



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 04:03 PM EST

PDB ID : 5DOX  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with Hygromycin-A at 3.1Å resolution  
Authors : Polikanov, Y.S.; Starosta, A.L.; Juetten, M.F.; Altman, R.B.; Terry, D.S.; Lu, W.; Burnett, B.J.; Dinos, G.; Reynolds, K.; Blanchard, S.C.; Steitz, T.A.; Wilson, D.N.  
Deposited on : 2015-09-11  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

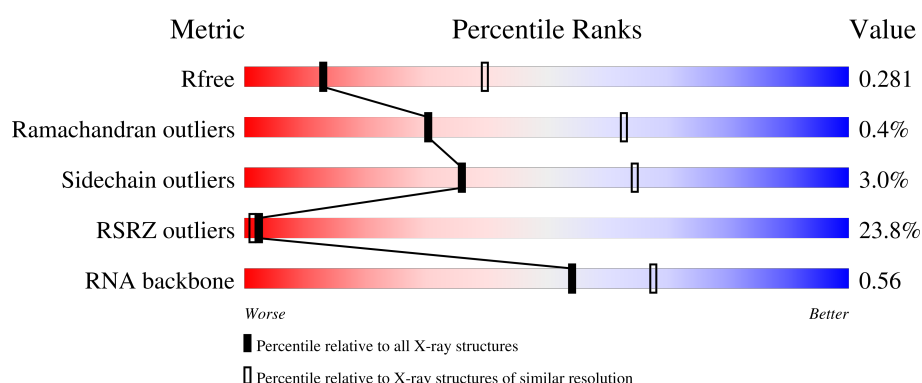
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1351 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)
RNA backbone	3690	1021 (3.36-2.84)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>11%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	2A	2915	<div> <div>8%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
2	1B	121	<div> <div>12%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
2	2B	121	<div> <div>12%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
3	1D	276	<div> <div>22%</div> <div>96%</div> <div>.</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	20% 97% ..
16	2U	118	7% 97% ..
17	1V	101	20% 97% .
17	2V	101	22% 97% .
18	1W	113	15% 97% ..
18	2W	113	4% 96% ..
19	1X	96	11% 99% .
19	2X	96	6% 97% ..
20	1Y	110	24% 95% ..
20	2Y	110	20% 96% ..
21	1Z	206	11% 94% ..
21	2Z	206	30% 97% .
22	10	85	20% 88% . 9%
22	20	85	20% 89% . 9%
23	11	98	26% 98% ..
23	21	98	19% 97% ..
24	12	72	21% 96% ..
24	22	72	15% 96% ..
25	13	60	25% 92% 7% .
25	23	60	7% 95% ..
26	14	71	42% 94% . .
26	24	71	48% 89% 8% .
27	15	60	8% 92% 7% .
27	25	60	7% 92% 7% .
28	16	54	22% 91% 7% .

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Mol	Chain	Length	Quality of chain
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	
40	2i	128	

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

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MG	1A	3453	-	-	-	X
53	MG	1A	3727	-	-	-	X
53	MG	1a	3039	-	-	-	X
53	MG	1n	101	-	-	-	X
53	MG	2a	1632	-	-	-	X
53	MG	2a	1633	-	-	-	X
53	MG	2a	1643	-	-	-	X
53	MG	2a	1692	-	-	-	X
53	MG	2a	1705	-	-	-	X



## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 289588 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	1A	761	Total Mg 761 761	0	0
53	1B	23	Total Mg 23 23	0	0
53	1D	8	Total Mg 8 8	0	0
53	1E	6	Total Mg 6 6	0	0
53	1F	6	Total Mg 6 6	0	0
53	1G	2	Total Mg 2 2	0	0
53	1H	2	Total Mg 2 2	0	0
53	1N	2	Total Mg 2 2	0	0
53	1P	3	Total Mg 3 3	0	0
53	1Q	4	Total Mg 4 4	0	0
53	1R	6	Total Mg 6 6	0	0
53	1T	4	Total Mg 4 4	0	0
53	1U	3	Total Mg 3 3	0	0
53	1V	2	Total Mg 2 2	0	0
53	1W	3	Total Mg 3 3	0	0
53	1Z	1	Total Mg 1 1	0	0
53	10	6	Total Mg 6 6	0	0
53	11	2	Total Mg 2 2	0	0
53	13	3	Total Mg 3 3	0	0
53	15	5	Total Mg 5 5	0	0
53	17	2	Total Mg 2 2	0	0
53	18	2	Total Mg 2 2	0	0

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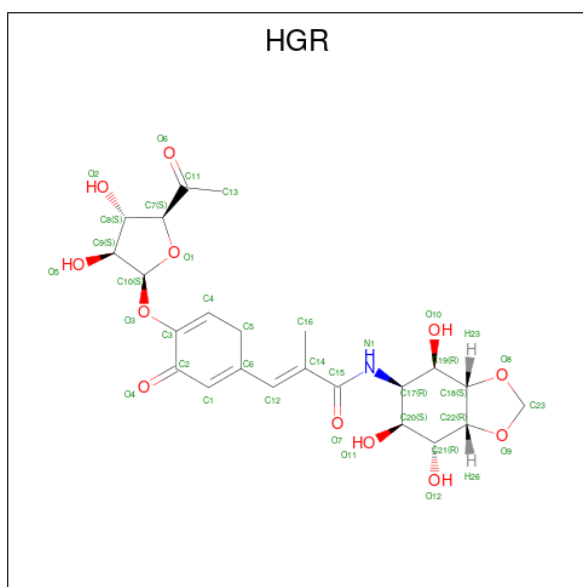
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	19	4	Total 4	Mg 4	0	0
53	1a	143	Total 143	Mg 143	0	0
53	1b	1	Total 1	Mg 1	0	0
53	1d	2	Total 2	Mg 2	0	0
53	1e	1	Total 1	Mg 1	0	0
53	1f	1	Total 1	Mg 1	0	0
53	1g	2	Total 2	Mg 2	0	0
53	1h	1	Total 1	Mg 1	0	0
53	1k	1	Total 1	Mg 1	0	0
53	1l	2	Total 2	Mg 2	0	0
53	1n	1	Total 1	Mg 1	0	0
53	1o	2	Total 2	Mg 2	0	0
53	1r	1	Total 1	Mg 1	0	0
53	1t	1	Total 1	Mg 1	0	0
53	2A	518	Total 518	Mg 518	0	0
53	2B	19	Total 19	Mg 19	0	0
53	2D	3	Total 3	Mg 3	0	0
53	2E	6	Total 6	Mg 6	0	0
53	2F	2	Total 2	Mg 2	0	0
53	2I	1	Total 1	Mg 1	0	0
53	2N	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	2O	2	Total 2	Mg 2	0	0
53	2P	1	Total 1	Mg 1	0	0
53	2Q	3	Total 3	Mg 3	0	0
53	2R	1	Total 1	Mg 1	0	0
53	2T	3	Total 3	Mg 3	0	0
53	2V	1	Total 1	Mg 1	0	0
53	2W	1	Total 1	Mg 1	0	0
53	2Y	1	Total 1	Mg 1	0	0
53	20	1	Total 1	Mg 1	0	0
53	28	2	Total 2	Mg 2	0	0
53	2a	129	Total 129	Mg 129	0	0
53	2e	1	Total 1	Mg 1	0	0
53	2k	1	Total 1	Mg 1	0	0
53	2l	1	Total 1	Mg 1	0	0
53	2t	1	Total 1	Mg 1	0	0

- Molecule 54 is Hygromycin A (three-letter code: HGR) (formula:  $C_{23}H_{29}NO_{12}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	1A	1	Total 36	C 23	N 1	O 12	0	0
54	2A	1	Total 36	C 23	N 1	O 12	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

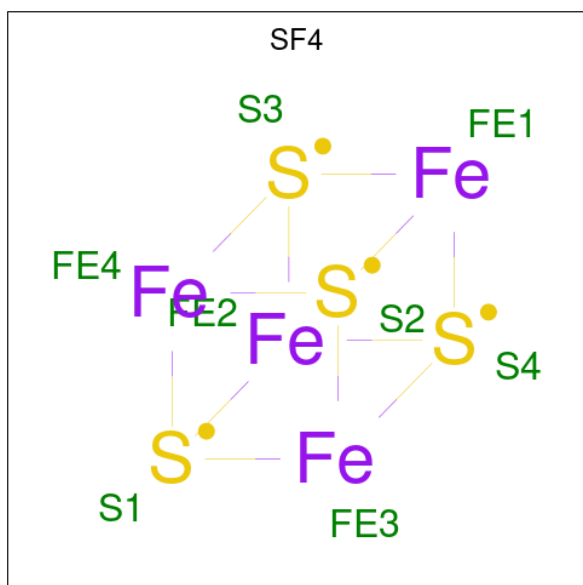
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1Y	1	Total Zn 1 1	0	0
55	14	1	Total Zn 1 1	0	0
55	15	1	Total Zn 1 1	0	0
55	16	1	Total Zn 1 1	0	0
55	19	1	Total Zn 1 1	0	0
55	1n	1	Total Zn 1 1	0	0
55	2Y	1	Total Zn 1 1	0	0
55	24	1	Total Zn 1 1	0	0
55	25	1	Total Zn 1 1	0	0
55	26	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	29	1	Total	Zn	0	0
			1	1		
55	2n	1	Total	Zn	0	0
			1	1		

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	1d	1	Total	Fe	S	0	0
			8	4	4		
56	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1448	Total	O	0	0
			1448	1448		
57	1B	37	Total	O	0	0
			37	37		
57	1D	23	Total	O	0	0
			23	23		
57	1E	20	Total	O	0	0
			20	20		
57	1F	20	Total	O	0	0
			20	20		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	6	Total 6	O 6	0	0
57	1H	4	Total 4	O 4	0	0
57	1I	2	Total 2	O 2	0	0
57	1N	24	Total 24	O 24	0	0
57	1O	4	Total 4	O 4	0	0
57	1P	9	Total 9	O 9	0	0
57	1Q	8	Total 8	O 8	0	0
57	1R	6	Total 6	O 6	0	0
57	1T	15	Total 15	O 15	0	0
57	1U	16	Total 16	O 16	0	0
57	1V	9	Total 9	O 9	0	0
57	1W	9	Total 9	O 9	0	0
57	1X	7	Total 7	O 7	0	0
57	1Y	5	Total 5	O 5	0	0
57	1Z	2	Total 2	O 2	0	0
57	10	10	Total 10	O 10	0	0
57	11	7	Total 7	O 7	0	0
57	12	2	Total 2	O 2	0	0
57	13	8	Total 8	O 8	0	0
57	14	1	Total 1	O 1	0	0
57	15	8	Total 8	O 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	16	1	Total 1	O 1	0	0
57	17	2	Total 2	O 2	0	0
57	18	3	Total 3	O 3	0	0
57	19	4	Total 4	O 4	0	0
57	1a	226	Total 226	O 226	0	0
57	1d	5	Total 5	O 5	0	0
57	1e	2	Total 2	O 2	0	0
57	1f	2	Total 2	O 2	0	0
57	1g	1	Total 1	O 1	0	0
57	1h	1	Total 1	O 1	0	0
57	1k	1	Total 1	O 1	0	0
57	1l	6	Total 6	O 6	0	0
57	1m	1	Total 1	O 1	0	0
57	1o	7	Total 7	O 7	0	0
57	1p	3	Total 3	O 3	0	0
57	1t	2	Total 2	O 2	0	0
57	1u	1	Total 1	O 1	0	0
57	2A	648	Total 648	O 648	0	0
57	2B	24	Total 24	O 24	0	0
57	2D	14	Total 14	O 14	0	0
57	2E	4	Total 4	O 4	0	0

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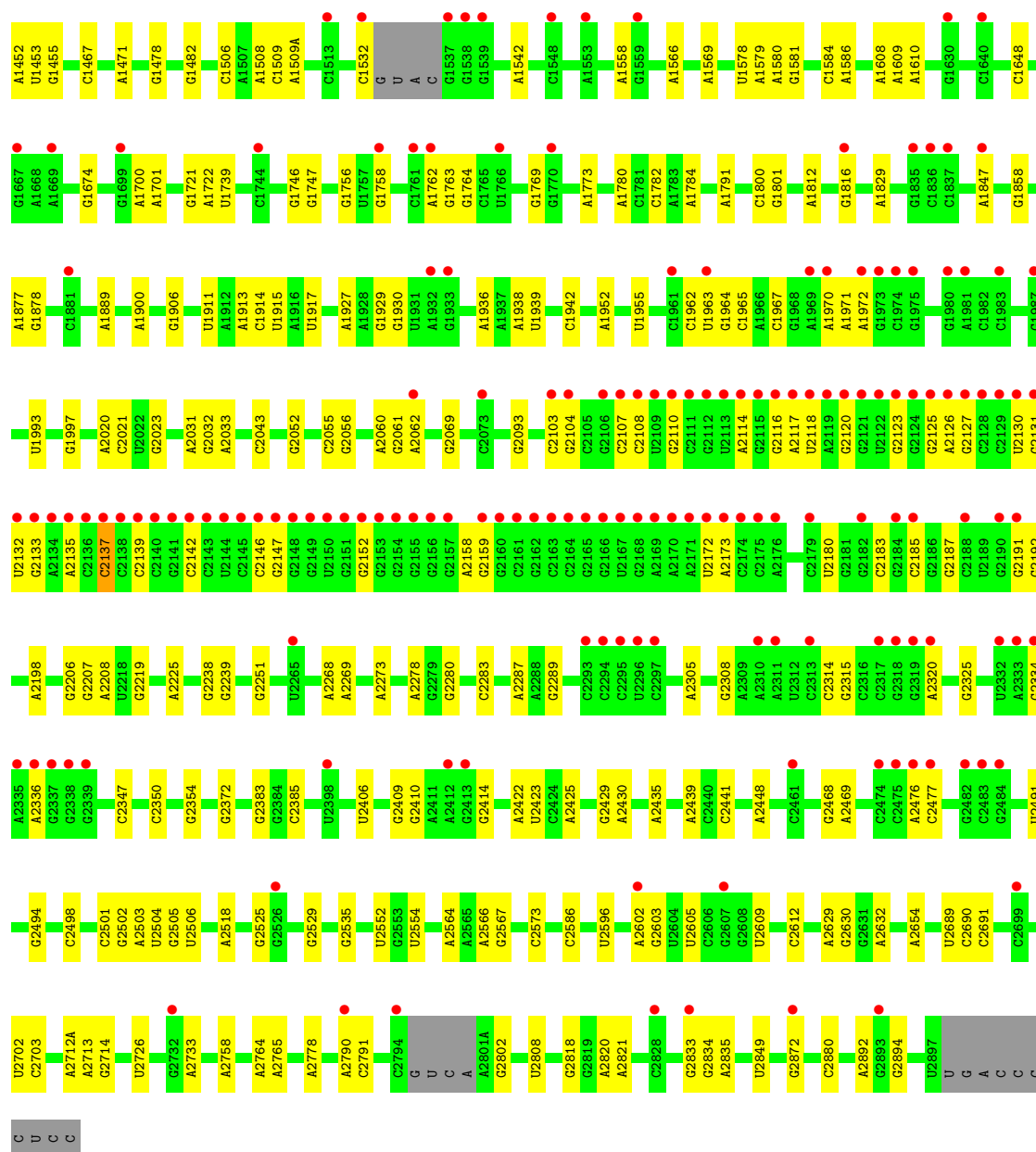
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			3	3		
57	2H	1	Total	O	0	0
			1	1		
57	2I	1	Total	O	0	0
			1	1		
57	2N	3	Total	O	0	0
			3	3		
57	2O	3	Total	O	0	0
			3	3		
57	2P	4	Total	O	0	0
			4	4		
57	2Q	4	Total	O	0	0
			4	4		
57	2R	4	Total	O	0	0
			4	4		
57	2S	1	Total	O	0	0
			1	1		
57	2T	5	Total	O	0	0
			5	5		
57	2U	3	Total	O	0	0
			3	3		
57	2W	3	Total	O	0	0
			3	3		
57	2X	2	Total	O	0	0
			2	2		
57	2Y	2	Total	O	0	0
			2	2		
57	2Z	3	Total	O	0	0
			3	3		
57	20	2	Total	O	0	0
			2	2		
57	21	2	Total	O	0	0
			2	2		
57	22	1	Total	O	0	0
			1	1		
57	23	1	Total	O	0	0
			1	1		
57	24	1	Total	O	0	0
			1	1		
57	25	1	Total	O	0	0
			1	1		

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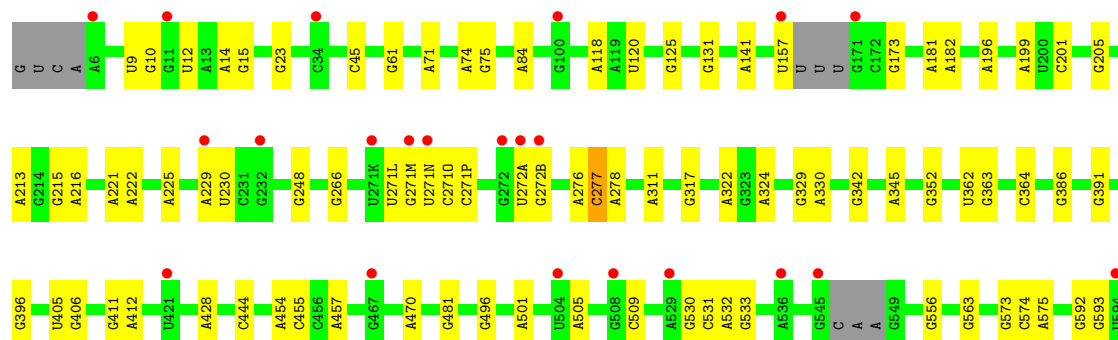
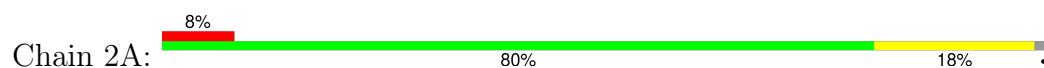
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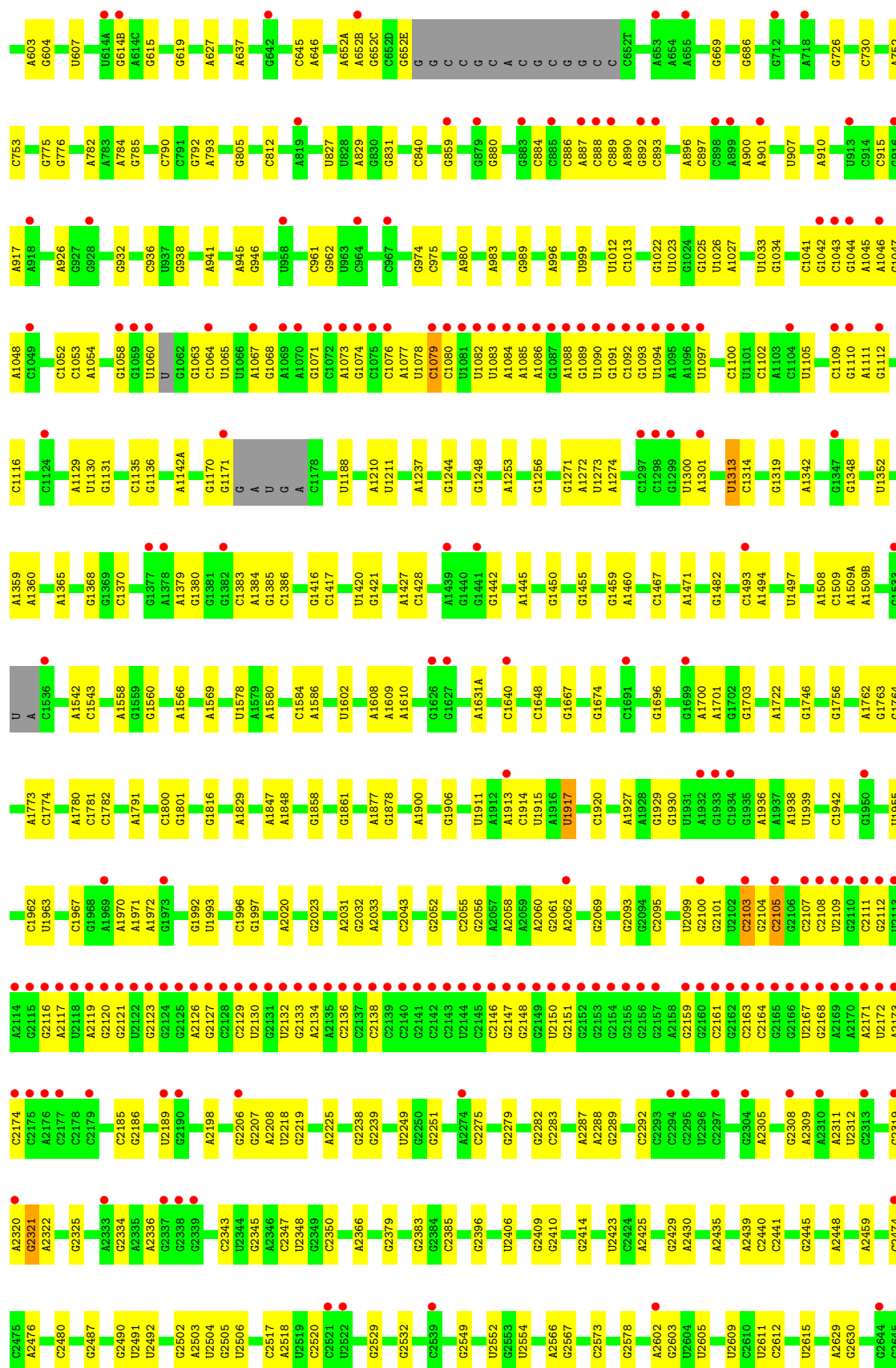
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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57	27	2	Total 2	O 2	0	0
57	28	3	Total 3	O 3	0	0
57	2a	179	Total 179	O 179	0	0
57	2d	1	Total 1	O 1	0	0
57	2e	2	Total 2	O 2	0	0
57	2f	3	Total 3	O 3	0	0
57	2l	3	Total 3	O 3	0	0
57	2m	1	Total 1	O 1	0	0
57	2o	1	Total 1	O 1	0	0
57	2p	1	Total 1	O 1	0	0
57	2q	1	Total 1	O 1	0	0
57	2r	3	Total 3	O 3	0	0
57	2t	3	Total 3	O 3	0	0

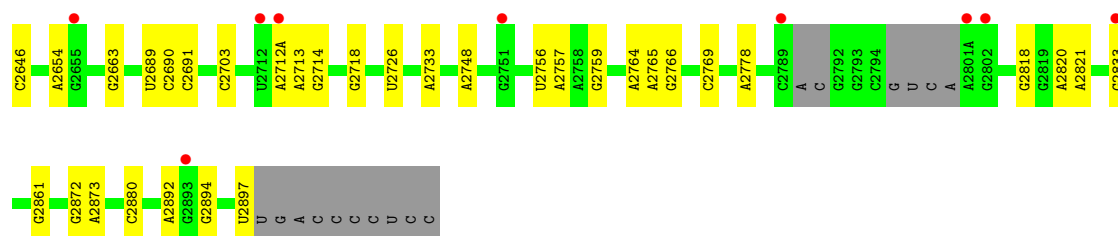




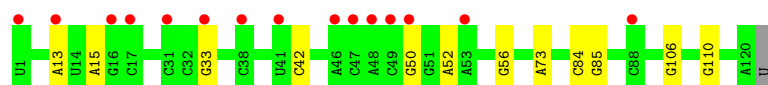
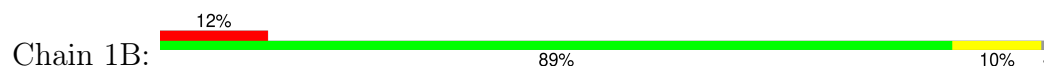
• Molecule 1: 23S Ribosomal RNA



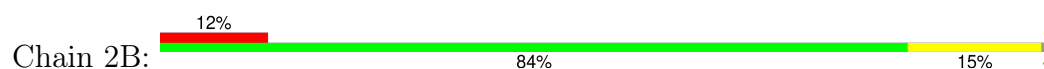




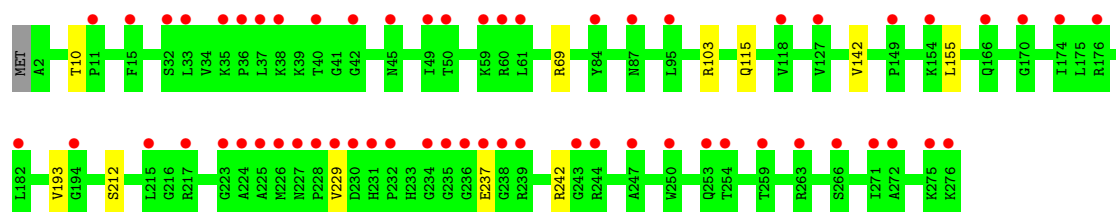
• Molecule 2: 5S Ribosomal RNA



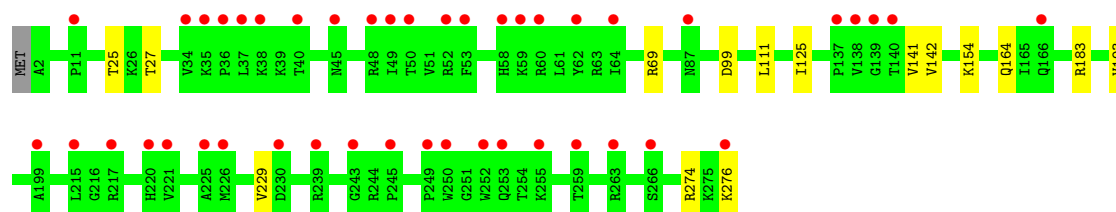
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

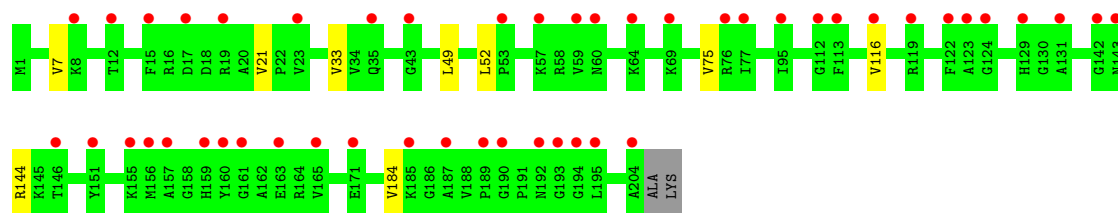


• Molecule 3: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L3

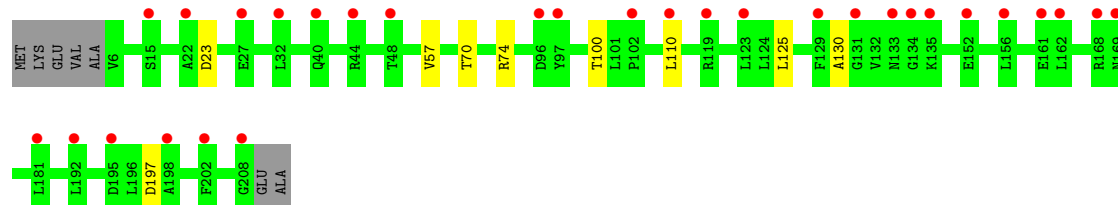




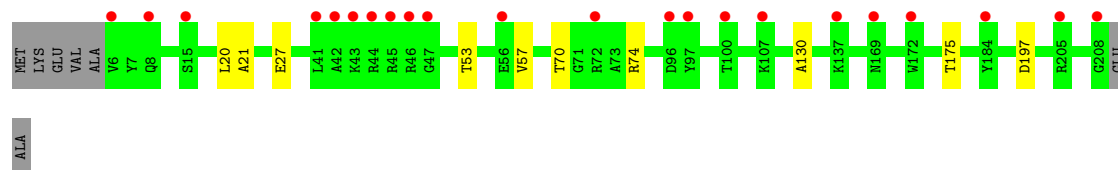
- Molecule 4: 50S ribosomal protein L3



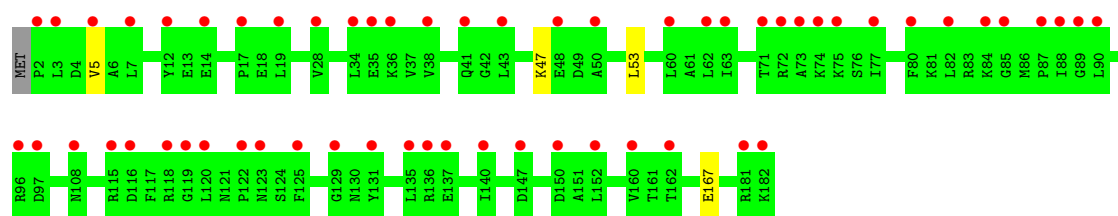
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4



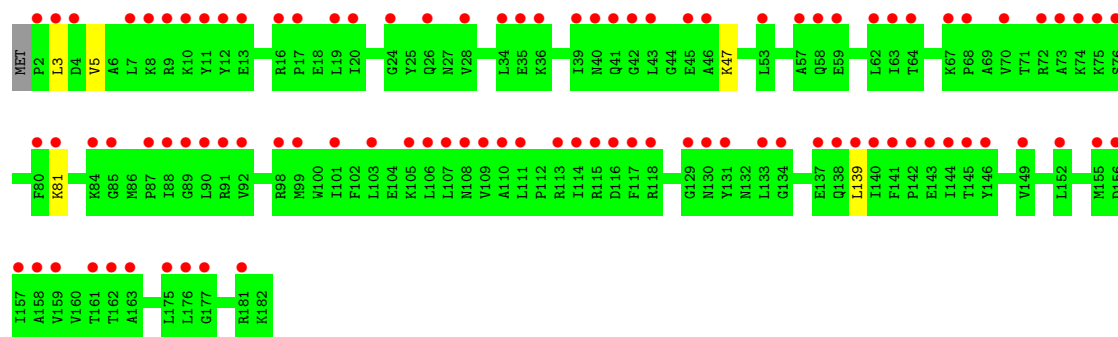
- Molecule 6: 50S ribosomal protein L5



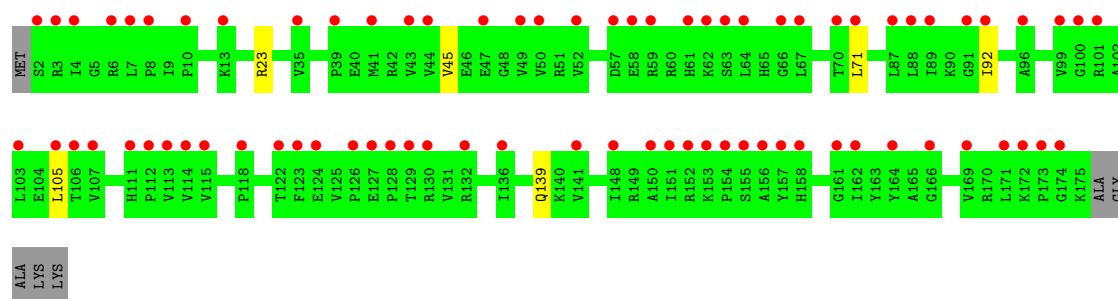
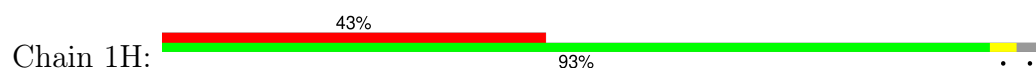
- Molecule 6: 50S ribosomal protein L5



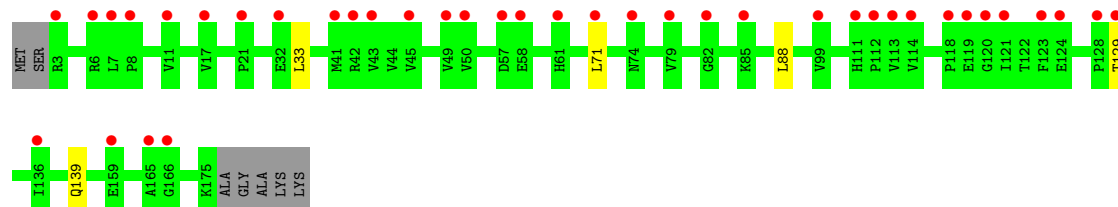




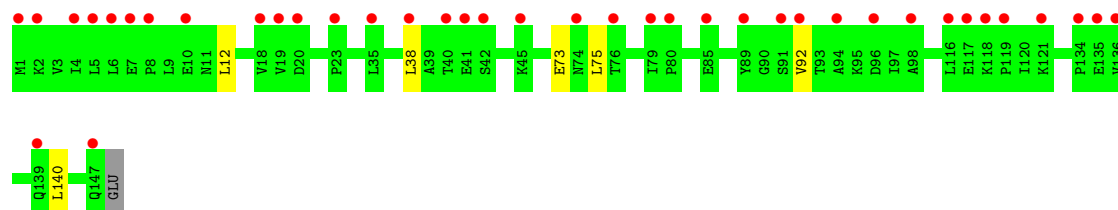
- Molecule 7: 50S ribosomal protein L6



- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9

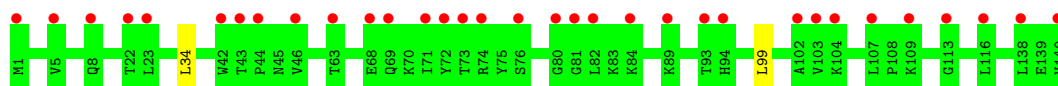




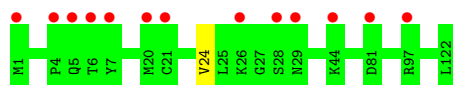
- Molecule 9: 50S ribosomal protein L13



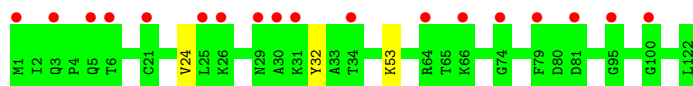
- Molecule 9: 50S ribosomal protein L13



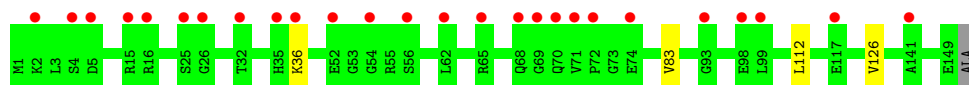
- Molecule 10: 50S ribosomal protein L14



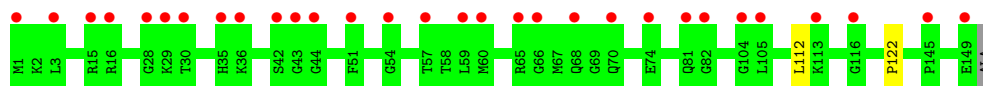
- Molecule 10: 50S ribosomal protein L14



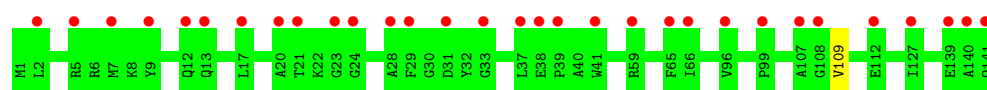
- Molecule 11: 50S ribosomal protein L15



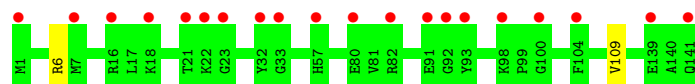
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16



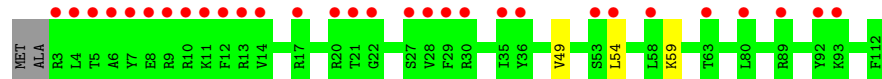
- Molecule 13: 50S ribosomal protein L17



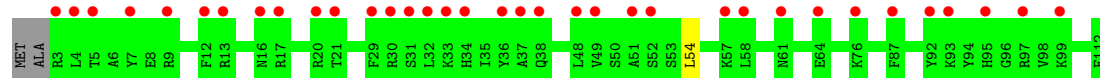
- Molecule 13: 50S ribosomal protein L17



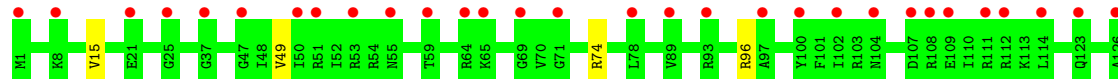
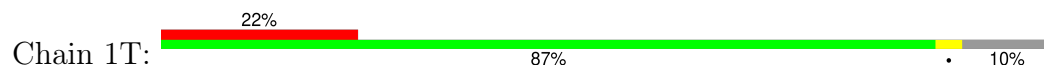
- Molecule 14: 50S ribosomal protein L18

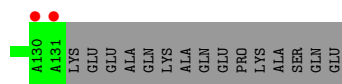


- Molecule 14: 50S ribosomal protein L18

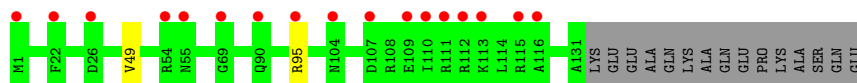
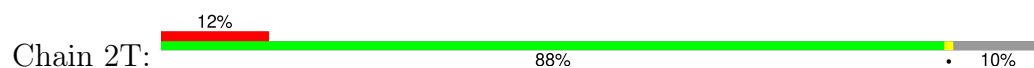


- Molecule 15: 50S ribosomal protein L19





- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



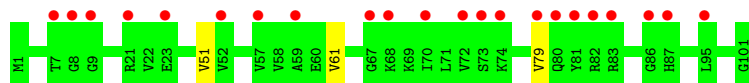
- Molecule 16: 50S ribosomal protein L20



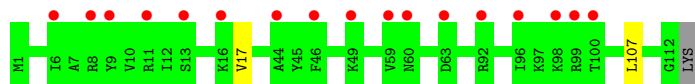
- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



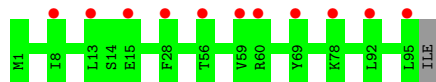
- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22



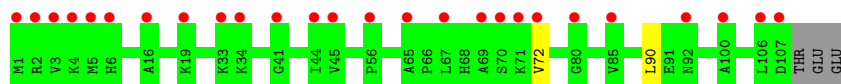
- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



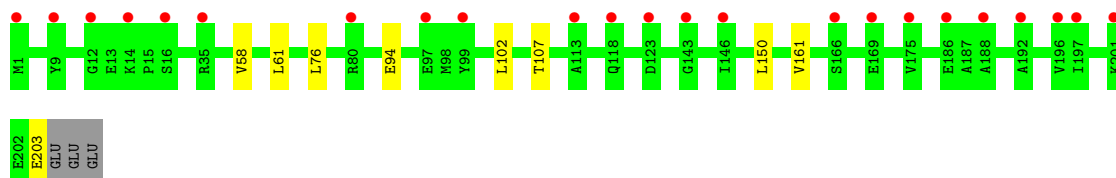
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

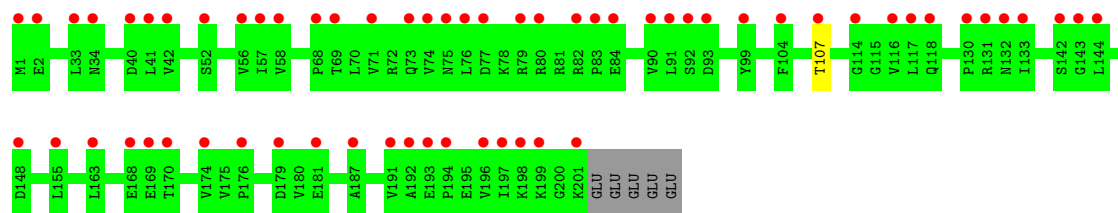


- Molecule 21: 50S ribosomal protein L25

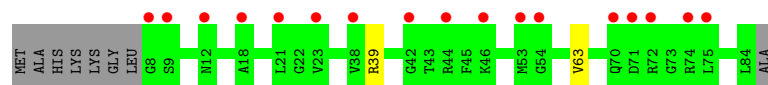
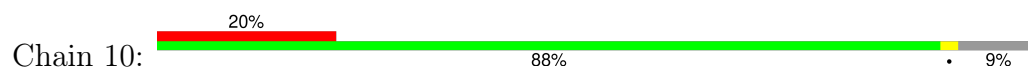


- Molecule 21: 50S ribosomal protein L25

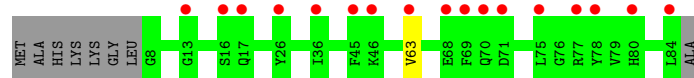
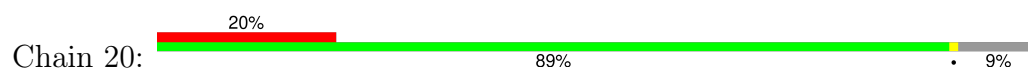




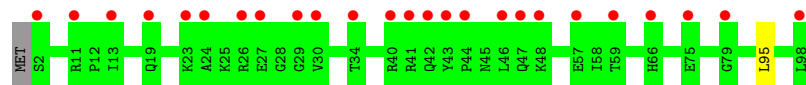
- Molecule 22: 50S ribosomal protein L27



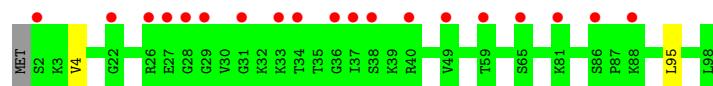
- Molecule 22: 50S ribosomal protein L27



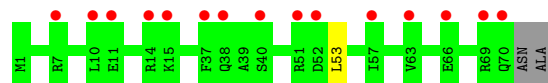
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28

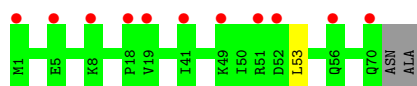


- Molecule 24: 50S ribosomal protein L29

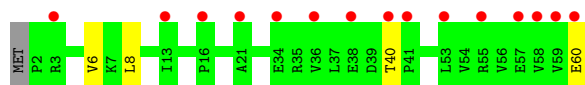
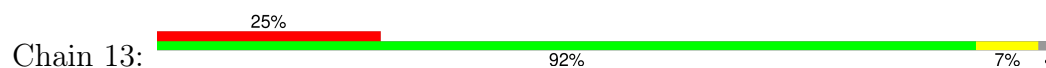


- Molecule 24: 50S ribosomal protein L29

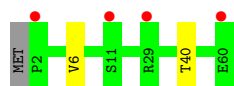




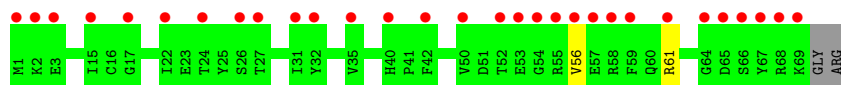
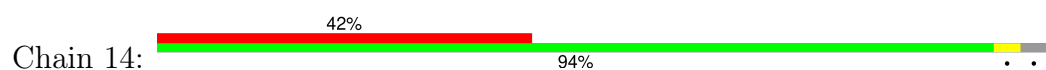
- Molecule 25: 50S ribosomal protein L30



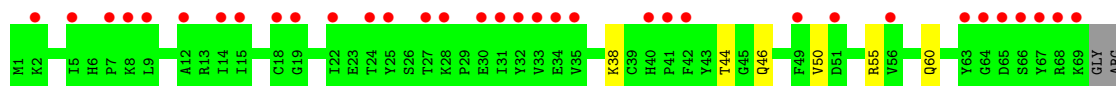
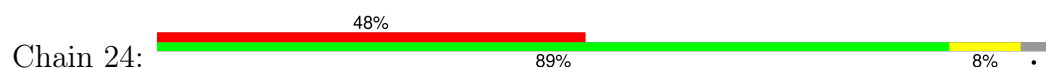
- Molecule 25: 50S ribosomal protein L30



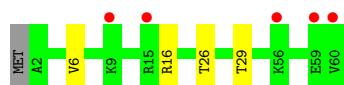
- Molecule 26: 50S ribosomal protein L31



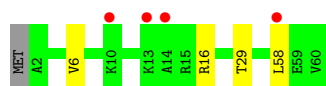
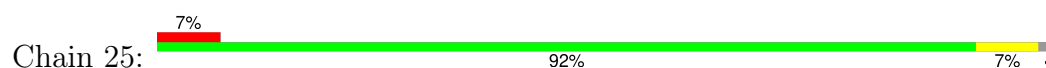
- Molecule 26: 50S ribosomal protein L31



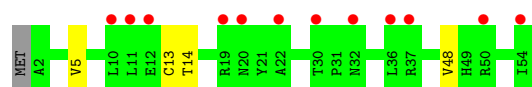
- Molecule 27: 50S ribosomal protein L32



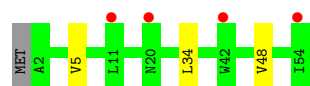
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



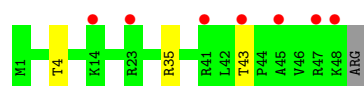
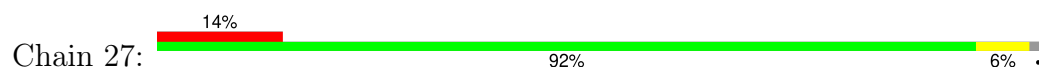
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



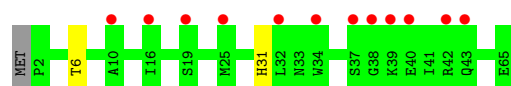
- Molecule 29: 50S ribosomal protein L34



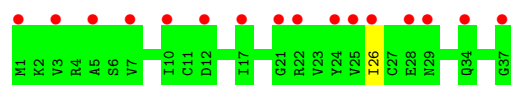
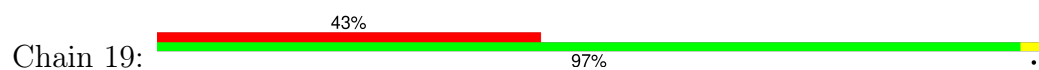
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

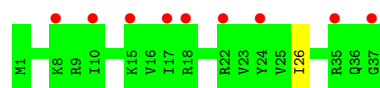


- Molecule 31: 50S ribosomal protein L36

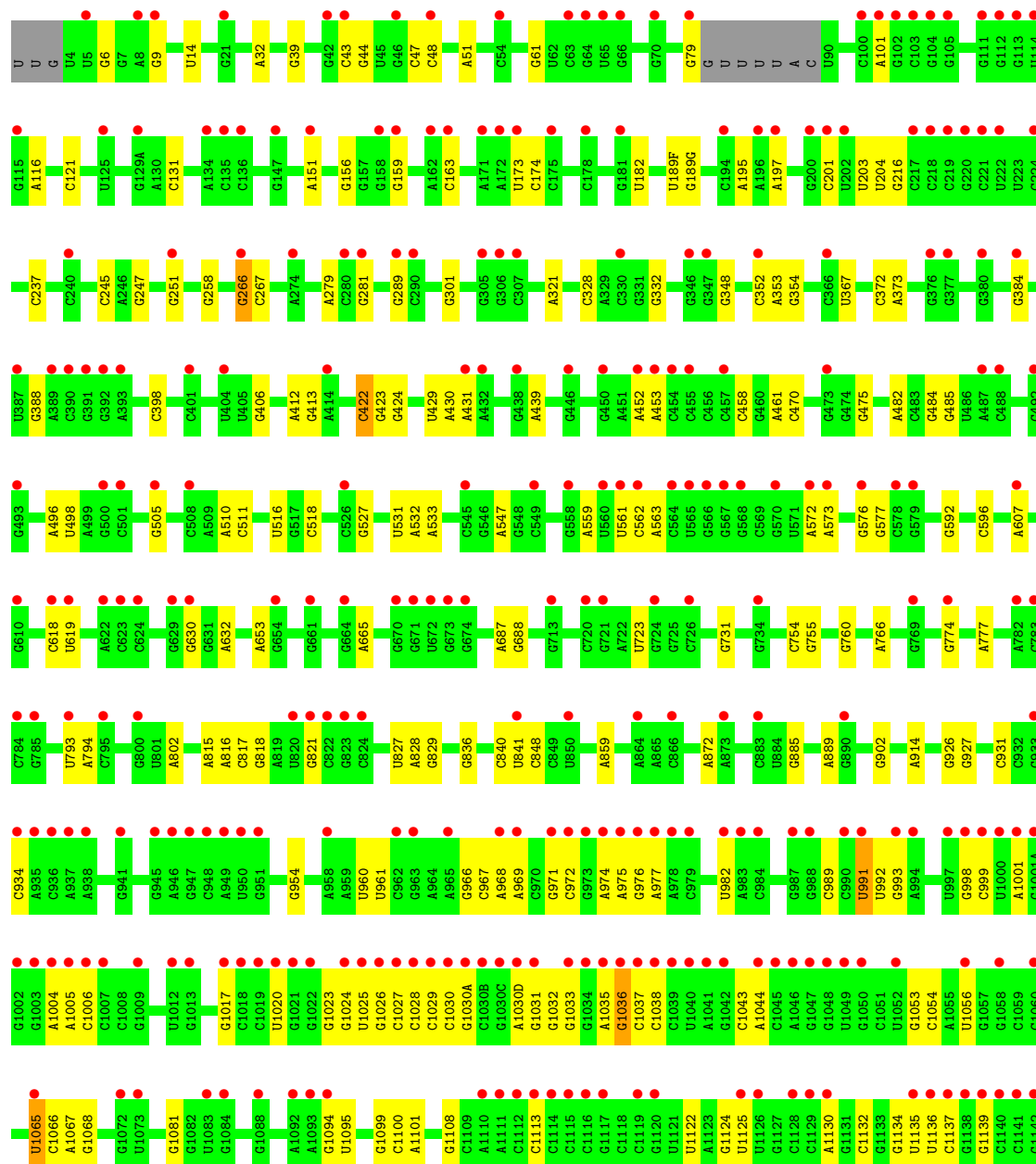
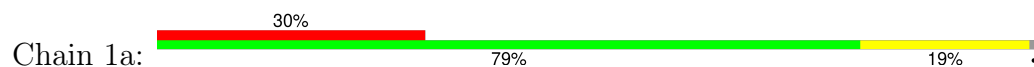


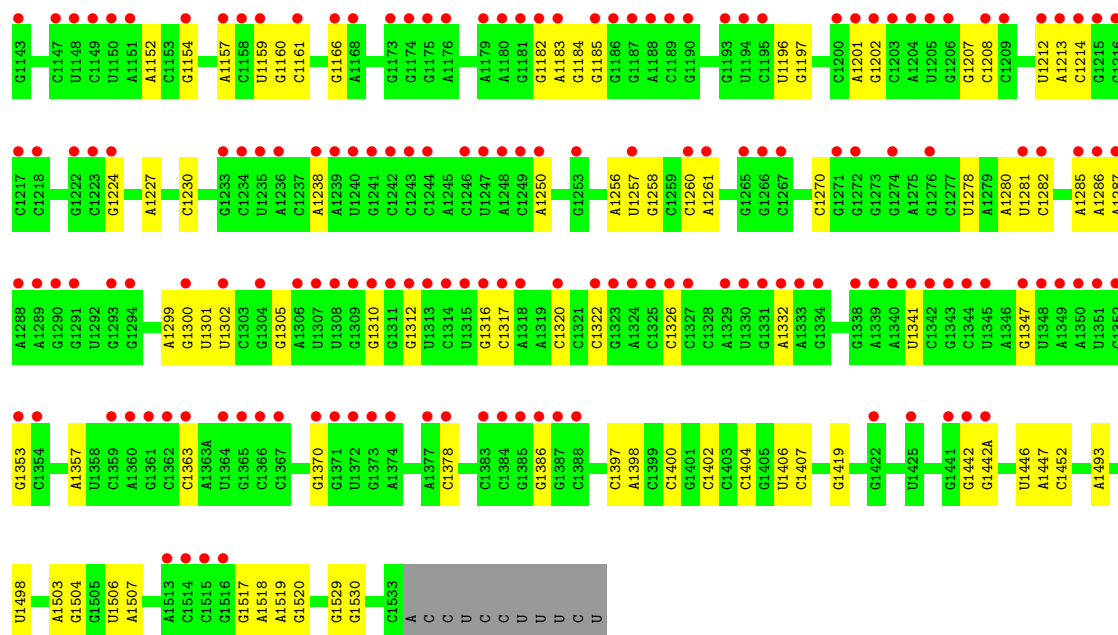


- Molecule 31: 50S ribosomal protein L36

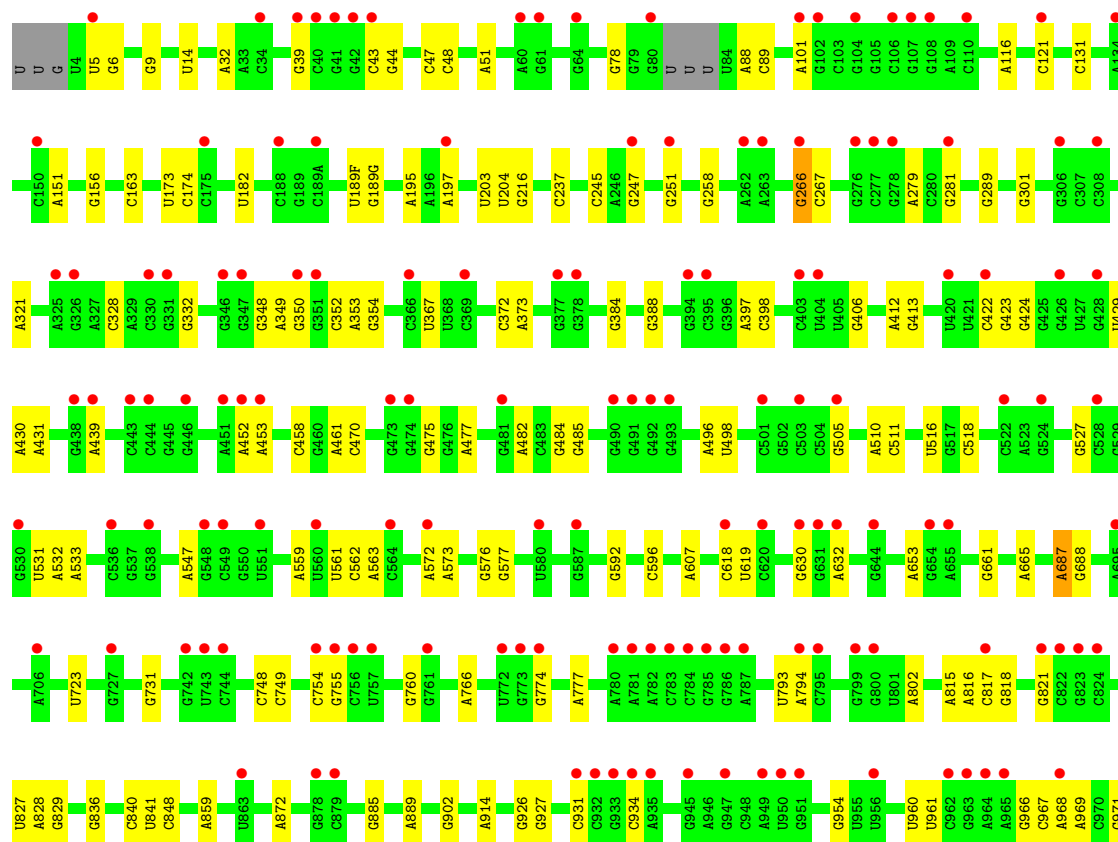
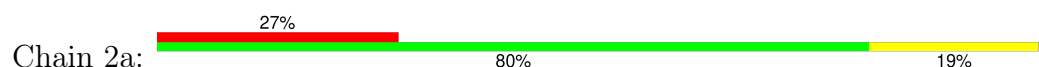


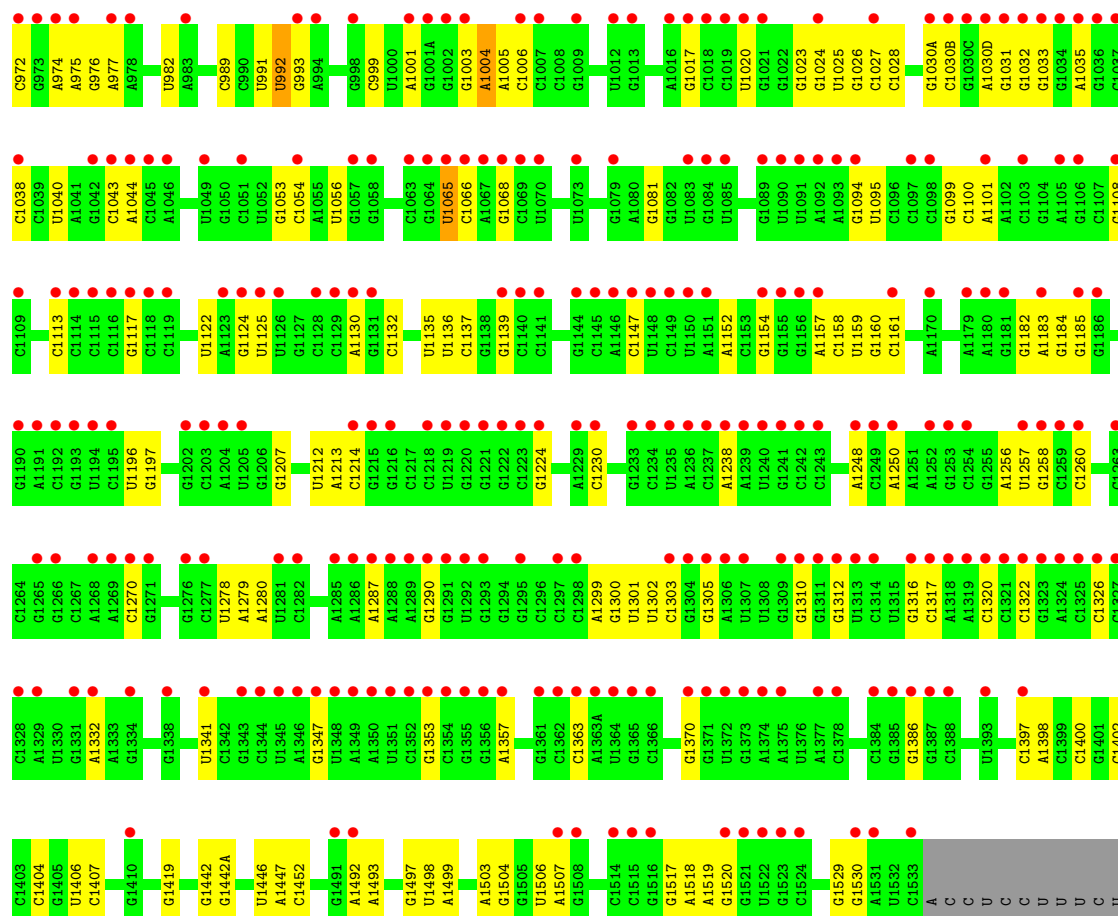
- Molecule 32: 16S Ribosomal RNA



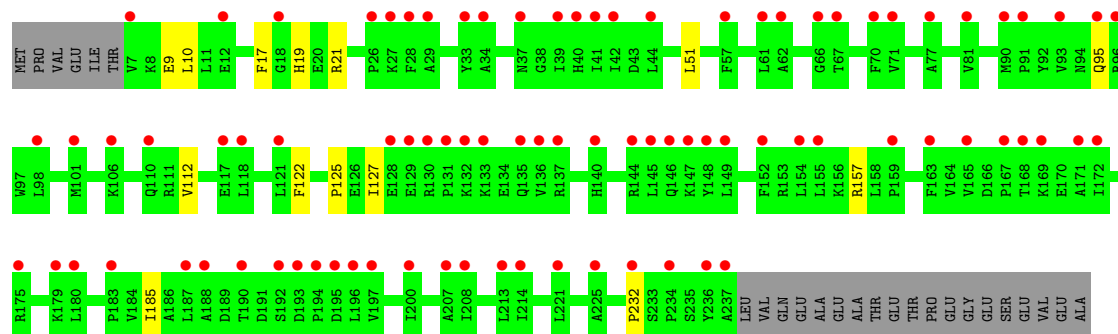
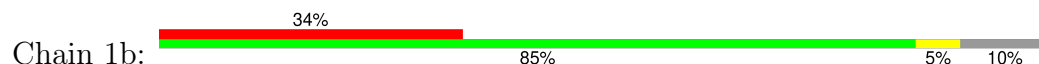


• Molecule 32: 16S Ribosomal RNA

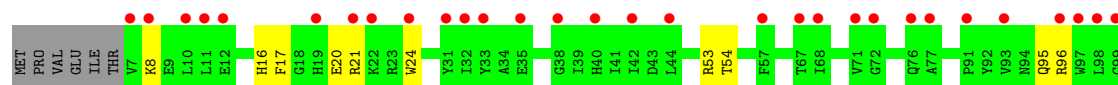
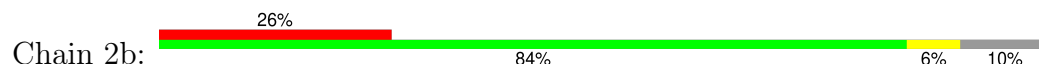


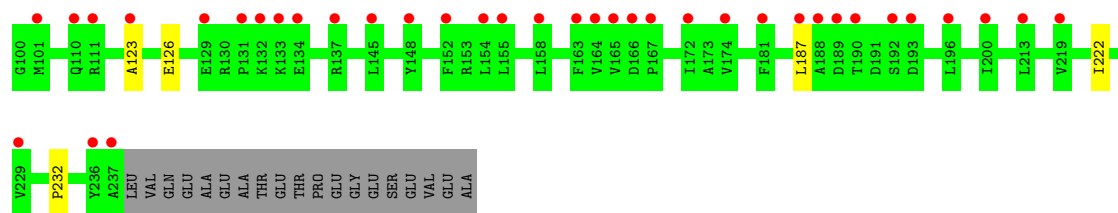


• Molecule 33: 30S ribosomal protein S2

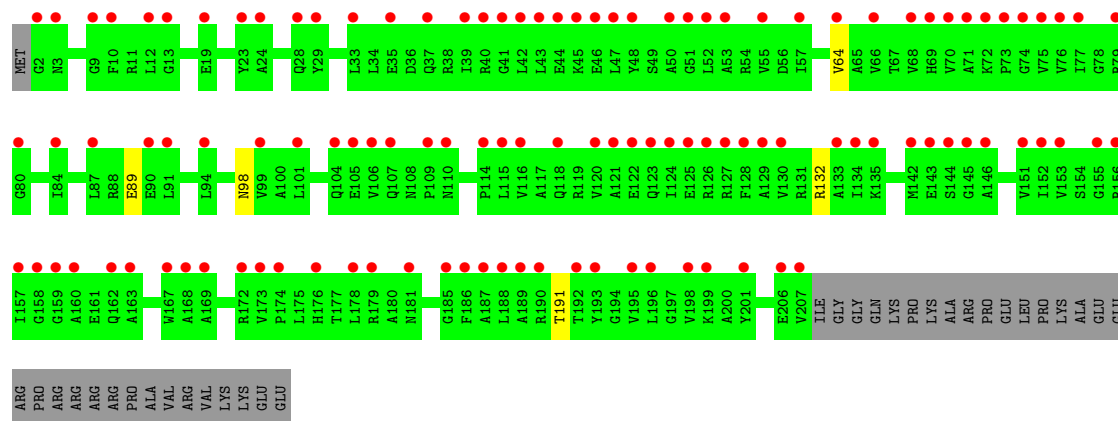
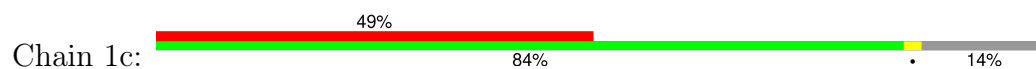


• Molecule 33: 30S ribosomal protein S2

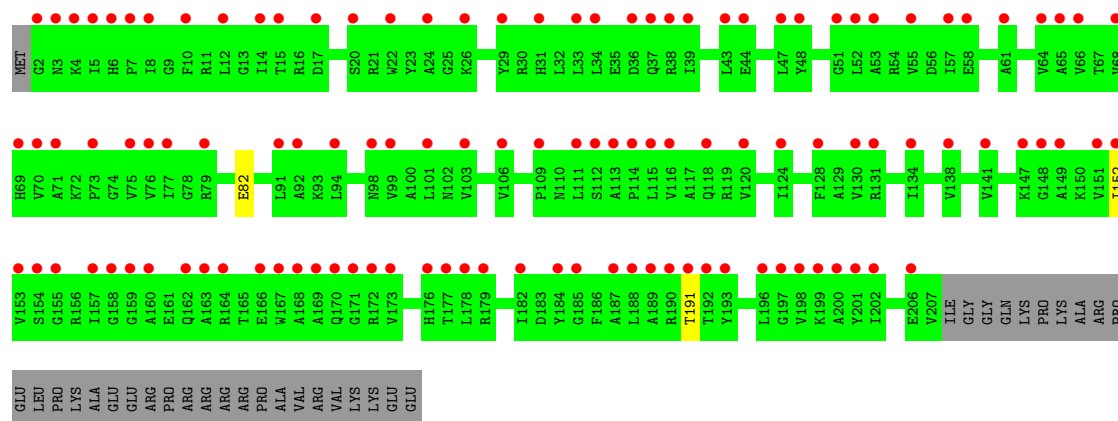
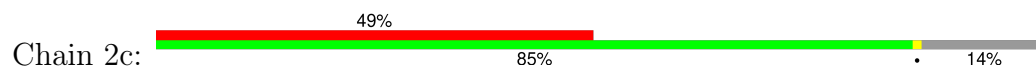




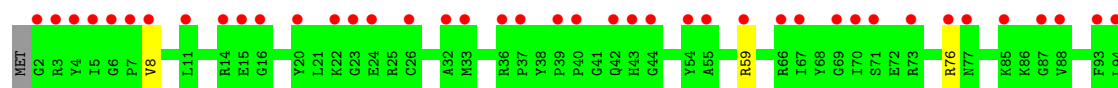
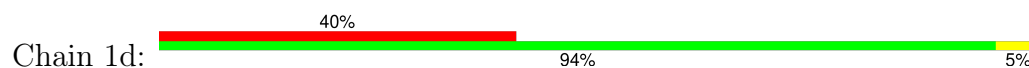
• Molecule 34: 30S ribosomal protein S3

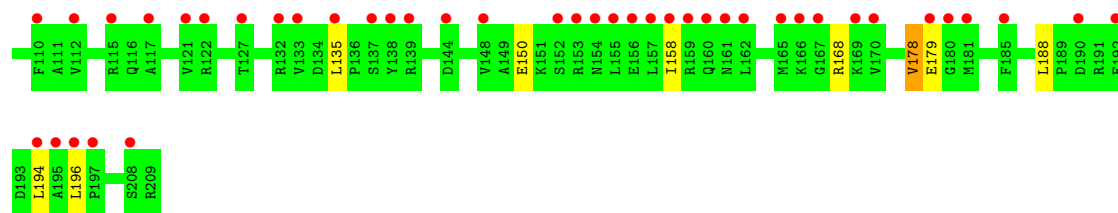


• Molecule 34: 30S ribosomal protein S3

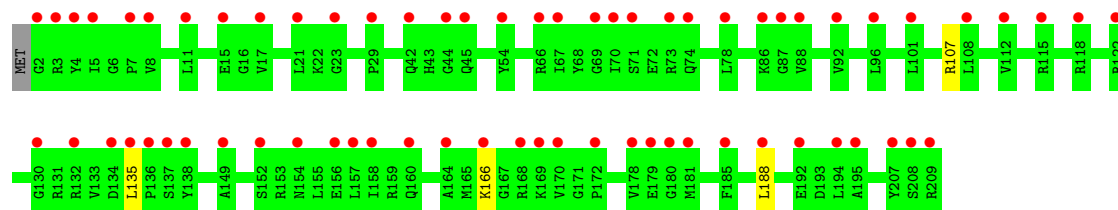


• Molecule 35: 30S ribosomal protein S4

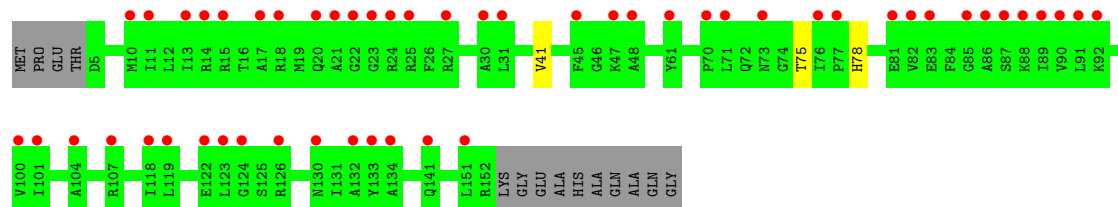
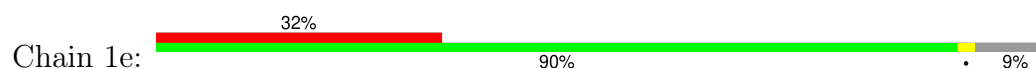




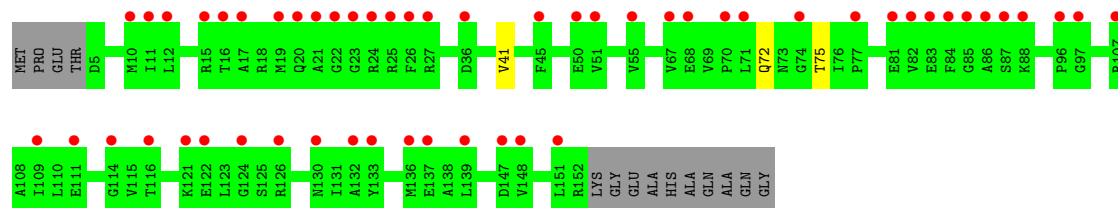
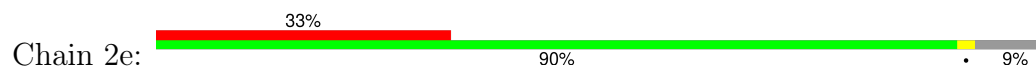
• Molecule 35: 30S ribosomal protein S4



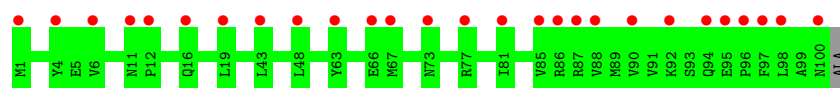
• Molecule 36: 30S ribosomal protein S5



• Molecule 36: 30S ribosomal protein S5

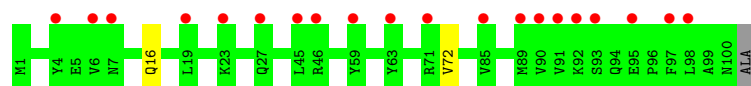


• Molecule 37: 30S ribosomal protein S6

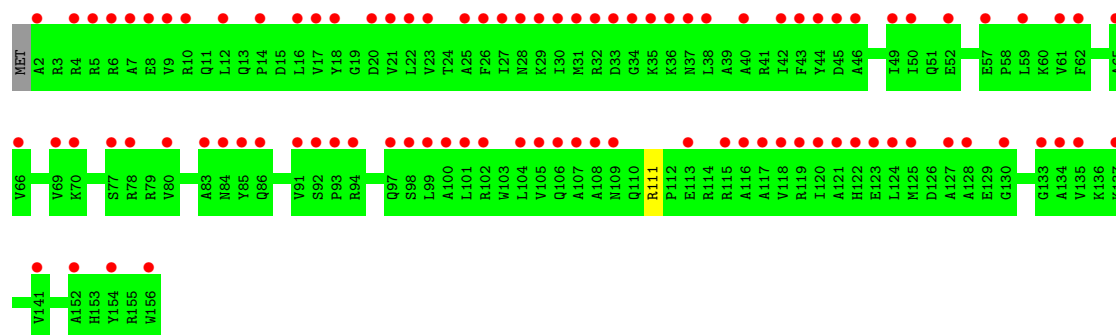


• Molecule 37: 30S ribosomal protein S6

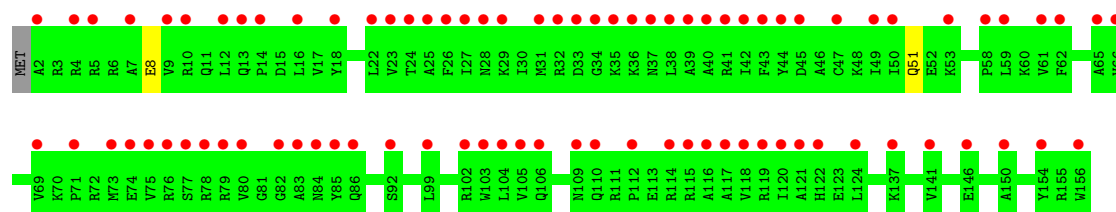




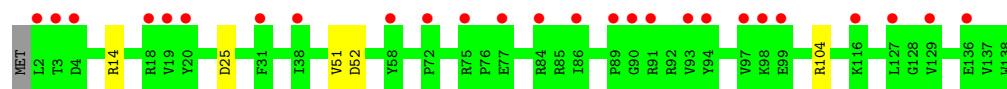
- Molecule 38: 30S ribosomal protein S7



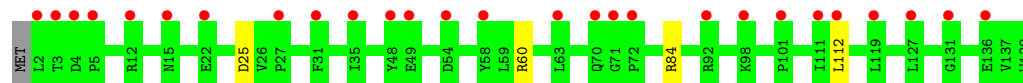
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

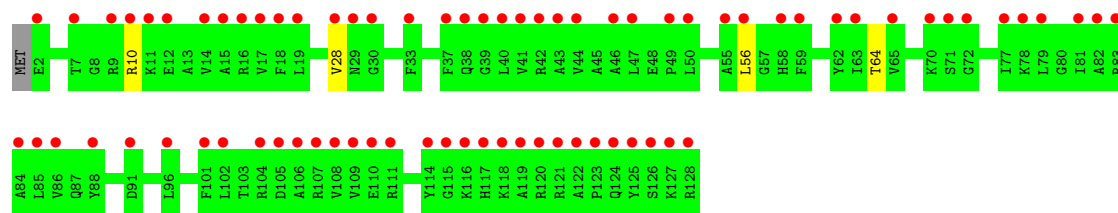


- Molecule 39: 30S ribosomal protein S8

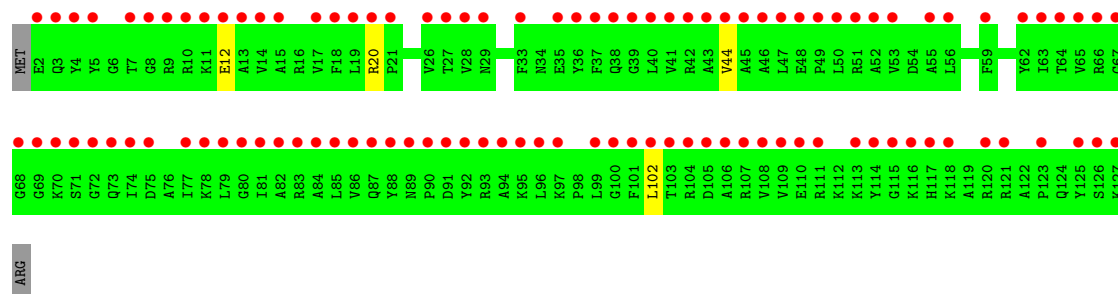
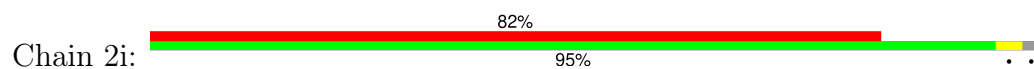


- Molecule 40: 30S ribosomal protein S9

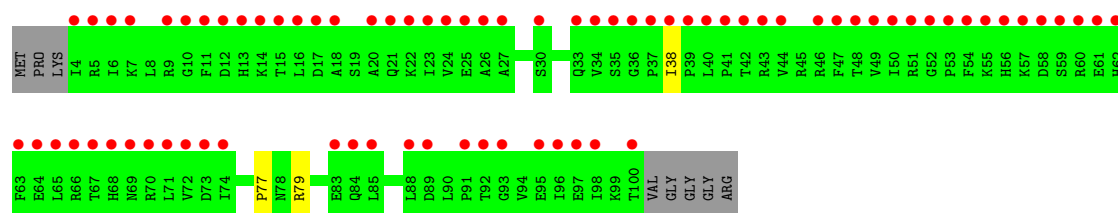
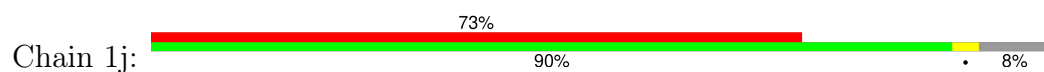




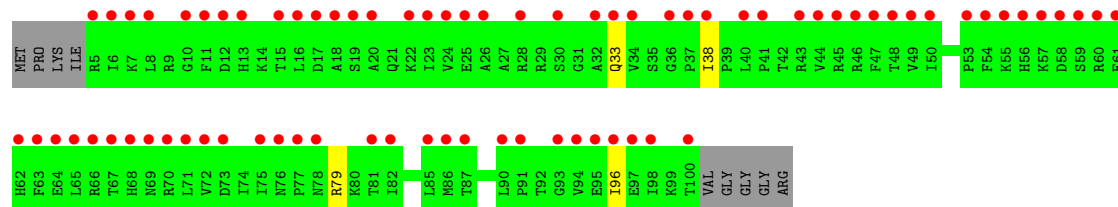
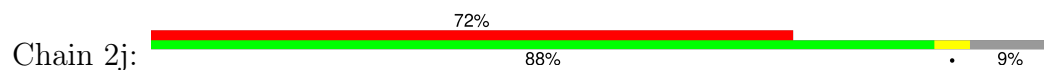
• Molecule 40: 30S ribosomal protein S9



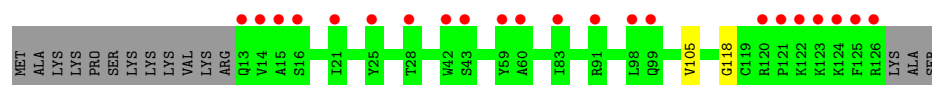
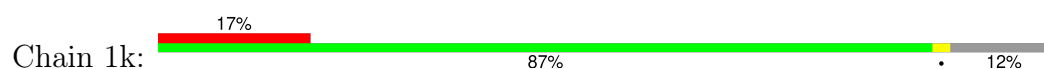
• Molecule 41: 30S ribosomal protein S10



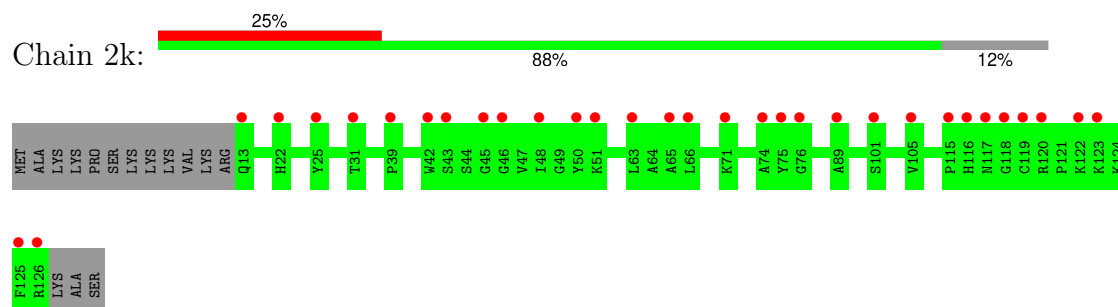
• Molecule 41: 30S ribosomal protein S10



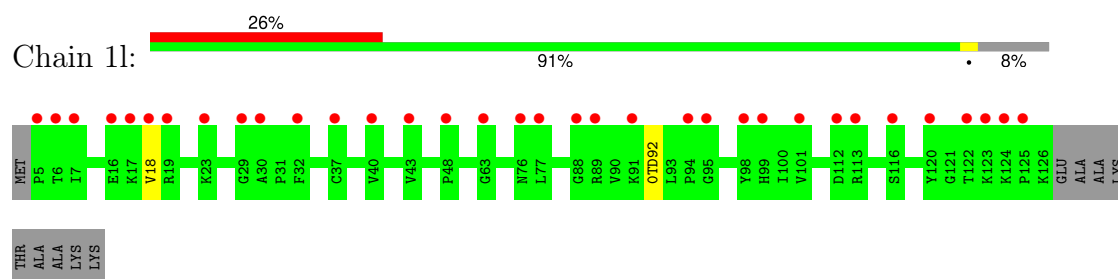
• Molecule 42: 30S ribosomal protein S11



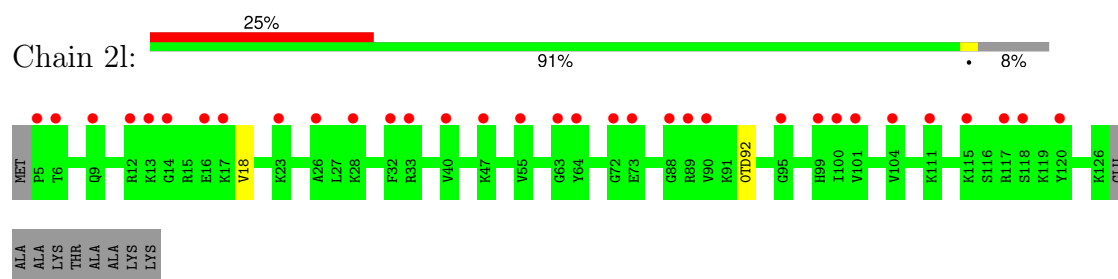
- Molecule 42: 30S ribosomal protein S11



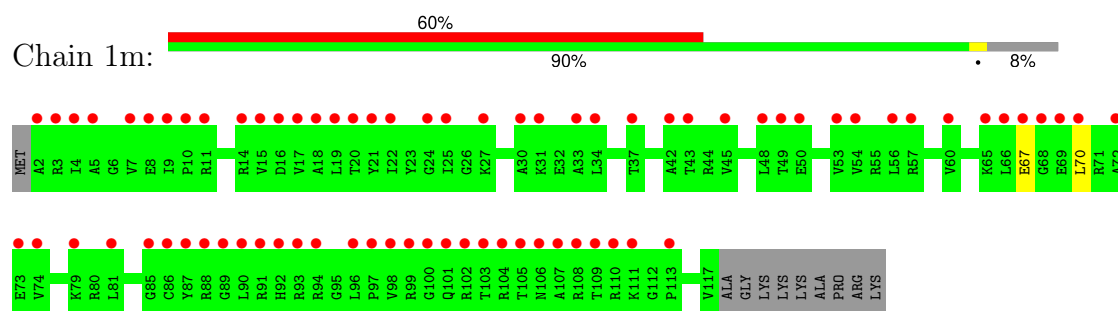
- Molecule 43: 30S ribosomal protein S12



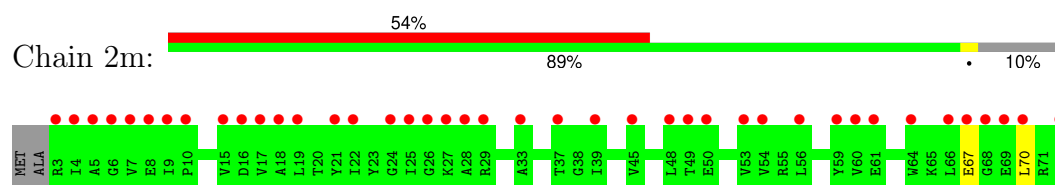
- Molecule 43: 30S ribosomal protein S12



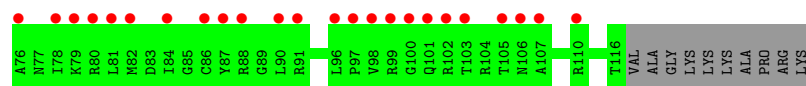
- Molecule 44: 30S ribosomal protein S13



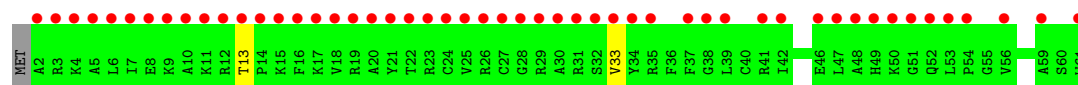
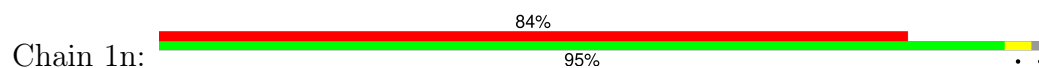
- Molecule 44: 30S ribosomal protein S13



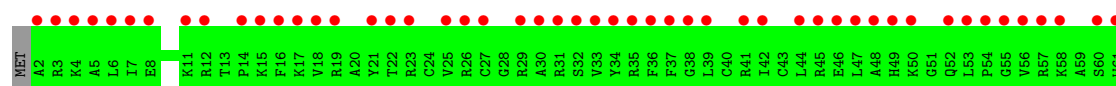
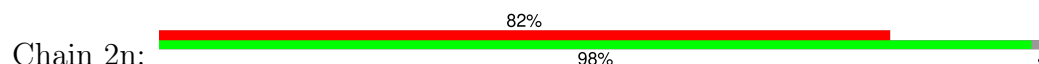




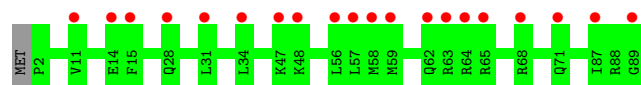
- Molecule 45: 30S ribosomal protein S14 type Z



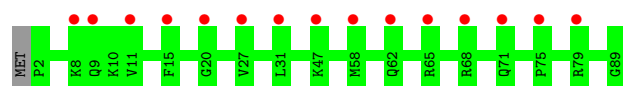
- Molecule 45: 30S ribosomal protein S14 type Z



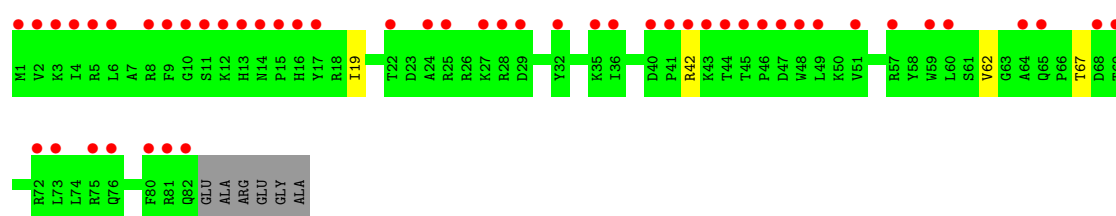
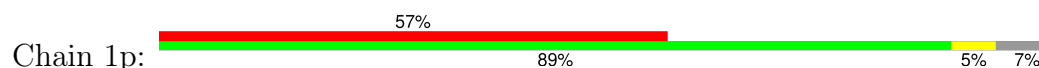
- Molecule 46: 30S ribosomal protein S15



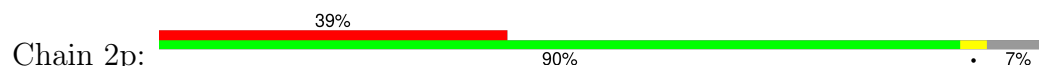
- Molecule 46: 30S ribosomal protein S15

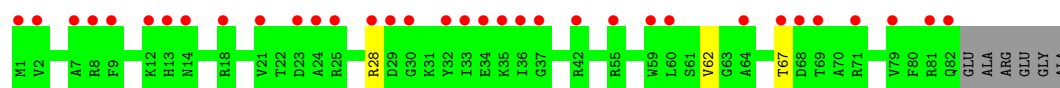


- Molecule 47: 30S ribosomal protein S16

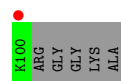
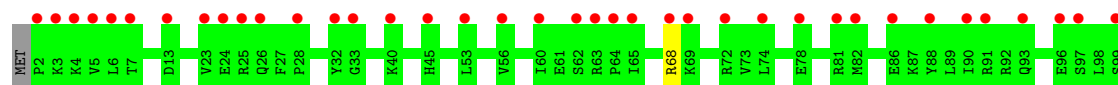


- Molecule 47: 30S ribosomal protein S16

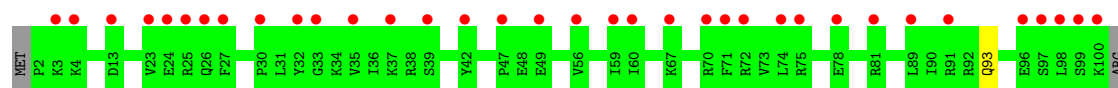




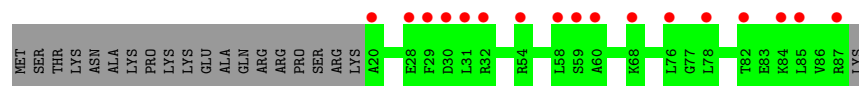
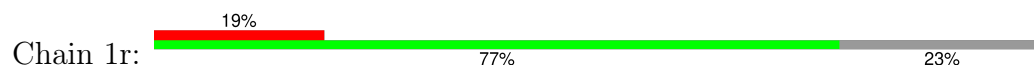
- Molecule 48: 30S ribosomal protein S17



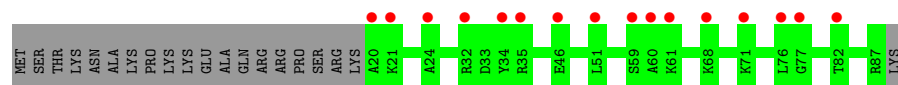
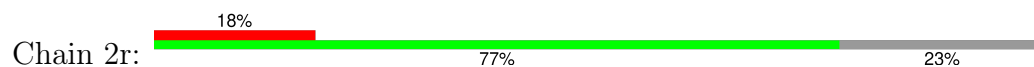
- Molecule 48: 30S ribosomal protein S17



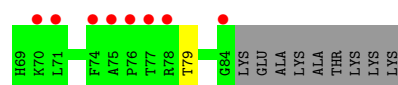
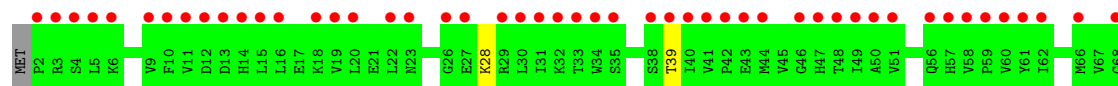
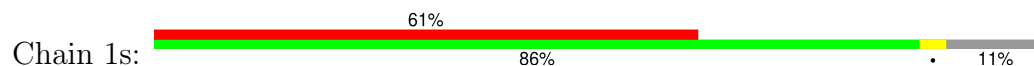
- Molecule 49: 30S ribosomal protein S18



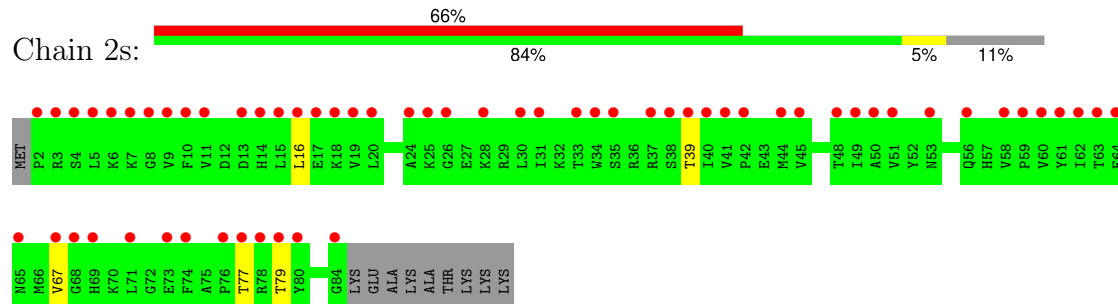
- Molecule 49: 30S ribosomal protein S18



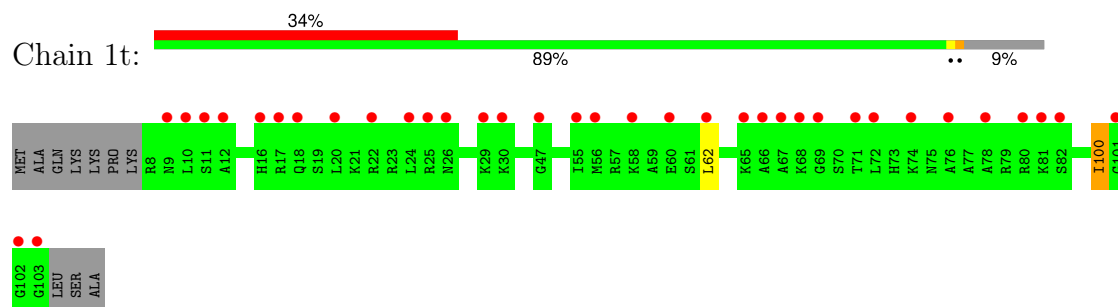
- Molecule 50: 30S ribosomal protein S19



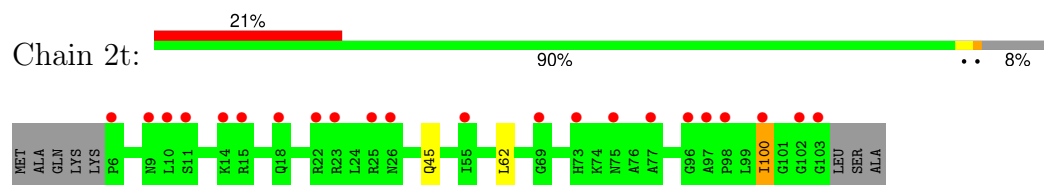
- Molecule 50: 30S ribosomal protein S19



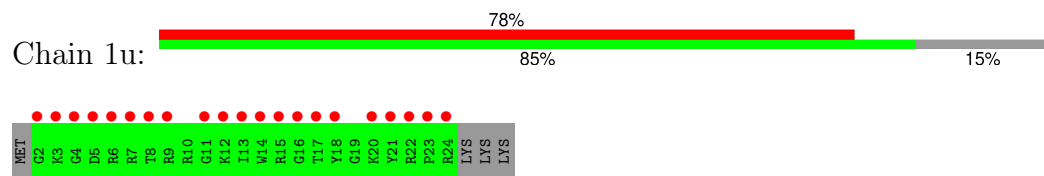
- Molecule 51: 30S ribosomal protein S20



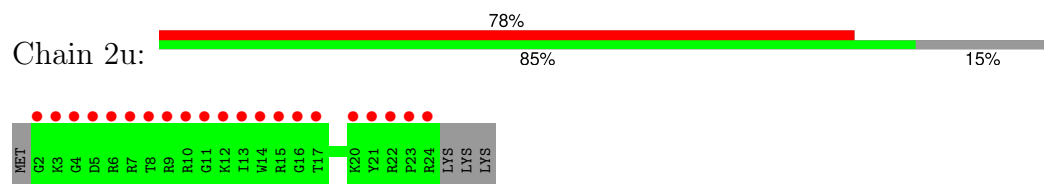
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.51Å 448.29Å 619.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	309.69 – 3.10 309.69 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (309.69-3.10) 99.8 (309.69-3.10)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.232 , 0.284 0.230 , 0.281	Depositor DCC
$R_{free}$ test set	52205 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.2	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 999.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	289588	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: M2G, OMG, 2MU, HGR, SF4, PSU, ZN, 0TD, MG, 5MU, 2MA, MA6, 4OC, 2MG, UR3, 5MC, 7MG

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	0.33	0/69029	0.75	11/107746 (0.0%)
1	2A	0.26	1/68901 (0.0%)	0.76	27/107544 (0.0%)
2	1B	0.26	0/2876	0.73	0/4486
2	2B	0.25	0/2878	0.74	0/4490
3	1D	0.26	0/2181	0.44	0/2940
3	2D	0.24	0/2186	0.45	0/2944
4	1E	0.28	0/1592	0.49	0/2149
4	2E	0.24	0/1592	0.49	0/2149
5	1F	0.27	0/1619	0.45	0/2193
5	2F	0.25	0/1615	0.46	0/2188
6	1G	0.23	0/1451	0.46	0/1961
6	2G	0.24	0/1449	0.46	0/1957
7	1H	0.25	0/1356	0.44	0/1834
7	2H	0.22	0/1350	0.45	0/1826
8	1I	0.23	0/1109	0.46	0/1512
8	2I	0.22	0/1091	0.45	0/1490
9	1N	0.28	0/1148	0.47	0/1547
9	2N	0.22	0/1144	0.43	0/1543
10	1O	0.28	0/943	0.46	0/1269
10	2O	0.24	0/943	0.43	0/1269
11	1P	0.26	0/1152	0.45	0/1533
11	2P	0.23	0/1152	0.46	0/1533
12	1Q	0.28	0/1143	0.45	0/1527
12	2Q	0.24	0/1143	0.44	0/1527
13	1R	0.27	0/982	0.46	0/1312
13	2R	0.25	0/982	0.46	0/1312
14	1S	0.24	0/887	0.47	0/1180
14	2S	0.25	0/880	0.44	0/1172
15	1T	0.26	0/1105	0.44	0/1477
15	2T	0.24	0/1097	0.43	0/1468
16	1U	0.30	0/977	0.42	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.26	0/977	0.41	0/1301
17	1V	0.30	0/786	0.44	0/1053
17	2V	0.25	0/782	0.45	0/1049
18	1W	0.30	0/897	0.47	0/1205
18	2W	0.26	0/897	0.45	0/1205
19	1X	0.29	0/764	0.45	0/1025
19	2X	0.26	0/764	0.45	0/1025
20	1Y	0.27	0/823	0.49	0/1099
20	2Y	0.24	0/823	0.44	0/1100
21	1Z	0.24	0/1620	0.45	0/2200
21	2Z	0.22	0/1590	0.44	0/2162
22	10	0.27	0/616	0.44	0/821
22	20	0.25	0/616	0.44	0/821
23	11	0.25	0/761	0.44	0/1013
23	21	0.25	0/766	0.44	0/1018
24	12	0.24	0/590	0.43	0/781
24	22	0.23	0/594	0.39	0/785
25	13	0.26	0/474	0.47	0/635
25	23	0.24	0/469	0.46	0/630
26	14	0.28	0/559	0.58	0/754
26	24	0.28	0/549	0.56	0/741
27	15	0.32	0/473	0.51	0/639
27	25	0.26	0/469	0.47	0/635
28	16	0.28	0/460	0.44	0/613
28	26	0.26	0/456	0.41	0/608
29	17	0.28	0/426	0.46	0/561
29	27	0.27	0/426	0.45	0/561
30	18	0.27	0/525	0.47	0/691
30	28	0.24	0/525	0.43	0/691
31	19	0.30	0/310	0.45	0/407
31	29	0.26	0/310	0.47	0/407
32	1a	0.25	0/35795	0.79	13/55864 (0.0%)
32	2a	0.24	0/35890	0.79	16/56012 (0.0%)
33	1b	0.24	0/1876	0.48	0/2533
33	2b	0.25	0/1860	0.48	0/2518
34	1c	0.23	0/1582	0.44	0/2137
34	2c	0.23	0/1566	0.44	0/2119
35	1d	0.23	0/1695	0.43	0/2274
35	2d	0.22	0/1698	0.42	0/2277
36	1e	0.23	0/1149	0.45	0/1548
36	2e	0.23	0/1149	0.47	0/1548
37	1f	0.24	0/827	0.42	0/1120
37	2f	0.23	0/829	0.43	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.23	0/1254	0.44	0/1683
38	2g	0.23	0/1248	0.41	0/1676
39	1h	0.22	0/1118	0.44	0/1506
39	2h	0.22	0/1108	0.45	0/1494
40	1i	0.24	0/1005	0.45	0/1351
40	2i	0.24	0/985	0.43	0/1329
41	1j	0.23	0/732	0.48	0/993
41	2j	0.24	0/723	0.48	0/984
42	1k	0.23	0/849	0.44	0/1150
42	2k	0.23	0/848	0.45	0/1149
43	1l	0.22	0/937	0.44	0/1260
43	2l	0.22	0/937	0.45	0/1260
44	1m	0.23	0/924	0.47	0/1242
44	2m	0.23	0/905	0.49	0/1217
45	1n	0.24	0/501	0.43	0/664
45	2n	0.23	0/501	0.40	0/664
46	1o	0.22	0/739	0.40	0/985
46	2o	0.22	0/739	0.41	0/985
47	1p	0.23	0/697	0.46	0/939
47	2p	0.22	0/693	0.44	0/935
48	1q	0.23	0/836	0.43	0/1117
48	2q	0.22	0/836	0.41	0/1117
49	1r	0.23	0/560	0.40	0/746
49	2r	0.23	0/560	0.40	0/746
50	1s	0.23	0/663	0.48	0/895
50	2s	0.24	0/660	0.51	0/893
51	1t	0.21	0/734	0.41	0/969
51	2t	0.21	0/736	0.41	0/976
52	1u	0.21	0/203	0.43	0/266
52	2u	0.21	0/203	0.43	0/266
All	All	0.27	1/308400 (0.0%)	0.70	67/461145 (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
3	2D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2104	G	N1-C2	-6.09	1.32	1.37

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2104	G	C5-C6-O6	14.27	137.16	128.60
1	2A	2185	C	N1-C2-O2	13.41	126.95	118.90
1	2A	2104	G	N3-C2-N2	12.71	128.80	119.90
1	1A	1042	G	OP1-P-O3'	-11.71	79.44	105.20
1	2A	2104	G	N1-C2-N2	-10.03	107.18	116.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2D	274	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%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	254 (93%)	18 (7%)	1 (0%)	30	63
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	25	58
4	2E	202/206 (98%)	195 (96%)	7 (4%)	0	100	100
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	25	58
5	2F	201/210 (96%)	198 (98%)	1 (0%)	2 (1%)	13	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	1G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	22	53
6	2G	179/182 (98%)	168 (94%)	9 (5%)	2 (1%)	12	39
7	1H	172/180 (96%)	166 (96%)	5 (3%)	1 (1%)	22	53
7	2H	171/180 (95%)	168 (98%)	3 (2%)	0	100	100
8	1I	145/148 (98%)	134 (92%)	10 (7%)	1 (1%)	19	51
8	2I	144/148 (97%)	135 (94%)	9 (6%)	0	100	100
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	19	51
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	19	51
12	1Q	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	1R	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
13	2R	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	14	45
14	2S	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	1T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
15	2T	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
17	2V	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
19	2X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	201/206 (98%)	194 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	2Z	199/206 (97%)	191 (96%)	8 (4%)	0	100	100
22	10	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
22	20	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
23	11	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
26	14	67/71 (94%)	57 (85%)	9 (13%)	1 (2%)	8	33
26	24	67/71 (94%)	55 (82%)	10 (15%)	2 (3%)	3	19
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	203 (89%)	20 (9%)	6 (3%)	4	21
33	2b	229/256 (90%)	205 (90%)	13 (6%)	11 (5%)	2	11
34	1c	204/239 (85%)	198 (97%)	6 (3%)	0	100	100
34	2c	204/239 (85%)	194 (95%)	10 (5%)	0	100	100
35	1d	206/209 (99%)	197 (96%)	7 (3%)	2 (1%)	13	42
35	2d	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	25	58
36	1e	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
36	2e	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
37	1f	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
37	2f	98/101 (97%)	97 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	1g	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
38	2g	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	19	51
39	1h	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
39	2h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
40	1i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16	48
40	2i	124/128 (97%)	114 (92%)	8 (6%)	2 (2%)	8	31
41	1j	95/105 (90%)	84 (88%)	9 (10%)	2 (2%)	5	25
41	2j	94/105 (90%)	87 (93%)	6 (6%)	1 (1%)	12	39
42	1k	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	7	29
42	2k	112/129 (87%)	107 (96%)	5 (4%)	0	100	100
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	114/126 (90%)	109 (96%)	4 (4%)	1 (1%)	14	45
44	2m	112/126 (89%)	109 (97%)	2 (2%)	1 (1%)	14	45
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
47	1p	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
47	2p	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
48	1q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	13	42
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
50	2s	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
51	1t	94/106 (89%)	91 (97%)	2 (2%)	1 (1%)	12	39
51	2t	96/106 (91%)	91 (95%)	4 (4%)	1 (1%)	13	42
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	21 (100%)	0	0	100	100
All	All	11440/12128 (94%)	10932 (96%)	458 (4%)	50 (0%)	30	63

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
26	14	56	VAL
33	1b	17	PHE
33	1b	21	ARG
33	1b	125	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	203 (95%)	11 (5%)	20	49
3	2D	215/218 (99%)	202 (94%)	13 (6%)	16	44
4	1E	164/166 (99%)	156 (95%)	8 (5%)	21	51
4	2E	164/166 (99%)	157 (96%)	7 (4%)	25	55
5	1F	160/166 (96%)	152 (95%)	8 (5%)	20	50
5	2F	159/166 (96%)	151 (95%)	8 (5%)	20	50
6	1G	144/156 (92%)	141 (98%)	3 (2%)	48	72
6	2G	142/156 (91%)	139 (98%)	3 (2%)	48	72
7	1H	144/148 (97%)	139 (96%)	5 (4%)	31	61
7	2H	143/148 (97%)	138 (96%)	5 (4%)	31	61
8	1I	111/124 (90%)	106 (96%)	5 (4%)	23	53
8	2I	108/124 (87%)	105 (97%)	3 (3%)	38	66
9	1N	119/119 (100%)	117 (98%)	2 (2%)	56	78
9	2N	118/119 (99%)	116 (98%)	2 (2%)	56	78
10	1O	100/100 (100%)	99 (99%)	1 (1%)	73	86
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36	64
11	1P	115/116 (99%)	112 (97%)	3 (3%)	41	68
11	2P	115/116 (99%)	114 (99%)	1 (1%)	75	88
12	1Q	111/111 (100%)	110 (99%)	1 (1%)	75	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	54	76
13	1R	101/101 (100%)	94 (93%)	7 (7%)	13	39
13	2R	101/101 (100%)	94 (93%)	7 (7%)	13	39
14	1S	87/88 (99%)	85 (98%)	2 (2%)	45	70
14	2S	85/88 (97%)	84 (99%)	1 (1%)	67	83
15	1T	115/127 (91%)	111 (96%)	4 (4%)	31	61
15	2T	113/127 (89%)	111 (98%)	2 (2%)	54	76
16	1U	93/94 (99%)	92 (99%)	1 (1%)	70	84
16	2U	93/94 (99%)	91 (98%)	2 (2%)	47	71
17	1V	81/82 (99%)	78 (96%)	3 (4%)	29	59
17	2V	80/82 (98%)	77 (96%)	3 (4%)	28	59
18	1W	90/92 (98%)	88 (98%)	2 (2%)	47	71
18	2W	90/92 (98%)	87 (97%)	3 (3%)	33	62
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	75 (97%)	2 (3%)	41	68
20	1Y	86/91 (94%)	84 (98%)	2 (2%)	45	70
20	2Y	86/91 (94%)	85 (99%)	1 (1%)	67	83
21	1Z	169/179 (94%)	160 (95%)	9 (5%)	19	48
21	2Z	165/179 (92%)	164 (99%)	1 (1%)	84	91
22	10	61/67 (91%)	59 (97%)	2 (3%)	33	62
22	20	61/67 (91%)	60 (98%)	1 (2%)	58	79
23	11	79/83 (95%)	78 (99%)	1 (1%)	65	82
23	21	81/83 (98%)	79 (98%)	2 (2%)	42	69
24	12	65/67 (97%)	64 (98%)	1 (2%)	60	80
24	22	66/67 (98%)	65 (98%)	1 (2%)	60	80
25	13	51/52 (98%)	47 (92%)	4 (8%)	10	35
25	23	50/52 (96%)	48 (96%)	2 (4%)	27	58
26	14	58/63 (92%)	57 (98%)	1 (2%)	56	78
26	24	54/63 (86%)	50 (93%)	4 (7%)	11	36
27	15	51/52 (98%)	47 (92%)	4 (8%)	10	35
27	25	50/52 (96%)	46 (92%)	4 (8%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	16	51/52 (98%)	47 (92%)	4 (8%)	10	35
28	26	50/52 (96%)	47 (94%)	3 (6%)	16	44
29	17	41/42 (98%)	39 (95%)	2 (5%)	21	51
29	27	41/42 (98%)	38 (93%)	3 (7%)	11	37
30	18	54/55 (98%)	53 (98%)	1 (2%)	52	75
30	28	54/55 (98%)	52 (96%)	2 (4%)	29	59
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	65
33	1b	191/220 (87%)	183 (96%)	8 (4%)	25	56
33	2b	187/220 (85%)	183 (98%)	4 (2%)	48	72
34	1c	144/188 (77%)	139 (96%)	5 (4%)	31	61
34	2c	140/188 (74%)	137 (98%)	3 (2%)	48	72
35	1d	171/181 (94%)	160 (94%)	11 (6%)	14	42
35	2d	172/181 (95%)	169 (98%)	3 (2%)	56	78
36	1e	114/123 (93%)	111 (97%)	3 (3%)	41	68
36	2e	114/123 (93%)	111 (97%)	3 (3%)	41	68
37	1f	85/90 (94%)	85 (100%)	0	100	100
37	2f	85/90 (94%)	83 (98%)	2 (2%)	44	70
38	1g	120/127 (94%)	119 (99%)	1 (1%)	79	89
38	2g	119/127 (94%)	118 (99%)	1 (1%)	79	89
39	1h	116/119 (98%)	111 (96%)	5 (4%)	25	55
39	2h	114/119 (96%)	110 (96%)	4 (4%)	31	61
40	1i	91/99 (92%)	88 (97%)	3 (3%)	33	62
40	2i	88/99 (89%)	86 (98%)	2 (2%)	45	70
41	1j	68/92 (74%)	67 (98%)	1 (2%)	60	80
41	2j	68/92 (74%)	65 (96%)	3 (4%)	24	54
42	1k	83/99 (84%)	83 (100%)	0	100	100
42	2k	83/99 (84%)	83 (100%)	0	100	100
43	1l	96/108 (89%)	95 (99%)	1 (1%)	73	86
43	2l	96/108 (89%)	95 (99%)	1 (1%)	73	86
44	1m	90/101 (89%)	89 (99%)	1 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	2m	87/101 (86%)	86 (99%)	1 (1%)	70	84
45	1n	49/50 (98%)	47 (96%)	2 (4%)	26	57
45	2n	49/50 (98%)	49 (100%)	0	100	100
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	78 (100%)	0	100	100
47	1p	69/74 (93%)	65 (94%)	4 (6%)	17	45
47	2p	68/74 (92%)	65 (96%)	3 (4%)	24	54
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	93 (99%)	1 (1%)	70	84
49	1r	59/77 (77%)	59 (100%)	0	100	100
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	68/80 (85%)	65 (96%)	3 (4%)	24	54
50	2s	67/80 (84%)	62 (92%)	5 (8%)	11	36
51	1t	71/82 (87%)	69 (97%)	2 (3%)	38	66
51	2t	70/82 (85%)	67 (96%)	3 (4%)	25	55
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9363/10064 (93%)	9084 (97%)	279 (3%)	36	64

5 of 279 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	26	5	VAL
30	28	31	HIS
40	2i	20	ARG
31	19	26	ILE
29	17	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
21	2Z	55	HIS
36	2e	78	HIS
21	2Z	132	ASN
33	2b	40	HIS

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Mol	Chain	Res	Type
41	2j	62	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	443 (15%)	15 (0%)
1	2A	2855/2915 (97%)	499 (17%)	24 (0%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	119/121 (98%)	18 (15%)	0
32	1a	1494/1521 (98%)	275 (18%)	0
32	2a	1498/1521 (98%)	275 (18%)	0
All	All	8947/9114 (98%)	1522 (17%)	39 (0%)

5 of 1522 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	15	G
1	1A	34	C
1	1A	45	C

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1420	U
1	2A	2321	G
1	2A	1442	G
1	2A	2171	A
1	2A	2689	U

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

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

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



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	5MC	2a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.14	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.64	3 (15%)	26,32,35	1.13	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	0.96	1 (4%)
32	5MC	2a	1400	32	19,22,23	1.70	3 (15%)	26,32,35	1.14	2 (7%)
32	5MC	1a	1407	32	19,22,23	1.66	2 (10%)	26,32,35	1.11	2 (7%)
32	MA6	2a	1519	32	19,26,27	1.05	1 (5%)	18,38,41	2.35	7 (38%)
32	5MC	1a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.12	2 (7%)
32	MA6	2a	1518	32	19,26,27	1.20	3 (15%)	18,38,41	2.21	5 (27%)
1	5MU	1A	1939	1	19,22,23	1.45	5 (26%)	27,32,35	2.30	6 (22%)
32	2MG	1a	1207	32	18,26,27	0.90	1 (5%)	16,38,41	1.48	4 (25%)
32	7MG	2a	527	32	23,26,27	1.29	3 (13%)	27,39,42	2.65	7 (25%)
1	2MU	1A	2552	53,1	19,22,24	1.21	2 (10%)	25,31,36	1.87	6 (24%)
1	4OC	1A	1920	1	19,22,24	0.78	0	25,31,35	0.80	0
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.07	4 (19%)
1	5MC	2A	1962	1	19,22,23	1.54	3 (15%)	26,32,35	1.12	2 (7%)
32	MA6	1a	1518	32	19,26,27	1.10	1 (5%)	18,38,41	2.23	7 (38%)
32	5MC	2a	1404	32	19,22,23	1.71	3 (15%)	26,32,35	1.14	3 (11%)
1	2MU	2A	2552	53,1	19,22,24	1.28	3 (15%)	25,31,36	1.92	5 (20%)
43	0TD	2l	92	43	8,9,10	4.54	2 (25%)	6,11,13	4.31	2 (33%)
1	PSU	2A	2605	1	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
1	OMG	1A	2251	1	19,26,27	0.90	1 (5%)	21,38,41	1.05	2 (9%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.92	1 (4%)
32	7MG	1a	527	32	23,26,27	1.31	3 (13%)	27,39,42	2.62	7 (25%)
1	5MC	1A	1942	1	19,22,23	1.62	3 (15%)	26,32,35	1.15	3 (11%)
32	PSU	2a	516	53,32	18,21,22	1.37	2 (11%)	21,30,33	2.07	5 (23%)
43	0TD	1l	92	43	8,9,10	4.52	2 (25%)	6,11,13	4.67	2 (33%)
1	4OC	2A	1920	1	19,22,24	0.82	0	25,31,35	1.05	1 (4%)
32	UR3	2a	1498	32	19,22,23	1.03	1 (5%)	26,32,35	1.73	3 (11%)
32	2MG	2a	1207	32	18,26,27	0.90	1 (5%)	16,38,41	1.21	2 (12%)
1	5MU	2A	1939	1	19,22,23	1.38	5 (26%)	27,32,35	2.18	6 (22%)
32	M2G	1a	966	32	20,27,28	1.34	2 (10%)	19,40,43	1.00	2 (10%)
32	M2G	2a	966	32	20,27,28	1.35	3 (15%)	19,40,43	0.99	1 (5%)
32	5MC	1a	967	32	19,22,23	1.64	2 (10%)	26,32,35	1.06	2 (7%)
1	5MC	1A	1962	1	19,22,23	1.66	3 (15%)	26,32,35	1.11	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MA	2A	2503	53,1	17,25,26	1.08	2 (11%)	16,37,40	1.28	3 (18%)
32	PSU	1a	516	53,32	18,21,22	1.37	2 (11%)	21,30,33	2.01	4 (19%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.01	4 (19%)
1	2MA	1A	2503	53,1	17,25,26	1.04	1 (5%)	16,37,40	1.23	3 (18%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.00	3 (14%)
1	PSU	1A	1917	53,1	18,21,22	1.36	2 (11%)	21,30,33	1.99	3 (14%)
32	5MC	1a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.15	2 (7%)
32	5MC	2a	967	32	19,22,23	1.75	3 (15%)	26,32,35	1.13	3 (11%)
32	UR3	1a	1498	32	19,22,23	1.02	2 (10%)	26,32,35	1.72	2 (7%)
1	PSU	1A	2605	1	18,21,22	1.41	3 (16%)	21,30,33	1.95	4 (19%)
1	5MU	2A	1915	1	19,22,23	1.42	5 (26%)	27,32,35	2.20	9 (33%)
32	MA6	1a	1519	32	19,26,27	1.10	2 (10%)	18,38,41	2.12	6 (33%)
1	5MU	1A	1915	53,1	19,22,23	1.43	6 (31%)	27,32,35	2.21	9 (33%)
1	OMG	2A	2251	53,1	19,26,27	0.90	1 (5%)	21,38,41	1.05	1 (4%)

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	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	2a	1400	32	-	4/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	6/7/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	7MG	2a	527	32	-	1/7/37/38	0/3/3/3
1	2MU	1A	2552	53,1	-	0/9/27/28	0/2/2/2
1	4OC	1A	1920	1	-	1/9/27/30	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MU	2A	2552	53,1	-	1/9/27/28	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1	-	0/5/27/28	0/3/3/3
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	7MG	1a	527	32	-	3/7/37/38	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	53,32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
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	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	2/7/25/26	0/2/2/2
1	2MA	2A	2503	53,1	-	3/3/25/26	0/3/3/3
32	PSU	1a	516	53,32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	53,1	-	1/3/25/26	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	53,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	1/7/29/30	0/3/3/3
1	5MU	1A	1915	53,1	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	53,1	-	0/5/27/28	0/3/3/3

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.34	1.69	1.82
43	1l	92	0TD	CB-SB	-12.20	1.70	1.82
32	2a	967	5MC	C5-C4	6.48	1.49	1.44
32	2a	1404	5MC	C5-C4	6.36	1.48	1.44
32	1a	1400	5MC	C5-C4	6.23	1.48	1.44

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-10.82	82.91	102.36
43	2l	92	0TD	CSB-SB-CB	-9.83	84.69	102.36
32	2a	527	7MG	N9-C4-N3	9.01	138.66	125.46
32	1a	527	7MG	N9-C4-N3	8.81	138.38	125.46
32	1a	1498	UR3	C4-N3-C2	-6.93	119.00	124.58

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
32	1a	1402	4OC	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CG-CB-SB-CSB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1734 ligands modelled in this entry, 1730 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	$\# Z  > 2$
56	SF4	1d	501	35	0,12,12	-	-	-		
56	SF4	2d	501	35	0,12,12	-	-	-		
54	HGR	1A	3749	-	39,39,39	2.41	9 (23%)	48,58,58	1.68	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	HGR	2A	3515	-	39,39,39	2.41	8 (20%)	48,58,58	1.74	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SF4	1d	501	35	-	-	0/6/5/5
56	SF4	2d	501	35	-	-	0/6/5/5
54	HGR	1A	3749	-	-	6/20/79/79	0/4/4/4
54	HGR	2A	3515	-	-	7/20/79/79	0/4/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2A	3515	HGR	C12-C14	9.17	1.55	1.33
54	1A	3749	HGR	C12-C14	9.13	1.55	1.33
54	2A	3515	HGR	C5-C4	-5.57	1.39	1.49
54	1A	3749	HGR	C5-C4	-5.55	1.39	1.49
54	1A	3749	HGR	C5-C6	-5.40	1.39	1.50

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2A	3515	HGR	C10-C9-C8	-5.20	95.82	102.29
54	1A	3749	HGR	C4-C5-C6	4.26	121.43	112.35
54	2A	3515	HGR	C4-C5-C6	4.19	121.29	112.35
54	1A	3749	HGR	C10-C9-C8	-3.71	97.66	102.29
54	2A	3515	HGR	O1-C10-C9	-3.61	100.39	104.98

There are no chirality outliers.

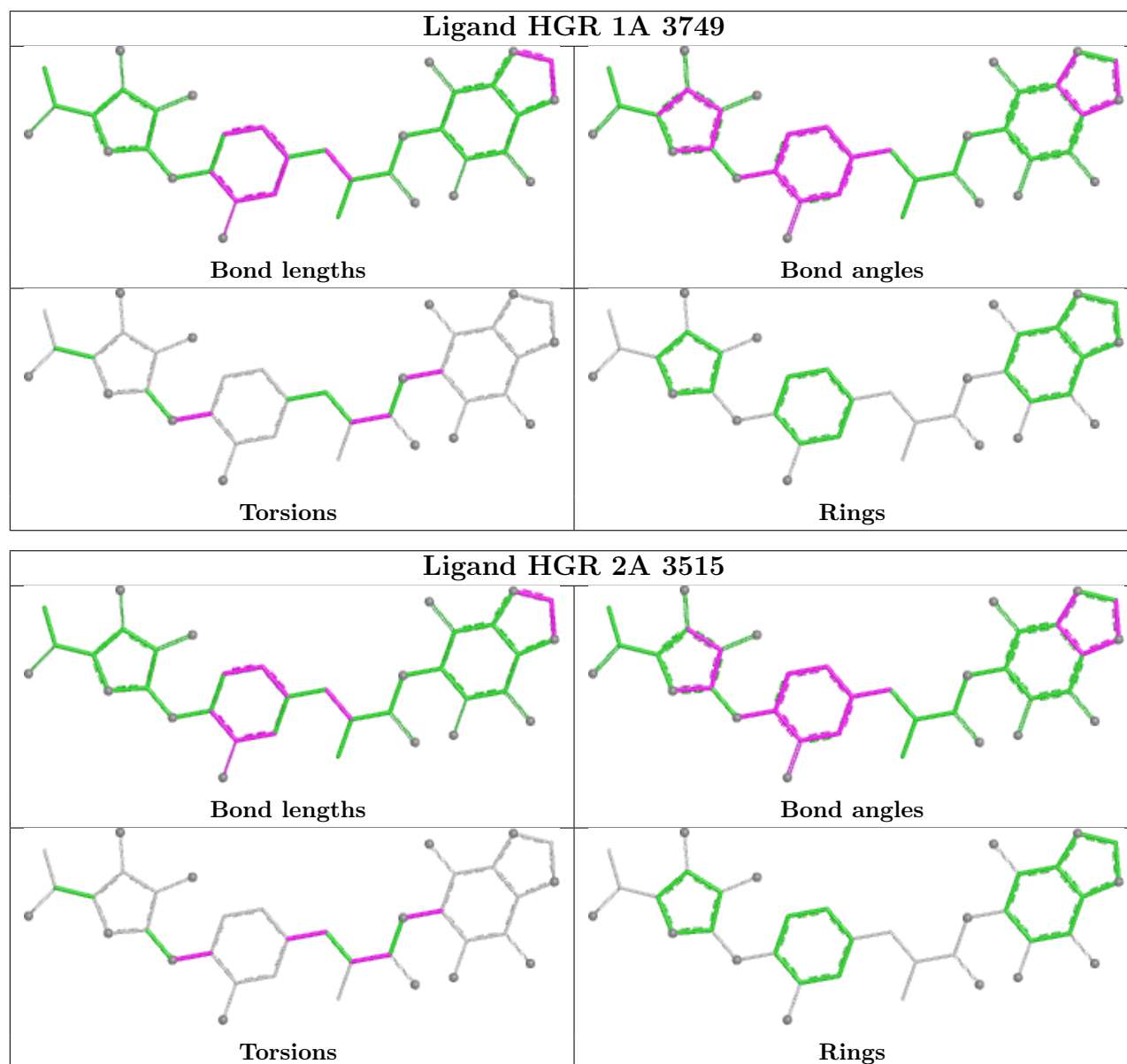
5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	2A	3515	HGR	C14-C12-C6-C1
54	1A	3749	HGR	C12-C14-C15-O7
54	1A	3749	HGR	C12-C14-C15-N1
54	2A	3515	HGR	C12-C14-C15-O7
54	2A	3515	HGR	C12-C14-C15-N1

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2861/2915 (98%)	1.09	331 (11%) 11 7	28, 61, 116, 129	0
1	2A	2856/2915 (97%)	0.68	224 (7%) 20 11	34, 66, 117, 137	0
2	1B	120/121 (99%)	1.01	15 (12%) 9 6	44, 84, 99, 108	0
2	2B	120/121 (99%)	1.11	14 (11%) 10 7	51, 90, 104, 111	0
3	1D	275/276 (99%)	1.49	60 (21%) 3 1	39, 63, 82, 98	0
3	2D	275/276 (99%)	1.14	44 (16%) 6 3	40, 66, 83, 99	0
4	1E	204/206 (99%)	1.38	48 (23%) 2 1	37, 64, 84, 99	0
4	2E	204/206 (99%)	0.79	15 (7%) 22 13	38, 68, 86, 102	0
5	1F	203/210 (96%)	1.24	30 (14%) 7 4	35, 71, 95, 116	0
5	2F	203/210 (96%)	1.04	22 (10%) 12 7	38, 75, 96, 118	0
6	1G	181/182 (99%)	1.79	58 (32%) 1 1	85, 105, 113, 120	0
6	2G	181/182 (99%)	2.36	98 (54%) 0 0	85, 107, 115, 123	0
7	1H	174/180 (96%)	1.98	77 (44%) 1 0	63, 84, 97, 104	0
7	2H	173/180 (96%)	1.38	39 (22%) 3 1	69, 89, 100, 106	0
8	1I	147/148 (99%)	1.47	39 (26%) 2 1	70, 97, 107, 111	0
8	2I	146/148 (98%)	1.22	28 (19%) 4 2	67, 98, 108, 111	0
9	1N	140/140 (100%)	0.89	14 (10%) 14 8	32, 49, 75, 93	0
9	2N	140/140 (100%)	1.47	33 (23%) 2 1	67, 86, 100, 108	0
10	1O	122/122 (100%)	0.80	13 (10%) 12 7	39, 61, 81, 88	0
10	2O	122/122 (100%)	1.27	18 (14%) 7 4	59, 80, 94, 101	0
11	1P	149/150 (99%)	1.37	26 (17%) 5 3	37, 75, 96, 103	0
11	2P	149/150 (99%)	1.28	30 (20%) 3 2	41, 79, 99, 107	0
12	1Q	141/141 (100%)	1.44	31 (21%) 3 1	45, 69, 85, 93	0
12	2Q	141/141 (100%)	1.13	20 (14%) 7 4	52, 75, 90, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.83	9 (7%) 21 12	38, 55, 71, 89	0
13	2R	118/118 (100%)	0.59	7 (5%) 29 18	41, 59, 73, 91	0
14	1S	110/112 (98%)	1.75	30 (27%) 2 1	62, 83, 97, 99	0
14	2S	110/112 (98%)	1.58	35 (31%) 1 1	67, 87, 100, 103	0
15	1T	131/146 (89%)	1.37	32 (24%) 2 1	53, 74, 95, 104	0
15	2T	131/146 (89%)	1.02	17 (12%) 9 5	59, 77, 96, 106	0
16	1U	116/118 (98%)	1.40	24 (20%) 3 2	34, 58, 80, 86	0
16	2U	116/118 (98%)	0.97	8 (6%) 24 14	43, 63, 85, 90	0
17	1V	101/101 (100%)	1.49	20 (19%) 3 2	39, 68, 86, 99	0
17	2V	101/101 (100%)	1.35	22 (21%) 3 1	45, 74, 91, 102	0
18	1W	112/113 (99%)	1.06	17 (15%) 6 3	34, 48, 75, 102	0
18	2W	112/113 (99%)	0.54	4 (3%) 46 27	39, 52, 80, 102	0
19	1X	95/96 (98%)	1.16	11 (11%) 11 7	40, 61, 84, 98	0
19	2X	95/96 (98%)	0.86	6 (6%) 27 16	45, 65, 87, 98	0
20	1Y	107/110 (97%)	1.71	26 (24%) 2 1	55, 75, 93, 103	0
20	2Y	107/110 (97%)	1.46	22 (20%) 3 2	63, 79, 96, 106	0
21	1Z	203/206 (98%)	1.05	23 (11%) 11 7	46, 76, 99, 114	0
21	2Z	201/206 (97%)	1.57	62 (30%) 1 1	71, 100, 110, 118	0
22	10	77/85 (90%)	1.36	17 (22%) 3 1	51, 65, 84, 88	0
22	20	77/85 (90%)	1.43	17 (22%) 3 1	57, 70, 87, 90	0
23	11	97/98 (98%)	1.54	25 (25%) 2 1	42, 70, 92, 99	0
23	21	97/98 (98%)	1.36	19 (19%) 4 2	45, 72, 94, 101	0
24	12	70/72 (97%)	1.39	15 (21%) 3 2	51, 74, 89, 103	0
24	22	70/72 (97%)	1.09	11 (15%) 6 3	56, 78, 91, 100	0
25	13	59/60 (98%)	1.46	15 (25%) 2 1	45, 64, 90, 106	0
25	23	59/60 (98%)	1.08	4 (6%) 25 14	53, 70, 92, 105	0
26	14	69/71 (97%)	1.81	30 (43%) 1 0	103, 112, 118, 122	0
26	24	69/71 (97%)	2.21	34 (49%) 0 0	102, 113, 119, 122	0
27	15	59/60 (98%)	0.83	5 (8%) 18 10	33, 53, 75, 91	0
27	25	59/60 (98%)	0.81	4 (6%) 25 14	38, 57, 76, 91	0
28	16	53/54 (98%)	1.35	12 (22%) 3 1	57, 69, 85, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.90	4 (7%)	22 12	61, 73, 89, 90	0
29	17	48/49 (97%)	0.98	6 (12%)	9 6	35, 44, 81, 96	0
29	27	48/49 (97%)	0.86	7 (14%)	7 4	37, 47, 81, 98	0
30	18	64/65 (98%)	1.37	15 (23%)	2 1	48, 63, 76, 86	0
30	28	64/65 (98%)	1.16	12 (18%)	4 2	54, 67, 79, 88	0
31	19	37/37 (100%)	1.90	16 (43%)	1 0	57, 70, 86, 91	0
31	29	37/37 (100%)	1.58	9 (24%)	2 1	65, 77, 90, 94	0
32	1a	1488/1521 (97%)	1.74	454 (30%)	1 1	69, 105, 124, 132	0
32	2a	1492/1521 (98%)	1.61	409 (27%)	2 1	70, 105, 124, 132	0
33	1b	231/256 (90%)	1.78	87 (37%)	1 0	98, 108, 115, 117	0
33	2b	231/256 (90%)	1.66	67 (29%)	1 1	98, 109, 115, 119	0
34	1c	206/239 (86%)	2.54	116 (56%)	0 0	102, 112, 118, 122	0
34	2c	206/239 (86%)	2.47	116 (56%)	0 0	102, 112, 117, 122	0
35	1d	208/209 (99%)	2.02	83 (39%)	1 0	89, 102, 111, 119	0
35	2d	208/209 (99%)	1.88	67 (32%)	1 0	88, 101, 111, 119	0
36	1e	148/162 (91%)	1.78	52 (35%)	1 0	80, 100, 107, 113	0
36	2e	148/162 (91%)	1.91	54 (36%)	1 0	82, 101, 108, 114	0
37	1f	100/101 (99%)	1.58	27 (27%)	2 1	82, 97, 106, 111	0
37	2f	100/101 (99%)	1.27	20 (20%)	3 2	84, 98, 107, 110	0
38	1g	155/156 (99%)	2.52	94 (60%)	0 0	103, 112, 118, 120	0
38	2g	155/156 (99%)	2.37	85 (54%)	0 0	103, 113, 118, 121	0
39	1h	137/138 (99%)	1.29	26 (18%)	4 2	88, 101, 108, 114	0
39	2h	137/138 (99%)	1.32	27 (19%)	3 2	88, 101, 108, 115	0
40	1i	127/128 (99%)	2.65	75 (59%)	0 0	100, 114, 120, 121	0
40	2i	126/128 (98%)	3.49	105 (83%)	0 0	100, 114, 120, 124	0
41	1j	97/105 (92%)	3.09	77 (79%)	0 0	102, 113, 120, 122	0
41	2j	96/105 (91%)	3.13	76 (79%)	0 0	105, 114, 120, 121	0
42	1k	114/129 (88%)	1.17	22 (19%)	4 2	79, 100, 112, 120	0
42	2k	114/129 (88%)	1.65	32 (28%)	2 1	84, 101, 109, 112	0
43	1l	121/132 (91%)	1.55	34 (28%)	2 1	78, 94, 102, 113	0
43	2l	121/132 (91%)	1.64	33 (27%)	2 1	79, 93, 102, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	116/126 (92%)	2.82	75 (64%)	0	0	102, 114, 119, 121	0
44	2m	114/126 (90%)	2.49	68 (59%)	0	0	105, 113, 118, 121	0
45	1n	60/61 (98%)	3.75	51 (85%)	0	0	103, 113, 119, 120	0
45	2n	60/61 (98%)	3.24	50 (83%)	0	0	104, 113, 119, 122	0
46	1o	88/89 (98%)	1.42	20 (22%)	3	1	78, 96, 106, 111	0
46	2o	88/89 (98%)	1.24	15 (17%)	5	3	81, 98, 107, 111	0
47	1p	82/88 (93%)	2.49	50 (60%)	0	0	93, 102, 111, 113	0
47	2p	82/88 (93%)	2.01	34 (41%)	1	0	92, 100, 108, 114	0
48	1q	99/105 (94%)	1.99	39 (39%)	1	0	88, 100, 108, 110	0
48	2q	99/105 (94%)	1.76	35 (35%)	1	0	87, 99, 107, 110	0
49	1r	68/88 (77%)	1.45	17 (25%)	2	1	85, 98, 107, 115	0
49	2r	68/88 (77%)	1.47	16 (23%)	2	1	91, 101, 109, 118	0
50	1s	83/93 (89%)	2.78	57 (68%)	0	0	105, 114, 119, 126	0
50	2s	83/93 (89%)	2.94	61 (73%)	0	0	100, 114, 121, 124	0
51	1t	96/106 (90%)	1.90	36 (37%)	1	0	90, 102, 110, 114	0
51	2t	98/106 (92%)	1.36	22 (22%)	3	1	77, 94, 105, 109	0
52	1u	23/27 (85%)	4.23	21 (91%)	0	0	109, 113, 117, 119	0
52	2u	23/27 (85%)	3.98	21 (91%)	0	0	108, 113, 119, 119	0
All	All	20573/21242 (96%)	1.42	4905 (23%)	2	1	28, 87, 118, 137	0

The worst 5 of 4905 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1091	G	18.9
1	1A	1093	G	17.9
1	1A	1087	G	17.1
1	1A	1072	C	16.4
1	1A	1089	G	15.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	5MC	1a	967	21/22	0.53	0.20	101,111,125,127	0
32	M2G	1a	966	25/26	0.68	0.18	96,110,117,129	0
32	5MC	2a	967	21/22	0.70	0.16	100,110,124,141	0
32	2MG	2a	1207	24/25	0.73	0.17	101,114,128,130	0
32	2MG	1a	1207	24/25	0.79	0.20	97,115,130,140	0
43	0TD	1l	92	10/11	0.80	0.19	76,97,100,136	0
1	5MU	2A	1915	21/22	0.81	0.13	89,104,108,127	0
32	M2G	2a	966	25/26	0.81	0.16	95,107,118,128	0
32	4OC	1a	1402	22/23	0.82	0.16	77,90,106,109	0
1	PSU	2A	1917	20/21	0.84	0.11	83,98,115,116	0
32	PSU	1a	516	20/21	0.84	0.11	92,103,110,110	0
32	5MC	2a	1400	21/22	0.84	0.17	87,100,110,117	0
1	PSU	1A	1917	20/21	0.85	0.12	83,98,110,113	0
32	5MC	1a	1400	21/22	0.86	0.14	72,98,109,116	0
32	7MG	2a	527	24/25	0.86	0.16	83,97,107,118	0
32	UR3	2a	1498	21/22	0.86	0.12	81,91,99,114	0
43	0TD	2l	92	10/11	0.86	0.16	79,94,103,117	0
1	PSU	2A	1911	20/21	0.87	0.10	80,92,102,104	0
1	4OC	2A	1920	21/23	0.87	0.11	86,93,100,101	0
1	5MU	1A	1915	21/22	0.87	0.12	91,100,109,124	0
1	PSU	1A	1911	20/21	0.88	0.11	82,93,98,102	0
32	PSU	2a	516	20/21	0.88	0.10	88,104,112,114	0
32	5MC	1a	1404	21/22	0.88	0.15	72,90,104,107	0
32	5MC	1a	1407	21/22	0.89	0.16	71,88,94,103	0
32	4OC	2a	1402	22/23	0.89	0.12	94,102,113,115	0
1	2MA	2A	2503	23/24	0.90	0.15	35,40,53,57	0
1	4OC	1A	1920	21/23	0.90	0.13	82,92,98,101	0
32	5MC	2a	1407	21/22	0.91	0.12	83,89,96,99	0
32	7MG	1a	527	24/25	0.91	0.13	85,94,100,105	0
32	5MC	2a	1404	21/22	0.91	0.12	70,87,106,107	0
32	UR3	1a	1498	21/22	0.92	0.11	80,88,95,99	0
1	2MA	1A	2503	23/24	0.93	0.18	31,36,45,65	0
1	5MU	1A	1939	21/22	0.93	0.13	42,55,63,65	0
32	MA6	1a	1519	24/25	0.93	0.17	61,84,94,101	0
1	5MC	1A	1962	21/22	0.93	0.17	49,70,83,86	0
1	5MU	2A	1939	21/22	0.93	0.15	45,59,65,67	0
32	MA6	2a	1518	24/25	0.93	0.12	56,95,102,108	0
32	MA6	2a	1519	24/25	0.93	0.17	78,91,99,106	0
1	5MC	2A	1962	21/22	0.93	0.14	51,71,84,90	0
1	2MU	2A	2552	21/23	0.94	0.12	38,47,60,60	0
1	PSU	2A	2605	20/21	0.94	0.13	36,51,56,56	0
32	MA6	1a	1518	24/25	0.94	0.13	58,81,89,95	0
1	OMG	2A	2251	24/25	0.94	0.13	43,54,59,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MC	1A	1942	21/22	0.94	0.11	50,71,80,88	0
1	2MU	1A	2552	21/23	0.95	0.14	37,44,57,60	0
1	PSU	1A	2605	20/21	0.95	0.12	33,49,55,60	0
1	5MC	2A	1942	21/22	0.95	0.09	57,73,79,89	0
1	OMG	1A	2251	24/25	0.96	0.12	34,50,55,60	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2B	216	1/1	0.46	0.35	81,81,81,81	0
53	MG	1a	3021	1/1	0.47	0.30	86,86,86,86	0
53	MG	1a	3092	1/1	0.49	0.26	104,104,104,104	0
53	MG	1a	3109	1/1	0.52	0.30	100,100,100,100	0
53	MG	2a	1705	1/1	0.54	0.71	91,91,91,91	0
53	MG	1A	3094	1/1	0.56	0.28	73,73,73,73	0
53	MG	1A	3446	1/1	0.59	0.29	76,76,76,76	0
53	MG	1A	3556	1/1	0.60	0.23	77,77,77,77	0
53	MG	1A	3545	1/1	0.61	0.32	89,89,89,89	0
53	MG	1A	3445	1/1	0.62	0.23	90,90,90,90	0
53	MG	1h	8001	1/1	0.62	0.19	88,88,88,88	0
53	MG	2D	301	1/1	0.64	0.31	76,76,76,76	0
53	MG	2A	3433	1/1	0.64	0.23	65,65,65,65	0
53	MG	2A	3164	1/1	0.65	0.30	57,57,57,57	0
53	MG	1a	3125	1/1	0.66	0.26	95,95,95,95	0
53	MG	1A	3062	1/1	0.66	0.21	71,71,71,71	0
53	MG	2A	3103	1/1	0.66	0.31	76,76,76,76	0
53	MG	2a	1640	1/1	0.66	0.16	84,84,84,84	0
53	MG	2a	1701	1/1	0.66	0.28	93,93,93,93	0
53	MG	1a	3089	1/1	0.66	0.31	72,72,72,72	0
53	MG	2a	1706	1/1	0.66	0.23	98,98,98,98	0
53	MG	1A	3574	1/1	0.67	0.29	82,82,82,82	0
53	MG	2a	1689	1/1	0.67	0.27	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3033	1/1	0.67	0.19	50,50,50,50	0
53	MG	2A	3387	1/1	0.67	0.19	69,69,69,69	0
53	MG	2a	1612	1/1	0.67	0.31	93,93,93,93	0
53	MG	1a	3002	1/1	0.68	0.14	96,96,96,96	0
53	MG	2A	3378	1/1	0.68	0.19	69,69,69,69	0
53	MG	1D	308	1/1	0.69	0.23	63,63,63,63	0
53	MG	2a	1694	1/1	0.69	0.14	74,74,74,74	0
53	MG	1A	3399	1/1	0.69	0.17	64,64,64,64	0
53	MG	2A	3427	1/1	0.69	0.14	84,84,84,84	0
53	MG	2A	3018	1/1	0.69	0.14	74,74,74,74	0
53	MG	1A	3374	1/1	0.70	0.15	68,68,68,68	0
53	MG	1A	3104	1/1	0.70	0.20	58,58,58,58	0
53	MG	1a	3047	1/1	0.70	0.27	80,80,80,80	0
53	MG	1A	3453	1/1	0.70	0.43	87,87,87,87	0
53	MG	1A	3718	1/1	0.70	0.22	76,76,76,76	0
53	MG	1A	3727	1/1	0.70	0.42	80,80,80,80	0
53	MG	1A	3526	1/1	0.70	0.32	89,89,89,89	0
53	MG	1a	3136	1/1	0.70	0.28	83,83,83,83	0
53	MG	1f	8001	1/1	0.70	0.27	86,86,86,86	0
53	MG	2A	3118	1/1	0.71	0.27	78,78,78,78	0
53	MG	2A	3075	1/1	0.71	0.16	73,73,73,73	0
53	MG	2A	3323	1/1	0.71	0.35	74,74,74,74	0
53	MG	1a	3086	1/1	0.71	0.20	77,77,77,77	0
53	MG	2a	1620	1/1	0.72	0.20	89,89,89,89	0
53	MG	1A	3598	1/1	0.72	0.17	109,109,109,109	0
53	MG	2B	214	1/1	0.72	0.17	53,53,53,53	0
53	MG	1r	3001	1/1	0.72	0.15	87,87,87,87	0
53	MG	1A	3732	1/1	0.72	0.29	76,76,76,76	0
53	MG	1a	3116	1/1	0.72	0.12	137,137,137,137	0
53	MG	2a	1617	1/1	0.72	0.23	71,71,71,71	0
53	MG	2A	3479	1/1	0.73	0.19	56,56,56,56	0
53	MG	2a	1633	1/1	0.73	0.41	103,103,103,103	0
53	MG	2B	205	1/1	0.73	0.21	73,73,73,73	0
53	MG	1A	3659	1/1	0.73	0.18	85,85,85,85	0
53	MG	1A	3510	1/1	0.73	0.29	41,41,41,41	0
53	MG	2A	3067	1/1	0.73	0.28	56,56,56,56	0
53	MG	1A	3614	1/1	0.73	0.25	64,64,64,64	0
53	MG	2A	3444	1/1	0.73	0.15	59,59,59,59	0
53	MG	2a	1716	1/1	0.73	0.28	85,85,85,85	0
53	MG	1A	3283	1/1	0.74	0.30	71,71,71,71	0
53	MG	2A	3425	1/1	0.74	0.14	68,68,68,68	0
53	MG	1G	8002	1/1	0.74	0.16	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3621	1/1	0.74	0.35	67,67,67,67	0
53	MG	1A	3469	1/1	0.74	0.16	77,77,77,77	0
53	MG	2a	1646	1/1	0.74	0.35	74,74,74,74	0
53	MG	2a	1650	1/1	0.75	0.15	80,80,80,80	0
53	MG	1A	3396	1/1	0.75	0.34	59,59,59,59	0
53	MG	1e	201	1/1	0.75	0.38	73,73,73,73	0
53	MG	1A	3030	1/1	0.75	0.25	61,61,61,61	0
53	MG	1a	3056	1/1	0.75	0.22	74,74,74,74	0
53	MG	1a	3059	1/1	0.75	0.24	92,92,92,92	0
53	MG	1B	3010	1/1	0.75	0.14	51,51,51,51	0
53	MG	1A	3516	1/1	0.76	0.22	53,53,53,53	0
53	MG	2a	1659	1/1	0.76	0.37	101,101,101,101	0
53	MG	1t	201	1/1	0.76	0.25	77,77,77,77	0
53	MG	2A	3088	1/1	0.76	0.22	67,67,67,67	0
53	MG	1g	3001	1/1	0.76	0.24	78,78,78,78	0
53	MG	2A	3023	1/1	0.76	0.31	63,63,63,63	0
53	MG	2a	1641	1/1	0.76	0.36	67,67,67,67	0
53	MG	1A	3133	1/1	0.76	0.19	69,69,69,69	0
53	MG	2a	1725	1/1	0.76	0.22	97,97,97,97	0
53	MG	2A	3368	1/1	0.77	0.19	77,77,77,77	0
53	MG	1A	3708	1/1	0.77	0.25	44,44,44,44	0
53	MG	1A	3542	1/1	0.77	0.21	78,78,78,78	0
53	MG	1Q	201	1/1	0.77	0.22	54,54,54,54	0
53	MG	1A	3413	1/1	0.77	0.18	57,57,57,57	0
53	MG	1A	3074	1/1	0.77	0.12	64,64,64,64	0
53	MG	1A	3531	1/1	0.77	0.34	78,78,78,78	0
53	MG	2A	3240	1/1	0.77	0.14	60,60,60,60	0
53	MG	2A	3055	1/1	0.77	0.15	59,59,59,59	0
53	MG	2a	1643	1/1	0.77	0.43	102,102,102,102	0
53	MG	1A	3013	1/1	0.78	0.33	69,69,69,69	0
53	MG	2A	3064	1/1	0.78	0.18	69,69,69,69	0
53	MG	1A	3295	1/1	0.78	0.22	57,57,57,57	0
53	MG	1a	3065	1/1	0.78	0.30	82,82,82,82	0
53	MG	1a	3068	1/1	0.78	0.18	90,90,90,90	0
53	MG	1A	3623	1/1	0.78	0.18	94,94,94,94	0
53	MG	2A	3478	1/1	0.78	0.15	81,81,81,81	0
53	MG	1A	3250	1/1	0.78	0.14	80,80,80,80	0
53	MG	2A	3502	1/1	0.78	0.29	94,94,94,94	0
53	MG	2a	1692	1/1	0.78	0.43	82,82,82,82	0
53	MG	1a	3039	1/1	0.78	0.40	62,62,62,62	0
53	MG	2a	1695	1/1	0.78	0.21	88,88,88,88	0
53	MG	2A	3223	1/1	0.78	0.28	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3394	1/1	0.78	0.21	61,61,61,61	0
53	MG	1a	3049	1/1	0.78	0.37	80,80,80,80	0
53	MG	2A	3337	1/1	0.78	0.28	53,53,53,53	0
53	MG	1a	3052	1/1	0.78	0.32	75,75,75,75	0
53	MG	2a	1632	1/1	0.79	0.47	89,89,89,89	0
53	MG	2A	3192	1/1	0.79	0.24	62,62,62,62	0
53	MG	1A	3084	1/1	0.79	0.10	73,73,73,73	0
53	MG	2A	3476	1/1	0.79	0.20	75,75,75,75	0
53	MG	2A	3227	1/1	0.79	0.25	71,71,71,71	0
53	MG	1l	202	1/1	0.79	0.13	81,81,81,81	0
53	MG	2A	3313	1/1	0.79	0.12	63,63,63,63	0
53	MG	1n	101	1/1	0.79	0.64	106,106,106,106	0
53	MG	2a	1688	1/1	0.79	0.19	82,82,82,82	0
53	MG	1a	3133	1/1	0.79	0.26	81,81,81,81	0
53	MG	1A	3370	1/1	0.79	0.11	57,57,57,57	0
53	MG	1a	3099	1/1	0.79	0.27	67,67,67,67	0
53	MG	28	8002	1/1	0.79	0.23	51,51,51,51	0
53	MG	2a	1700	1/1	0.79	0.18	80,80,80,80	0
53	MG	2a	1607	1/1	0.79	0.16	85,85,85,85	0
53	MG	2a	1611	1/1	0.79	0.18	97,97,97,97	0
53	MG	1a	3076	1/1	0.79	0.18	87,87,87,87	0
53	MG	2A	3135	1/1	0.79	0.27	65,65,65,65	0
53	MG	2a	1720	1/1	0.79	0.18	75,75,75,75	0
53	MG	2a	1723	1/1	0.79	0.20	77,77,77,77	0
53	MG	1a	3023	1/1	0.79	0.18	51,51,51,51	0
53	MG	2A	3242	1/1	0.80	0.14	62,62,62,62	0
53	MG	2A	3248	1/1	0.80	0.27	63,63,63,63	0
53	MG	2A	3267	1/1	0.80	0.15	70,70,70,70	0
53	MG	1a	3131	1/1	0.80	0.24	91,91,91,91	0
53	MG	1A	3026	1/1	0.80	0.15	48,48,48,48	0
53	MG	2A	3332	1/1	0.80	0.34	66,66,66,66	0
53	MG	1A	3136	1/1	0.80	0.23	63,63,63,63	0
53	MG	1A	3139	1/1	0.80	0.18	57,57,57,57	0
53	MG	1A	3197	1/1	0.80	0.17	74,74,74,74	0
53	MG	1a	3008	1/1	0.80	0.17	95,95,95,95	0
53	MG	2A	3413	1/1	0.80	0.33	71,71,71,71	0
53	MG	1a	3018	1/1	0.80	0.19	86,86,86,86	0
53	MG	2A	3117	1/1	0.80	0.30	73,73,73,73	0
53	MG	1A	3069	1/1	0.80	0.30	63,63,63,63	0
53	MG	2a	1671	1/1	0.80	0.28	70,70,70,70	0
53	MG	2A	3123	1/1	0.80	0.19	68,68,68,68	0
53	MG	1A	3257	1/1	0.80	0.28	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3270	1/1	0.80	0.18	62,62,62,62	0
53	MG	2A	3168	1/1	0.80	0.16	57,57,57,57	0
53	MG	2A	3493	1/1	0.80	0.20	52,52,52,52	0
53	MG	2a	1699	1/1	0.80	0.21	85,85,85,85	0
53	MG	1A	3102	1/1	0.80	0.13	85,85,85,85	0
53	MG	2A	3508	1/1	0.80	0.36	65,65,65,65	0
53	MG	2B	204	1/1	0.80	0.22	63,63,63,63	0
53	MG	2A	3216	1/1	0.80	0.33	65,65,65,65	0
53	MG	2a	1715	1/1	0.80	0.24	84,84,84,84	0
53	MG	2B	209	1/1	0.80	0.17	64,64,64,64	0
53	MG	2A	3008	1/1	0.80	0.25	60,60,60,60	0
53	MG	1A	3058	1/1	0.80	0.17	49,49,49,49	0
53	MG	1A	3591	1/1	0.80	0.23	61,61,61,61	0
53	MG	1A	3164	1/1	0.81	0.34	53,53,53,53	0
53	MG	1A	3465	1/1	0.81	0.17	62,62,62,62	0
53	MG	1A	3221	1/1	0.81	0.14	70,70,70,70	0
53	MG	1A	3275	1/1	0.81	0.14	38,38,38,38	0
53	MG	1T	204	1/1	0.81	0.17	83,83,83,83	0
53	MG	1A	3184	1/1	0.81	0.12	55,55,55,55	0
53	MG	1A	3525	1/1	0.81	0.24	73,73,73,73	0
53	MG	2A	3010	1/1	0.81	0.31	67,67,67,67	0
53	MG	2a	1682	1/1	0.81	0.14	76,76,76,76	0
53	MG	1A	3287	1/1	0.81	0.15	49,49,49,49	0
53	MG	1A	3251	1/1	0.81	0.18	59,59,59,59	0
53	MG	1a	3111	1/1	0.81	0.15	78,78,78,78	0
53	MG	2A	3249	1/1	0.81	0.21	64,64,64,64	0
53	MG	1a	3113	1/1	0.81	0.16	97,97,97,97	0
53	MG	2A	3269	1/1	0.81	0.32	75,75,75,75	0
53	MG	1A	3535	1/1	0.81	0.16	68,68,68,68	0
53	MG	1a	3036	1/1	0.81	0.23	88,88,88,88	0
53	MG	1A	3713	1/1	0.81	0.30	54,54,54,54	0
53	MG	1A	3541	1/1	0.81	0.19	72,72,72,72	0
53	MG	2a	1713	1/1	0.81	0.12	100,100,100,100	0
53	MG	2a	1714	1/1	0.81	0.20	101,101,101,101	0
53	MG	2A	3363	1/1	0.81	0.10	52,52,52,52	0
53	MG	1A	3360	1/1	0.81	0.29	77,77,77,77	0
53	MG	2A	3111	1/1	0.81	0.18	63,63,63,63	0
53	MG	1A	3362	1/1	0.81	0.14	63,63,63,63	0
53	MG	1A	3739	1/1	0.81	0.15	36,36,36,36	0
53	MG	2k	3001	1/1	0.81	0.17	86,86,86,86	0
53	MG	1a	3045	1/1	0.82	0.17	76,76,76,76	0
53	MG	1A	3323	1/1	0.82	0.31	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1B	3015	1/1	0.82	0.21	64,64,64,64	0
53	MG	2A	3071	1/1	0.82	0.15	68,68,68,68	0
53	MG	2a	1623	1/1	0.82	0.12	66,66,66,66	0
53	MG	1A	3175	1/1	0.82	0.27	54,54,54,54	0
53	MG	2A	3078	1/1	0.82	0.15	62,62,62,62	0
53	MG	2A	3081	1/1	0.82	0.32	82,82,82,82	0
53	MG	1A	3630	1/1	0.82	0.22	70,70,70,70	0
53	MG	1a	3057	1/1	0.82	0.78	88,88,88,88	0
53	MG	2A	3385	1/1	0.82	0.20	71,71,71,71	0
53	MG	2A	3109	1/1	0.82	0.12	67,67,67,67	0
53	MG	1A	3042	1/1	0.82	0.16	53,53,53,53	0
53	MG	1A	3128	1/1	0.82	0.28	60,60,60,60	0
53	MG	15	102	1/1	0.82	0.15	47,47,47,47	0
53	MG	2a	1683	1/1	0.82	0.32	89,89,89,89	0
53	MG	2A	3120	1/1	0.82	0.27	64,64,64,64	0
53	MG	1A	3567	1/1	0.82	0.14	97,97,97,97	0
53	MG	1A	3429	1/1	0.82	0.13	63,63,63,63	0
53	MG	2A	3161	1/1	0.82	0.18	54,54,54,54	0
53	MG	1A	3027	1/1	0.82	0.08	66,66,66,66	0
53	MG	1A	3378	1/1	0.82	0.15	72,72,72,72	0
53	MG	2A	3184	1/1	0.82	0.13	52,52,52,52	0
53	MG	1A	3387	1/1	0.82	0.16	46,46,46,46	0
53	MG	2B	202	1/1	0.82	0.37	85,85,85,85	0
53	MG	1a	3103	1/1	0.82	0.16	81,81,81,81	0
53	MG	2A	3016	1/1	0.82	0.15	70,70,70,70	0
53	MG	1a	3033	1/1	0.82	0.16	83,83,83,83	0
53	MG	1A	3761	1/1	0.82	0.15	64,64,64,64	0
53	MG	2A	3030	1/1	0.82	0.17	73,73,73,73	0
53	MG	1B	3002	1/1	0.82	0.12	76,76,76,76	0
53	MG	2O	201	1/1	0.82	0.15	48,48,48,48	0
53	MG	2A	3050	1/1	0.82	0.14	45,45,45,45	0
53	MG	2A	3253	1/1	0.82	0.14	54,54,54,54	0
53	MG	2A	3082	1/1	0.83	0.38	69,69,69,69	0
53	MG	1A	3319	1/1	0.83	0.19	70,70,70,70	0
53	MG	1A	3466	1/1	0.83	0.15	87,87,87,87	0
53	MG	2A	3104	1/1	0.83	0.40	79,79,79,79	0
53	MG	1U	201	1/1	0.83	0.45	45,45,45,45	0
53	MG	1A	3206	1/1	0.83	0.22	67,67,67,67	0
53	MG	1a	3066	1/1	0.83	0.17	74,74,74,74	0
53	MG	1A	3264	1/1	0.83	0.23	68,68,68,68	0
53	MG	1A	3014	1/1	0.83	0.36	52,52,52,52	0
53	MG	2A	3398	1/1	0.83	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3589	1/1	0.83	0.18	91,91,91,91	0
53	MG	1a	3087	1/1	0.83	0.11	87,87,87,87	0
53	MG	2A	3138	1/1	0.83	0.29	55,55,55,55	0
53	MG	2a	1658	1/1	0.83	0.30	74,74,74,74	0
53	MG	1A	3227	1/1	0.83	0.40	61,61,61,61	0
53	MG	2A	3434	1/1	0.83	0.26	57,57,57,57	0
53	MG	2A	3437	1/1	0.83	0.20	83,83,83,83	0
53	MG	1A	3745	1/1	0.83	0.28	81,81,81,81	0
53	MG	1a	3025	1/1	0.83	0.24	84,84,84,84	0
53	MG	1a	3026	1/1	0.83	0.27	65,65,65,65	0
53	MG	2A	3189	1/1	0.83	0.14	55,55,55,55	0
53	MG	1a	3107	1/1	0.83	0.17	92,92,92,92	0
53	MG	1A	3436	1/1	0.83	0.18	49,49,49,49	0
53	MG	2A	3045	1/1	0.83	0.23	61,61,61,61	0
53	MG	1a	3110	1/1	0.83	0.13	82,82,82,82	0
53	MG	1A	3130	1/1	0.83	0.13	63,63,63,63	0
53	MG	1A	3112	1/1	0.83	0.15	70,70,70,70	0
53	MG	2B	208	1/1	0.83	0.17	79,79,79,79	0
53	MG	2a	1712	1/1	0.83	0.14	103,103,103,103	0
53	MG	1a	3044	1/1	0.83	0.15	61,61,61,61	0
53	MG	2B	212	1/1	0.83	0.22	71,71,71,71	0
53	MG	1B	3012	1/1	0.83	0.14	64,64,64,64	0
53	MG	1A	3538	1/1	0.83	0.15	65,65,65,65	0
53	MG	1A	3255	1/1	0.83	0.15	57,57,57,57	0
53	MG	1A	3650	1/1	0.83	0.14	42,42,42,42	0
53	MG	2Q	3001	1/1	0.83	0.24	66,66,66,66	0
53	MG	2A	3304	1/1	0.83	0.11	57,57,57,57	0
53	MG	2t	201	1/1	0.83	0.47	80,80,80,80	0
53	MG	1A	3279	1/1	0.84	0.28	53,53,53,53	0
53	MG	1A	3330	1/1	0.84	0.15	66,66,66,66	0
53	MG	2A	3422	1/1	0.84	0.16	72,72,72,72	0
53	MG	1A	3060	1/1	0.84	0.18	53,53,53,53	0
53	MG	1g	3002	1/1	0.84	0.09	83,83,83,83	0
53	MG	1a	3029	1/1	0.84	0.19	72,72,72,72	0
53	MG	2a	1642	1/1	0.84	0.10	70,70,70,70	0
53	MG	1A	3496	1/1	0.84	0.16	73,73,73,73	0
53	MG	1A	3561	1/1	0.84	0.56	70,70,70,70	0
53	MG	2A	3229	1/1	0.84	0.23	72,72,72,72	0
53	MG	2A	3235	1/1	0.84	0.18	53,53,53,53	0
53	MG	1A	3239	1/1	0.84	0.15	56,56,56,56	0
53	MG	2a	1661	1/1	0.84	0.22	87,87,87,87	0
53	MG	1A	3715	1/1	0.84	0.13	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3364	1/1	0.84	0.18	82,82,82,82	0
53	MG	2A	3105	1/1	0.84	0.44	74,74,74,74	0
53	MG	1A	3719	1/1	0.84	0.17	71,71,71,71	0
53	MG	1Z	8001	1/1	0.84	0.18	58,58,58,58	0
53	MG	2A	3115	1/1	0.84	0.18	47,47,47,47	0
53	MG	2A	3287	1/1	0.84	0.21	63,63,63,63	0
53	MG	1A	3431	1/1	0.84	0.27	62,62,62,62	0
53	MG	1a	3055	1/1	0.84	0.17	74,74,74,74	0
53	MG	2B	211	1/1	0.84	0.15	62,62,62,62	0
53	MG	2A	3316	1/1	0.84	0.12	46,46,46,46	0
53	MG	2B	213	1/1	0.84	0.27	70,70,70,70	0
53	MG	2A	3027	1/1	0.84	0.12	63,63,63,63	0
53	MG	1A	3273	1/1	0.84	0.22	50,50,50,50	0
53	MG	1A	3303	1/1	0.84	0.19	52,52,52,52	0
53	MG	2I	3001	1/1	0.84	0.12	81,81,81,81	0
53	MG	1a	3009	1/1	0.84	0.25	70,70,70,70	0
53	MG	2A	3147	1/1	0.84	0.23	53,53,53,53	0
53	MG	2A	3376	1/1	0.84	0.20	77,77,77,77	0
53	MG	2A	3152	1/1	0.84	0.20	48,48,48,48	0
53	MG	2A	3382	1/1	0.84	0.14	51,51,51,51	0
53	MG	1A	3306	1/1	0.84	0.11	56,56,56,56	0
53	MG	1A	3100	1/1	0.84	0.59	36,36,36,36	0
53	MG	15	106	1/1	0.85	0.15	86,86,86,86	0
53	MG	1A	3519	1/1	0.85	0.24	75,75,75,75	0
53	MG	2a	1626	1/1	0.85	0.11	72,72,72,72	0
53	MG	1a	3003	1/1	0.85	0.16	77,77,77,77	0
53	MG	1A	3363	1/1	0.85	0.21	60,60,60,60	0
53	MG	2a	1634	1/1	0.85	0.38	78,78,78,78	0
53	MG	2a	1638	1/1	0.85	0.35	74,74,74,74	0
53	MG	2A	3236	1/1	0.85	0.22	42,42,42,42	0
53	MG	2A	3441	1/1	0.85	0.14	57,57,57,57	0
53	MG	2A	3239	1/1	0.85	0.18	73,73,73,73	0
53	MG	1A	3076	1/1	0.85	0.19	60,60,60,60	0
53	MG	1a	3069	1/1	0.85	0.17	75,75,75,75	0
53	MG	1A	3174	1/1	0.85	0.37	44,44,44,44	0
53	MG	2a	1653	1/1	0.85	0.21	67,67,67,67	0
53	MG	2A	3489	1/1	0.85	0.14	55,55,55,55	0
53	MG	1A	3748	1/1	0.85	0.12	62,62,62,62	0
53	MG	1A	3760	1/1	0.85	0.28	42,42,42,42	0
53	MG	2a	1667	1/1	0.85	0.39	74,74,74,74	0
53	MG	1A	3038	1/1	0.85	0.21	35,35,35,35	0
53	MG	1A	3010	1/1	0.85	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3095	1/1	0.85	0.13	67,67,67,67	0
53	MG	2a	1687	1/1	0.85	0.17	76,76,76,76	0
53	MG	1A	3633	1/1	0.85	0.21	57,57,57,57	0
53	MG	1a	3106	1/1	0.85	0.15	74,74,74,74	0
53	MG	1A	3200	1/1	0.85	0.27	55,55,55,55	0
53	MG	2a	1693	1/1	0.85	0.23	82,82,82,82	0
53	MG	1A	3096	1/1	0.85	0.14	62,62,62,62	0
53	MG	2A	3144	1/1	0.85	0.34	49,49,49,49	0
53	MG	1a	3040	1/1	0.85	0.12	76,76,76,76	0
53	MG	2A	3350	1/1	0.85	0.39	72,72,72,72	0
53	MG	2A	3151	1/1	0.85	0.17	64,64,64,64	0
53	MG	1A	3551	1/1	0.85	0.12	58,58,58,58	0
53	MG	2F	301	1/1	0.85	0.40	62,62,62,62	0
53	MG	2A	3047	1/1	0.85	0.11	59,59,59,59	0
53	MG	1A	3490	1/1	0.85	0.25	48,48,48,48	0
53	MG	1A	3714	1/1	0.85	0.21	74,74,74,74	0
53	MG	2A	3182	1/1	0.85	0.21	58,58,58,58	0
53	MG	1A	3057	1/1	0.85	0.30	47,47,47,47	0
53	MG	1A	3031	1/1	0.85	0.17	56,56,56,56	0
53	MG	1l	3002	1/1	0.85	0.20	51,51,51,51	0
53	MG	2a	1724	1/1	0.85	0.33	91,91,91,91	0
53	MG	2a	1614	1/1	0.85	0.15	84,84,84,84	0
53	MG	2a	1616	1/1	0.85	0.17	92,92,92,92	0
53	MG	2l	3001	1/1	0.85	0.20	53,53,53,53	0
53	MG	1A	3228	1/1	0.85	0.15	65,65,65,65	0
53	MG	2a	1605	1/1	0.86	0.15	82,82,82,82	0
53	MG	2a	1606	1/1	0.86	0.13	55,55,55,55	0
53	MG	2A	3344	1/1	0.86	0.43	54,54,54,54	0
53	MG	2A	3346	1/1	0.86	0.26	68,68,68,68	0
53	MG	1a	3067	1/1	0.86	0.20	80,80,80,80	0
53	MG	1A	3609	1/1	0.86	0.23	56,56,56,56	0
53	MG	2a	1615	1/1	0.86	0.12	79,79,79,79	0
53	MG	1A	3332	1/1	0.86	0.18	61,61,61,61	0
53	MG	1a	3072	1/1	0.86	0.24	83,83,83,83	0
53	MG	1A	3346	1/1	0.86	0.27	71,71,71,71	0
53	MG	2A	3381	1/1	0.86	0.09	69,69,69,69	0
53	MG	1a	3078	1/1	0.86	0.14	65,65,65,65	0
53	MG	2a	1627	1/1	0.86	0.14	78,78,78,78	0
53	MG	1a	3080	1/1	0.86	0.25	66,66,66,66	0
53	MG	2A	3015	1/1	0.86	0.23	45,45,45,45	0
53	MG	2A	3396	1/1	0.86	0.23	68,68,68,68	0
53	MG	1A	3098	1/1	0.86	0.13	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3153	1/1	0.86	0.17	59,59,59,59	0
53	MG	1A	3113	1/1	0.86	0.33	63,63,63,63	0
53	MG	2A	3020	1/1	0.86	0.13	54,54,54,54	0
53	MG	1a	3088	1/1	0.86	0.20	107,107,107,107	0
53	MG	2A	3430	1/1	0.86	0.13	63,63,63,63	0
53	MG	1A	3546	1/1	0.86	0.21	77,77,77,77	0
53	MG	1B	3005	1/1	0.86	0.18	52,52,52,52	0
53	MG	1B	3008	1/1	0.86	0.28	69,69,69,69	0
53	MG	2A	3039	1/1	0.86	0.17	51,51,51,51	0
53	MG	2A	3443	1/1	0.86	0.23	88,88,88,88	0
53	MG	1A	3648	1/1	0.86	0.69	73,73,73,73	0
53	MG	2A	3449	1/1	0.86	0.15	59,59,59,59	0
53	MG	2a	1675	1/1	0.86	0.15	83,83,83,83	0
53	MG	1B	3011	1/1	0.86	0.13	58,58,58,58	0
53	MG	1A	3548	1/1	0.86	0.50	69,69,69,69	0
53	MG	1A	3236	1/1	0.86	0.17	64,64,64,64	0
53	MG	2A	3234	1/1	0.86	0.12	73,73,73,73	0
53	MG	1A	3707	1/1	0.86	0.59	38,38,38,38	0
53	MG	2A	3494	1/1	0.86	0.10	66,66,66,66	0
53	MG	1A	3078	1/1	0.86	0.13	67,67,67,67	0
53	MG	1A	3315	1/1	0.86	0.12	53,53,53,53	0
53	MG	2A	3509	1/1	0.86	0.14	61,61,61,61	0
53	MG	2A	3072	1/1	0.86	0.20	71,71,71,71	0
53	MG	1A	3081	1/1	0.86	0.36	46,46,46,46	0
53	MG	1A	3569	1/1	0.86	0.25	67,67,67,67	0
53	MG	1A	3717	1/1	0.86	0.19	79,79,79,79	0
53	MG	1A	3210	1/1	0.86	0.14	60,60,60,60	0
53	MG	1a	3134	1/1	0.86	0.16	94,94,94,94	0
53	MG	2A	3094	1/1	0.86	0.17	76,76,76,76	0
53	MG	2A	3271	1/1	0.86	0.23	49,49,49,49	0
53	MG	2A	3282	1/1	0.86	0.53	59,59,59,59	0
53	MG	2B	215	1/1	0.86	0.12	69,69,69,69	0
53	MG	1a	3135	1/1	0.86	0.19	105,105,105,105	0
53	MG	1A	3447	1/1	0.86	0.24	59,59,59,59	0
53	MG	1a	3141	1/1	0.86	0.18	70,70,70,70	0
53	MG	1A	3720	1/1	0.86	0.09	53,53,53,53	0
53	MG	2e	3001	1/1	0.86	0.35	74,74,74,74	0
53	MG	1a	3062	1/1	0.86	0.13	69,69,69,69	0
53	MG	1A	3050	1/1	0.86	0.21	78,78,78,78	0
53	MG	1A	3464	1/1	0.86	0.18	36,36,36,36	0
53	MG	2A	3019	1/1	0.87	0.10	60,60,60,60	0
53	MG	1A	3116	1/1	0.87	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3361	1/1	0.87	0.28	69,69,69,69	0
53	MG	1A	3521	1/1	0.87	0.13	64,64,64,64	0
53	MG	2A	3029	1/1	0.87	0.13	59,59,59,59	0
53	MG	1A	3126	1/1	0.87	0.16	55,55,55,55	0
53	MG	1a	3081	1/1	0.87	0.29	63,63,63,63	0
53	MG	1A	3308	1/1	0.87	0.25	68,68,68,68	0
53	MG	1A	3592	1/1	0.87	0.16	49,49,49,49	0
53	MG	1a	3006	1/1	0.87	0.10	85,85,85,85	0
53	MG	2A	3048	1/1	0.87	0.11	64,64,64,64	0
53	MG	2A	3257	1/1	0.87	0.14	60,60,60,60	0
53	MG	1A	3721	1/1	0.87	0.15	69,69,69,69	0
53	MG	2a	1602	1/1	0.87	0.10	88,88,88,88	0
53	MG	1A	3310	1/1	0.87	0.71	49,49,49,49	0
53	MG	2A	3063	1/1	0.87	0.23	41,41,41,41	0
53	MG	1a	3014	1/1	0.87	0.08	88,88,88,88	0
53	MG	2a	1608	1/1	0.87	0.11	94,94,94,94	0
53	MG	2A	3286	1/1	0.87	0.26	56,56,56,56	0
53	MG	1A	3728	1/1	0.87	0.12	77,77,77,77	0
53	MG	2A	3290	1/1	0.87	0.23	49,49,49,49	0
53	MG	1a	3104	1/1	0.87	0.11	92,92,92,92	0
53	MG	1A	3731	1/1	0.87	0.22	71,71,71,71	0
53	MG	1A	3599	1/1	0.87	0.29	54,54,54,54	0
53	MG	1A	3314	1/1	0.87	0.24	57,57,57,57	0
53	MG	1A	3161	1/1	0.87	0.22	51,51,51,51	0
53	MG	1A	3747	1/1	0.87	0.14	58,58,58,58	0
53	MG	2A	3342	1/1	0.87	0.13	61,61,61,61	0
53	MG	2a	1629	1/1	0.87	0.15	61,61,61,61	0
53	MG	1A	3463	1/1	0.87	0.29	48,48,48,48	0
53	MG	1a	3115	1/1	0.87	0.13	82,82,82,82	0
53	MG	2A	3349	1/1	0.87	0.17	62,62,62,62	0
53	MG	1A	3163	1/1	0.87	0.27	54,54,54,54	0
53	MG	1a	3117	1/1	0.87	0.10	78,78,78,78	0
53	MG	1a	3120	1/1	0.87	0.10	92,92,92,92	0
53	MG	2A	3369	1/1	0.87	0.11	56,56,56,56	0
53	MG	1A	3629	1/1	0.87	0.18	59,59,59,59	0
53	MG	1A	3384	1/1	0.87	0.13	30,30,30,30	0
53	MG	1A	3099	1/1	0.87	0.13	64,64,64,64	0
53	MG	2a	1652	1/1	0.87	0.34	80,80,80,80	0
53	MG	1B	3007	1/1	0.87	0.17	43,43,43,43	0
53	MG	1A	3642	1/1	0.87	0.19	88,88,88,88	0
53	MG	1a	3048	1/1	0.87	0.21	66,66,66,66	0
53	MG	1A	3052	1/1	0.87	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2a	1662	1/1	0.87	0.25	74,74,74,74	0
53	MG	2A	3132	1/1	0.87	0.28	56,56,56,56	0
53	MG	2A	3406	1/1	0.87	0.21	49,49,49,49	0
53	MG	1A	3549	1/1	0.87	0.27	63,63,63,63	0
53	MG	1A	3063	1/1	0.87	0.24	36,36,36,36	0
53	MG	2A	3143	1/1	0.87	0.27	47,47,47,47	0
53	MG	1A	3676	1/1	0.87	0.14	89,89,89,89	0
53	MG	2A	3145	1/1	0.87	0.15	55,55,55,55	0
53	MG	1A	3680	1/1	0.87	0.14	41,41,41,41	0
53	MG	2A	3148	1/1	0.87	0.28	60,60,60,60	0
53	MG	2A	3150	1/1	0.87	0.12	46,46,46,46	0
53	MG	1E	305	1/1	0.87	0.19	79,79,79,79	0
53	MG	1a	3060	1/1	0.87	0.20	81,81,81,81	0
53	MG	1A	3703	1/1	0.87	0.17	62,62,62,62	0
53	MG	2A	3445	1/1	0.87	0.13	46,46,46,46	0
53	MG	1a	3063	1/1	0.87	0.10	73,73,73,73	0
53	MG	1N	3001	1/1	0.87	0.36	77,77,77,77	0
53	MG	2A	3165	1/1	0.87	0.11	54,54,54,54	0
53	MG	2a	1709	1/1	0.87	0.11	105,105,105,105	0
53	MG	2A	3004	1/1	0.87	0.14	53,53,53,53	0
53	MG	2A	3170	1/1	0.87	0.17	61,61,61,61	0
53	MG	2A	3180	1/1	0.87	0.15	59,59,59,59	0
53	MG	2A	3006	1/1	0.87	0.10	51,51,51,51	0
53	MG	1P	203	1/1	0.87	0.09	72,72,72,72	0
53	MG	2A	3503	1/1	0.87	0.15	67,67,67,67	0
53	MG	2a	1722	1/1	0.87	0.15	78,78,78,78	0
53	MG	1A	3555	1/1	0.87	0.25	35,35,35,35	0
53	MG	1A	3262	1/1	0.87	0.32	55,55,55,55	0
53	MG	2A	3213	1/1	0.87	0.23	64,64,64,64	0
53	MG	2a	1729	1/1	0.87	0.18	65,65,65,65	0
53	MG	2B	203	1/1	0.87	0.11	76,76,76,76	0
53	MG	1A	3359	1/1	0.87	0.18	66,66,66,66	0
53	MG	1a	3070	1/1	0.87	0.27	69,69,69,69	0
53	MG	2A	3226	1/1	0.87	0.18	49,49,49,49	0
53	MG	2A	3327	1/1	0.88	0.23	51,51,51,51	0
53	MG	2N	8001	1/1	0.88	0.10	68,68,68,68	0
53	MG	1a	3015	1/1	0.88	0.18	73,73,73,73	0
53	MG	2O	202	1/1	0.88	0.19	47,47,47,47	0
53	MG	1A	3118	1/1	0.88	0.21	53,53,53,53	0
53	MG	2Y	502	1/1	0.88	0.15	57,57,57,57	0
53	MG	2A	3341	1/1	0.88	0.17	45,45,45,45	0
53	MG	1A	3025	1/1	0.88	0.28	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3615	1/1	0.88	0.23	73,73,73,73	0
53	MG	1A	3008	1/1	0.88	0.16	57,57,57,57	0
53	MG	2A	3025	1/1	0.88	0.18	58,58,58,58	0
53	MG	1A	3036	1/1	0.88	0.20	76,76,76,76	0
53	MG	1A	3628	1/1	0.88	0.20	58,58,58,58	0
53	MG	2A	3364	1/1	0.88	0.14	68,68,68,68	0
53	MG	1A	3131	1/1	0.88	0.21	68,68,68,68	0
53	MG	2A	3160	1/1	0.88	0.26	53,53,53,53	0
53	MG	2A	3374	1/1	0.88	0.10	48,48,48,48	0
53	MG	1A	3105	1/1	0.88	0.11	66,66,66,66	0
53	MG	2A	3163	1/1	0.88	0.18	55,55,55,55	0
53	MG	2A	3036	1/1	0.88	0.20	55,55,55,55	0
53	MG	1A	3004	1/1	0.88	0.09	42,42,42,42	0
53	MG	2A	3384	1/1	0.88	0.10	45,45,45,45	0
53	MG	1A	3067	1/1	0.88	0.09	66,66,66,66	0
53	MG	1a	3043	1/1	0.88	0.17	90,90,90,90	0
53	MG	2A	3392	1/1	0.88	0.24	51,51,51,51	0
53	MG	1A	3372	1/1	0.88	0.22	59,59,59,59	0
53	MG	1A	3258	1/1	0.88	0.14	40,40,40,40	0
53	MG	2a	1639	1/1	0.88	0.24	69,69,69,69	0
53	MG	2A	3403	1/1	0.88	0.18	69,69,69,69	0
53	MG	1A	3651	1/1	0.88	0.15	78,78,78,78	0
53	MG	2A	3409	1/1	0.88	0.13	53,53,53,53	0
53	MG	2A	3188	1/1	0.88	0.29	66,66,66,66	0
53	MG	2A	3420	1/1	0.88	0.21	54,54,54,54	0
53	MG	1A	3207	1/1	0.88	0.30	49,49,49,49	0
53	MG	1A	3662	1/1	0.88	0.15	82,82,82,82	0
53	MG	2A	3201	1/1	0.88	0.34	62,62,62,62	0
53	MG	1a	3123	1/1	0.88	0.10	81,81,81,81	0
53	MG	2A	3068	1/1	0.88	0.14	59,59,59,59	0
53	MG	1A	3674	1/1	0.88	0.21	82,82,82,82	0
53	MG	1A	3476	1/1	0.88	0.15	39,39,39,39	0
53	MG	2a	1663	1/1	0.88	0.17	62,62,62,62	0
53	MG	1A	3479	1/1	0.88	0.18	58,58,58,58	0
53	MG	1A	3681	1/1	0.88	0.22	63,63,63,63	0
53	MG	1A	3557	1/1	0.88	0.22	55,55,55,55	0
53	MG	2a	1680	1/1	0.88	0.41	56,56,56,56	0
53	MG	1A	3560	1/1	0.88	0.27	66,66,66,66	0
53	MG	2A	3446	1/1	0.88	0.12	59,59,59,59	0
53	MG	2a	1684	1/1	0.88	0.12	75,75,75,75	0
53	MG	1A	3208	1/1	0.88	0.20	47,47,47,47	0
53	MG	1A	3491	1/1	0.88	0.13	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3095	1/1	0.88	0.19	71,71,71,71	0
53	MG	2A	3099	1/1	0.88	0.15	46,46,46,46	0
53	MG	1A	3316	1/1	0.88	0.41	68,68,68,68	0
53	MG	2A	3491	1/1	0.88	0.21	71,71,71,71	0
53	MG	10	104	1/1	0.88	0.11	57,57,57,57	0
53	MG	2A	3252	1/1	0.88	0.29	42,42,42,42	0
53	MG	1A	3573	1/1	0.88	0.17	92,92,92,92	0
53	MG	1A	3266	1/1	0.88	0.14	65,65,65,65	0
53	MG	1A	3515	1/1	0.88	0.20	75,75,75,75	0
53	MG	19	104	1/1	0.88	0.52	49,49,49,49	0
53	MG	2A	3514	1/1	0.88	0.28	50,50,50,50	0
53	MG	1A	3144	1/1	0.88	0.35	48,48,48,48	0
53	MG	2A	3276	1/1	0.88	0.13	57,57,57,57	0
53	MG	1A	3083	1/1	0.88	0.31	61,61,61,61	0
53	MG	2A	3119	1/1	0.88	0.14	72,72,72,72	0
53	MG	1A	3274	1/1	0.88	0.17	61,61,61,61	0
53	MG	1a	3079	1/1	0.88	0.19	73,73,73,73	0
53	MG	2A	3295	1/1	0.88	0.11	54,54,54,54	0
53	MG	1A	3345	1/1	0.88	0.33	56,56,56,56	0
53	MG	1A	3602	1/1	0.88	0.11	50,50,50,50	0
53	MG	2A	3314	1/1	0.88	0.18	55,55,55,55	0
53	MG	2A	3136	1/1	0.88	0.24	62,62,62,62	0
53	MG	2A	3320	1/1	0.88	0.32	73,73,73,73	0
53	MG	2A	3321	1/1	0.88	0.17	47,47,47,47	0
53	MG	2E	301	1/1	0.88	0.26	45,45,45,45	0
53	MG	1A	3606	1/1	0.88	0.16	58,58,58,58	0
53	MG	2A	3049	1/1	0.89	0.10	57,57,57,57	0
53	MG	1A	3657	1/1	0.89	0.11	44,44,44,44	0
53	MG	1a	3083	1/1	0.89	0.09	59,59,59,59	0
53	MG	2A	3061	1/1	0.89	0.17	65,65,65,65	0
53	MG	1A	3428	1/1	0.89	0.24	39,39,39,39	0
53	MG	2A	3245	1/1	0.89	0.17	46,46,46,46	0
53	MG	2B	207	1/1	0.89	0.14	62,62,62,62	0
53	MG	1W	201	1/1	0.89	0.19	47,47,47,47	0
53	MG	1A	3543	1/1	0.89	0.11	60,60,60,60	0
53	MG	1A	3544	1/1	0.89	0.40	64,64,64,64	0
53	MG	2A	3069	1/1	0.89	0.18	60,60,60,60	0
53	MG	10	106	1/1	0.89	0.19	78,78,78,78	0
53	MG	1A	3328	1/1	0.89	0.47	61,61,61,61	0
53	MG	1A	3007	1/1	0.89	0.17	56,56,56,56	0
53	MG	1A	3002	1/1	0.89	0.10	51,51,51,51	0
53	MG	2B	217	1/1	0.89	0.10	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3274	1/1	0.89	0.15	71,71,71,71	0
53	MG	2A	3080	1/1	0.89	0.17	66,66,66,66	0
53	MG	18	101	1/1	0.89	0.38	68,68,68,68	0
53	MG	1A	3692	1/1	0.89	0.13	36,36,36,36	0
53	MG	1a	3108	1/1	0.89	0.11	61,61,61,61	0
53	MG	2A	3089	1/1	0.89	0.09	71,71,71,71	0
53	MG	2A	3090	1/1	0.89	0.22	77,77,77,77	0
53	MG	2P	201	1/1	0.89	0.20	49,49,49,49	0
53	MG	2A	3091	1/1	0.89	0.29	68,68,68,68	0
53	MG	2A	3307	1/1	0.89	0.23	69,69,69,69	0
53	MG	2A	3093	1/1	0.89	0.49	64,64,64,64	0
53	MG	2a	1601	1/1	0.89	0.11	71,71,71,71	0
53	MG	1A	3442	1/1	0.89	0.29	68,68,68,68	0
53	MG	1A	3706	1/1	0.89	0.11	71,71,71,71	0
53	MG	2A	3319	1/1	0.89	0.21	50,50,50,50	0
53	MG	2A	3098	1/1	0.89	0.15	54,54,54,54	0
53	MG	1A	3028	1/1	0.89	0.19	61,61,61,61	0
53	MG	2A	3322	1/1	0.89	0.23	53,53,53,53	0
53	MG	1A	3048	1/1	0.89	0.20	48,48,48,48	0
53	MG	1A	3710	1/1	0.89	0.10	52,52,52,52	0
53	MG	1A	3350	1/1	0.89	0.26	59,59,59,59	0
53	MG	1A	3351	1/1	0.89	0.18	40,40,40,40	0
53	MG	2A	3338	1/1	0.89	0.09	49,49,49,49	0
53	MG	1A	3354	1/1	0.89	0.20	63,63,63,63	0
53	MG	1A	3356	1/1	0.89	0.24	41,41,41,41	0
53	MG	2a	1625	1/1	0.89	0.18	69,69,69,69	0
53	MG	1A	3017	1/1	0.89	0.13	56,56,56,56	0
53	MG	1A	3215	1/1	0.89	0.29	59,59,59,59	0
53	MG	1A	3153	1/1	0.89	0.21	52,52,52,52	0
53	MG	2a	1631	1/1	0.89	0.10	59,59,59,59	0
53	MG	1A	3470	1/1	0.89	0.19	71,71,71,71	0
53	MG	2A	3353	1/1	0.89	0.11	64,64,64,64	0
53	MG	2A	3122	1/1	0.89	0.10	47,47,47,47	0
53	MG	1a	3031	1/1	0.89	0.22	75,75,75,75	0
53	MG	2A	3131	1/1	0.89	0.35	34,34,34,34	0
53	MG	1A	3585	1/1	0.89	0.16	55,55,55,55	0
53	MG	1A	3586	1/1	0.89	0.24	41,41,41,41	0
53	MG	1a	3143	1/1	0.89	0.20	79,79,79,79	0
53	MG	1A	3158	1/1	0.89	0.12	55,55,55,55	0
53	MG	1A	3065	1/1	0.89	0.17	52,52,52,52	0
53	MG	1a	3042	1/1	0.89	0.40	64,64,64,64	0
53	MG	2A	3383	1/1	0.89	0.15	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3485	1/1	0.89	0.13	72,72,72,72	0
53	MG	1A	3744	1/1	0.89	0.12	74,74,74,74	0
53	MG	1A	3232	1/1	0.89	0.17	60,60,60,60	0
53	MG	1A	3066	1/1	0.89	0.20	54,54,54,54	0
53	MG	1A	3305	1/1	0.89	0.13	60,60,60,60	0
53	MG	1A	3509	1/1	0.89	0.13	77,77,77,77	0
53	MG	1A	3607	1/1	0.89	0.14	86,86,86,86	0
53	MG	2A	3156	1/1	0.89	0.14	50,50,50,50	0
53	MG	2A	3157	1/1	0.89	0.13	55,55,55,55	0
53	MG	2a	1679	1/1	0.89	0.11	74,74,74,74	0
53	MG	1a	3053	1/1	0.89	0.08	60,60,60,60	0
53	MG	2A	3414	1/1	0.89	0.09	70,70,70,70	0
53	MG	1A	3051	1/1	0.89	0.12	60,60,60,60	0
53	MG	1A	3243	1/1	0.89	0.14	50,50,50,50	0
53	MG	2a	1686	1/1	0.89	0.14	88,88,88,88	0
53	MG	2A	3014	1/1	0.89	0.26	53,53,53,53	0
53	MG	2A	3426	1/1	0.89	0.16	56,56,56,56	0
53	MG	1A	3125	1/1	0.89	0.12	49,49,49,49	0
53	MG	1A	3005	1/1	0.89	0.36	51,51,51,51	0
53	MG	2A	3432	1/1	0.89	0.09	62,62,62,62	0
53	MG	1A	3180	1/1	0.89	0.22	57,57,57,57	0
53	MG	2A	3171	1/1	0.89	0.17	62,62,62,62	0
53	MG	2A	3435	1/1	0.89	0.22	88,88,88,88	0
53	MG	1A	3625	1/1	0.89	0.24	49,49,49,49	0
53	MG	1A	3070	1/1	0.89	0.20	74,74,74,74	0
53	MG	1A	3191	1/1	0.89	0.32	31,31,31,31	0
53	MG	2A	3187	1/1	0.89	0.19	45,45,45,45	0
53	MG	1B	3018	1/1	0.89	0.15	69,69,69,69	0
53	MG	1A	3402	1/1	0.89	0.10	50,50,50,50	0
53	MG	2A	3447	1/1	0.89	0.12	72,72,72,72	0
53	MG	1A	3533	1/1	0.89	0.12	90,90,90,90	0
53	MG	2A	3453	1/1	0.89	0.18	66,66,66,66	0
53	MG	2A	3198	1/1	0.89	0.21	40,40,40,40	0
53	MG	1A	3403	1/1	0.89	0.11	68,68,68,68	0
53	MG	1A	3537	1/1	0.89	0.21	59,59,59,59	0
53	MG	1A	3072	1/1	0.89	0.32	58,58,58,58	0
53	MG	1A	3426	1/1	0.89	0.16	56,56,56,56	0
53	MG	2A	3492	1/1	0.89	0.19	83,83,83,83	0
53	MG	2A	3042	1/1	0.89	0.26	62,62,62,62	0
53	MG	1Q	202	1/1	0.89	0.13	50,50,50,50	0
53	MG	1R	205	1/1	0.89	0.10	25,25,25,25	0
53	MG	2A	3230	1/1	0.89	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1T	202	1/1	0.89	0.13	83,83,83,83	0
53	MG	2A	3127	1/1	0.90	0.36	66,66,66,66	0
53	MG	1U	202	1/1	0.90	0.13	49,49,49,49	0
53	MG	1A	3282	1/1	0.90	0.38	61,61,61,61	0
53	MG	2A	3133	1/1	0.90	0.16	63,63,63,63	0
53	MG	2A	3325	1/1	0.90	0.21	53,53,53,53	0
53	MG	1A	3091	1/1	0.90	0.07	76,76,76,76	0
53	MG	2A	3331	1/1	0.90	0.19	65,65,65,65	0
53	MG	10	103	1/1	0.90	0.16	39,39,39,39	0
53	MG	2A	3011	1/1	0.90	0.25	52,52,52,52	0
53	MG	1A	3254	1/1	0.90	0.22	48,48,48,48	0
53	MG	10	105	1/1	0.90	0.18	62,62,62,62	0
53	MG	1A	3132	1/1	0.90	0.08	49,49,49,49	0
53	MG	2T	203	1/1	0.90	0.12	52,52,52,52	0
53	MG	11	3001	1/1	0.90	0.21	73,73,73,73	0
53	MG	2A	3345	1/1	0.90	0.15	55,55,55,55	0
53	MG	1A	3302	1/1	0.90	0.44	63,63,63,63	0
53	MG	1A	3622	1/1	0.90	0.12	55,55,55,55	0
53	MG	2A	3022	1/1	0.90	0.12	67,67,67,67	0
53	MG	1A	3024	1/1	0.90	0.53	62,62,62,62	0
53	MG	2A	3362	1/1	0.90	0.20	51,51,51,51	0
53	MG	1A	3486	1/1	0.90	0.18	52,52,52,52	0
53	MG	2a	1609	1/1	0.90	0.11	60,60,60,60	0
53	MG	1A	3487	1/1	0.90	0.15	45,45,45,45	0
53	MG	1A	3554	1/1	0.90	0.20	66,66,66,66	0
53	MG	1a	3082	1/1	0.90	0.10	70,70,70,70	0
53	MG	1A	3119	1/1	0.90	0.16	31,31,31,31	0
53	MG	2A	3034	1/1	0.90	0.07	60,60,60,60	0
53	MG	1A	3417	1/1	0.90	0.18	59,59,59,59	0
53	MG	2a	1619	1/1	0.90	0.12	81,81,81,81	0
53	MG	1A	3422	1/1	0.90	0.17	22,22,22,22	0
53	MG	2a	1621	1/1	0.90	0.09	88,88,88,88	0
53	MG	2a	1622	1/1	0.90	0.15	83,83,83,83	0
53	MG	1A	3644	1/1	0.90	0.14	78,78,78,78	0
53	MG	2a	1624	1/1	0.90	0.11	55,55,55,55	0
53	MG	1a	3010	1/1	0.90	0.09	83,83,83,83	0
53	MG	1a	3090	1/1	0.90	0.12	88,88,88,88	0
53	MG	1A	3041	1/1	0.90	0.44	59,59,59,59	0
53	MG	1a	3097	1/1	0.90	0.18	82,82,82,82	0
53	MG	1A	3649	1/1	0.90	0.14	72,72,72,72	0
53	MG	2A	3052	1/1	0.90	0.21	66,66,66,66	0
53	MG	2A	3053	1/1	0.90	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1a	3016	1/1	0.90	0.27	77,77,77,77	0
53	MG	2A	3058	1/1	0.90	0.28	52,52,52,52	0
53	MG	1A	3034	1/1	0.90	0.23	50,50,50,50	0
53	MG	1a	3019	1/1	0.90	0.18	81,81,81,81	0
53	MG	1A	3562	1/1	0.90	0.27	70,70,70,70	0
53	MG	1A	3655	1/1	0.90	0.22	77,77,77,77	0
53	MG	2A	3220	1/1	0.90	0.11	37,37,37,37	0
53	MG	1B	3006	1/1	0.90	0.08	47,47,47,47	0
53	MG	2a	1647	1/1	0.90	0.12	64,64,64,64	0
53	MG	1A	3514	1/1	0.90	0.17	83,83,83,83	0
53	MG	2a	1651	1/1	0.90	0.19	76,76,76,76	0
53	MG	1a	3027	1/1	0.90	0.21	65,65,65,65	0
53	MG	2A	3428	1/1	0.90	0.16	83,83,83,83	0
53	MG	2a	1655	1/1	0.90	0.23	78,78,78,78	0
53	MG	1A	3145	1/1	0.90	0.34	26,26,26,26	0
53	MG	2A	3073	1/1	0.90	0.14	61,61,61,61	0
53	MG	2A	3231	1/1	0.90	0.21	49,49,49,49	0
53	MG	2A	3232	1/1	0.90	0.19	47,47,47,47	0
53	MG	1a	3030	1/1	0.90	0.10	59,59,59,59	0
53	MG	2a	1665	1/1	0.90	0.18	76,76,76,76	0
53	MG	2a	1666	1/1	0.90	0.17	66,66,66,66	0
53	MG	2A	3436	1/1	0.90	0.11	61,61,61,61	0
53	MG	2a	1670	1/1	0.90	0.21	67,67,67,67	0
53	MG	1A	3011	1/1	0.90	0.32	49,49,49,49	0
53	MG	1a	3032	1/1	0.90	0.24	56,56,56,56	0
53	MG	1A	3433	1/1	0.90	0.23	47,47,47,47	0
53	MG	1A	3675	1/1	0.90	0.11	63,63,63,63	0
53	MG	1A	3271	1/1	0.90	0.11	44,44,44,44	0
53	MG	1A	3129	1/1	0.90	0.17	54,54,54,54	0
53	MG	1a	3132	1/1	0.90	0.12	65,65,65,65	0
53	MG	2A	3448	1/1	0.90	0.21	80,80,80,80	0
53	MG	1a	3041	1/1	0.90	0.12	96,96,96,96	0
53	MG	1D	301	1/1	0.90	0.10	59,59,59,59	0
53	MG	1A	3367	1/1	0.90	0.21	35,35,35,35	0
53	MG	2A	3256	1/1	0.90	0.17	58,58,58,58	0
53	MG	1A	3088	1/1	0.90	0.12	71,71,71,71	0
53	MG	1a	3137	1/1	0.90	0.21	86,86,86,86	0
53	MG	1a	3138	1/1	0.90	0.17	115,115,115,115	0
53	MG	1F	302	1/1	0.90	0.18	43,43,43,43	0
53	MG	2A	3272	1/1	0.90	0.10	41,41,41,41	0
53	MG	1a	3142	1/1	0.90	0.21	57,57,57,57	0
53	MG	1A	3694	1/1	0.90	0.20	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3108	1/1	0.90	0.27	54,54,54,54	0
53	MG	2A	3504	1/1	0.90	0.12	74,74,74,74	0
53	MG	2A	3284	1/1	0.90	0.27	56,56,56,56	0
53	MG	1H	202	1/1	0.90	0.09	50,50,50,50	0
53	MG	1A	3321	1/1	0.90	0.11	54,54,54,54	0
53	MG	2A	3112	1/1	0.90	0.13	37,37,37,37	0
53	MG	1A	3595	1/1	0.90	0.19	68,68,68,68	0
53	MG	2A	3300	1/1	0.90	0.08	41,41,41,41	0
53	MG	1A	3245	1/1	0.90	0.12	48,48,48,48	0
53	MG	2B	206	1/1	0.90	0.12	74,74,74,74	0
53	MG	1A	3162	1/1	0.90	0.30	51,51,51,51	0
53	MG	2A	3312	1/1	0.90	0.23	70,70,70,70	0
53	MG	1A	3601	1/1	0.90	0.11	43,43,43,43	0
53	MG	1A	3712	1/1	0.90	0.13	53,53,53,53	0
53	MG	2A	3315	1/1	0.90	0.32	59,59,59,59	0
53	MG	1A	3383	1/1	0.90	0.24	71,71,71,71	0
53	MG	1A	3281	1/1	0.90	0.12	56,56,56,56	0
53	MG	1A	3137	1/1	0.91	0.10	40,40,40,40	0
53	MG	19	103	1/1	0.91	0.26	47,47,47,47	0
53	MG	2A	3268	1/1	0.91	0.25	60,60,60,60	0
53	MG	2A	3519	1/1	0.91	0.12	70,70,70,70	0
53	MG	1A	3329	1/1	0.91	0.24	37,37,37,37	0
53	MG	1A	3189	1/1	0.91	0.22	26,26,26,26	0
53	MG	1A	3117	1/1	0.91	0.16	63,63,63,63	0
53	MG	1a	3004	1/1	0.91	0.11	65,65,65,65	0
53	MG	2A	3092	1/1	0.91	0.26	68,68,68,68	0
53	MG	1A	3461	1/1	0.91	0.15	86,86,86,86	0
53	MG	1A	3194	1/1	0.91	0.15	51,51,51,51	0
53	MG	1A	3583	1/1	0.91	0.12	53,53,53,53	0
53	MG	2A	3097	1/1	0.91	0.20	67,67,67,67	0
53	MG	2A	3288	1/1	0.91	0.09	32,32,32,32	0
53	MG	1A	3141	1/1	0.91	0.17	62,62,62,62	0
53	MG	2A	3291	1/1	0.91	0.16	45,45,45,45	0
53	MG	1A	3348	1/1	0.91	0.21	51,51,51,51	0
53	MG	1A	3020	1/1	0.91	0.15	35,35,35,35	0
53	MG	2A	3301	1/1	0.91	0.11	45,45,45,45	0
53	MG	1A	3723	1/1	0.91	0.10	62,62,62,62	0
53	MG	2A	3306	1/1	0.91	0.17	68,68,68,68	0
53	MG	1A	3724	1/1	0.91	0.08	38,38,38,38	0
53	MG	2A	3309	1/1	0.91	0.17	50,50,50,50	0
53	MG	1A	3267	1/1	0.91	0.12	42,42,42,42	0
53	MG	1a	3020	1/1	0.91	0.09	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3205	1/1	0.91	0.12	40,40,40,40	0
53	MG	1A	3021	1/1	0.91	0.25	27,27,27,27	0
53	MG	2A	3114	1/1	0.91	0.15	78,78,78,78	0
53	MG	1A	3149	1/1	0.91	0.24	31,31,31,31	0
53	MG	1A	3736	1/1	0.91	0.16	68,68,68,68	0
53	MG	1A	3151	1/1	0.91	0.17	62,62,62,62	0
53	MG	1a	3028	1/1	0.91	0.12	59,59,59,59	0
53	MG	1A	3743	1/1	0.91	0.19	65,65,65,65	0
53	MG	2a	1603	1/1	0.91	0.24	79,79,79,79	0
53	MG	2A	3324	1/1	0.91	0.23	51,51,51,51	0
53	MG	1A	3152	1/1	0.91	0.09	30,30,30,30	0
53	MG	2A	3326	1/1	0.91	0.13	55,55,55,55	0
53	MG	1A	3211	1/1	0.91	0.13	50,50,50,50	0
53	MG	1d	502	1/1	0.91	0.10	58,58,58,58	0
53	MG	1A	3213	1/1	0.91	0.21	64,64,64,64	0
53	MG	2A	3336	1/1	0.91	0.28	66,66,66,66	0
53	MG	1A	3016	1/1	0.91	0.27	66,66,66,66	0
53	MG	1a	3034	1/1	0.91	0.12	61,61,61,61	0
53	MG	2A	3340	1/1	0.91	0.11	53,53,53,53	0
53	MG	1A	3757	1/1	0.91	0.36	51,51,51,51	0
53	MG	1a	3037	1/1	0.91	0.08	84,84,84,84	0
53	MG	2A	3343	1/1	0.91	0.31	50,50,50,50	0
53	MG	2A	3137	1/1	0.91	0.13	56,56,56,56	0
53	MG	1A	3064	1/1	0.91	0.16	57,57,57,57	0
53	MG	1A	3368	1/1	0.91	0.13	62,62,62,62	0
53	MG	2A	3348	1/1	0.91	0.16	58,58,58,58	0
53	MG	1A	3369	1/1	0.91	0.23	47,47,47,47	0
53	MG	1B	3003	1/1	0.91	0.19	60,60,60,60	0
53	MG	1A	3618	1/1	0.91	0.18	81,81,81,81	0
53	MG	2A	3354	1/1	0.91	0.13	68,68,68,68	0
53	MG	2A	3358	1/1	0.91	0.13	49,49,49,49	0
53	MG	1A	3511	1/1	0.91	0.12	67,67,67,67	0
53	MG	2A	3149	1/1	0.91	0.12	52,52,52,52	0
53	MG	1A	3512	1/1	0.91	0.11	64,64,64,64	0
53	MG	2a	1636	1/1	0.91	0.14	60,60,60,60	0
53	MG	1a	3046	1/1	0.91	0.10	65,65,65,65	0
53	MG	1A	3285	1/1	0.91	0.10	46,46,46,46	0
53	MG	1A	3223	1/1	0.91	0.21	71,71,71,71	0
53	MG	1A	3290	1/1	0.91	0.12	51,51,51,51	0
53	MG	2A	3377	1/1	0.91	0.11	50,50,50,50	0
53	MG	1A	3377	1/1	0.91	0.19	60,60,60,60	0
53	MG	2a	1645	1/1	0.91	0.09	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3294	1/1	0.91	0.27	39,39,39,39	0
53	MG	1a	3054	1/1	0.91	0.26	76,76,76,76	0
53	MG	2a	1648	1/1	0.91	0.24	52,52,52,52	0
53	MG	2A	3162	1/1	0.91	0.32	52,52,52,52	0
53	MG	1A	3085	1/1	0.91	0.17	58,58,58,58	0
53	MG	1A	3086	1/1	0.91	0.18	58,58,58,58	0
53	MG	2A	3386	1/1	0.91	0.08	55,55,55,55	0
53	MG	2a	1654	1/1	0.91	0.07	67,67,67,67	0
53	MG	1D	303	1/1	0.91	0.10	58,58,58,58	0
53	MG	1A	3073	1/1	0.91	0.12	62,62,62,62	0
53	MG	1A	3647	1/1	0.91	0.12	66,66,66,66	0
53	MG	2a	1660	1/1	0.91	0.08	64,64,64,64	0
53	MG	1a	3061	1/1	0.91	0.12	78,78,78,78	0
53	MG	1F	301	1/1	0.91	0.13	28,28,28,28	0
53	MG	2A	3405	1/1	0.91	0.15	49,49,49,49	0
53	MG	1A	3388	1/1	0.91	0.41	53,53,53,53	0
53	MG	1F	303	1/1	0.91	0.16	40,40,40,40	0
53	MG	1A	3012	1/1	0.91	0.37	47,47,47,47	0
53	MG	2A	3038	1/1	0.91	0.08	56,56,56,56	0
53	MG	1A	3171	1/1	0.91	0.12	46,46,46,46	0
53	MG	1A	3307	1/1	0.91	0.22	34,34,34,34	0
53	MG	2a	1676	1/1	0.91	0.10	58,58,58,58	0
53	MG	1A	3241	1/1	0.91	0.15	50,50,50,50	0
53	MG	1A	3309	1/1	0.91	0.32	46,46,46,46	0
53	MG	2A	3206	1/1	0.91	0.09	48,48,48,48	0
53	MG	2A	3211	1/1	0.91	0.27	50,50,50,50	0
53	MG	1A	3409	1/1	0.91	0.12	30,30,30,30	0
53	MG	2A	3214	1/1	0.91	0.22	35,35,35,35	0
53	MG	1A	3173	1/1	0.91	0.26	48,48,48,48	0
53	MG	2A	3217	1/1	0.91	0.20	64,64,64,64	0
53	MG	1A	3312	1/1	0.91	0.23	44,44,44,44	0
53	MG	2a	1691	1/1	0.91	0.47	76,76,76,76	0
53	MG	1A	3421	1/1	0.91	0.28	40,40,40,40	0
53	MG	1A	3059	1/1	0.91	0.14	76,76,76,76	0
53	MG	1A	3248	1/1	0.91	0.14	55,55,55,55	0
53	MG	1A	3114	1/1	0.91	0.15	66,66,66,66	0
53	MG	2A	3060	1/1	0.91	0.09	52,52,52,52	0
53	MG	1A	3687	1/1	0.91	0.17	74,74,74,74	0
53	MG	1a	3085	1/1	0.91	0.09	45,45,45,45	0
53	MG	2a	1702	1/1	0.91	0.09	62,62,62,62	0
53	MG	2a	1704	1/1	0.91	0.08	110,110,110,110	0
53	MG	1A	3317	1/1	0.91	0.23	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3065	1/1	0.91	0.14	37,37,37,37	0
53	MG	1A	3077	1/1	0.91	0.20	51,51,51,51	0
53	MG	2A	3452	1/1	0.91	0.18	67,67,67,67	0
53	MG	1A	3252	1/1	0.91	0.10	60,60,60,60	0
53	MG	1A	3704	1/1	0.91	0.12	53,53,53,53	0
53	MG	2A	3070	1/1	0.91	0.31	57,57,57,57	0
53	MG	2A	3244	1/1	0.91	0.10	48,48,48,48	0
53	MG	2A	3482	1/1	0.91	0.23	72,72,72,72	0
53	MG	1A	3705	1/1	0.91	0.10	42,42,42,42	0
53	MG	1a	3091	1/1	0.91	0.14	62,62,62,62	0
53	MG	1A	3322	1/1	0.91	0.27	47,47,47,47	0
53	MG	2A	3250	1/1	0.91	0.10	51,51,51,51	0
53	MG	2a	1727	1/1	0.91	0.16	76,76,76,76	0
53	MG	1A	3558	1/1	0.91	0.09	53,53,53,53	0
53	MG	1A	3181	1/1	0.91	0.28	65,65,65,65	0
53	MG	2A	3255	1/1	0.91	0.09	71,71,71,71	0
53	MG	17	101	1/1	0.91	0.11	38,38,38,38	0
53	MG	2A	3507	1/1	0.91	0.28	93,93,93,93	0
54	HGR	2A	3515	36/36	0.91	0.17	36,61,70,76	0
55	ZN	2n	501	1/1	0.91	0.16	160,160,160,160	0
53	MG	1A	3758	1/1	0.92	0.16	66,66,66,66	0
53	MG	1A	3518	1/1	0.92	0.09	37,37,37,37	0
53	MG	1A	3411	1/1	0.92	0.12	32,32,32,32	0
53	MG	1A	3337	1/1	0.92	0.31	26,26,26,26	0
53	MG	1A	3522	1/1	0.92	0.12	70,70,70,70	0
53	MG	1A	3342	1/1	0.92	0.28	72,72,72,72	0
53	MG	1A	3632	1/1	0.92	0.11	68,68,68,68	0
53	MG	1A	3040	1/1	0.92	0.20	57,57,57,57	0
53	MG	1A	3527	1/1	0.92	0.14	56,56,56,56	0
53	MG	1A	3528	1/1	0.92	0.14	72,72,72,72	0
53	MG	1A	3177	1/1	0.92	0.25	35,35,35,35	0
53	MG	2B	218	1/1	0.92	0.11	62,62,62,62	0
53	MG	1A	3347	1/1	0.92	0.12	52,52,52,52	0
53	MG	2A	3317	1/1	0.92	0.24	59,59,59,59	0
53	MG	2A	3318	1/1	0.92	0.10	63,63,63,63	0
53	MG	2F	302	1/1	0.92	0.08	64,64,64,64	0
53	MG	1A	3019	1/1	0.92	0.09	53,53,53,53	0
53	MG	1B	3017	1/1	0.92	0.11	54,54,54,54	0
53	MG	1A	3289	1/1	0.92	0.14	39,39,39,39	0
53	MG	1A	3253	1/1	0.92	0.17	65,65,65,65	0
53	MG	1A	3015	1/1	0.92	0.22	48,48,48,48	0
53	MG	1D	307	1/1	0.92	0.21	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3009	1/1	0.92	0.17	57,57,57,57	0
53	MG	2W	3001	1/1	0.92	0.10	58,58,58,58	0
53	MG	1A	3435	1/1	0.92	0.15	46,46,46,46	0
53	MG	1E	304	1/1	0.92	0.12	43,43,43,43	0
53	MG	2A	3330	1/1	0.92	0.30	47,47,47,47	0
53	MG	2A	3013	1/1	0.92	0.14	80,80,80,80	0
53	MG	1A	3087	1/1	0.92	0.45	61,61,61,61	0
53	MG	1A	3256	1/1	0.92	0.07	52,52,52,52	0
53	MG	1A	3667	1/1	0.92	0.14	36,36,36,36	0
53	MG	1A	3216	1/1	0.92	0.43	55,55,55,55	0
53	MG	1A	3185	1/1	0.92	0.23	51,51,51,51	0
53	MG	1A	3259	1/1	0.92	0.24	39,39,39,39	0
53	MG	2a	1610	1/1	0.92	0.14	74,74,74,74	0
53	MG	1A	3448	1/1	0.92	0.11	64,64,64,64	0
53	MG	1A	3452	1/1	0.92	0.12	63,63,63,63	0
53	MG	2a	1613	1/1	0.92	0.12	83,83,83,83	0
53	MG	2A	3158	1/1	0.92	0.29	54,54,54,54	0
53	MG	1A	3552	1/1	0.92	0.11	72,72,72,72	0
53	MG	1A	3688	1/1	0.92	0.10	76,76,76,76	0
53	MG	2A	3028	1/1	0.92	0.08	57,57,57,57	0
53	MG	1Q	203	1/1	0.92	0.10	35,35,35,35	0
53	MG	1A	3160	1/1	0.92	0.13	51,51,51,51	0
53	MG	2A	3351	1/1	0.92	0.10	59,59,59,59	0
53	MG	2A	3031	1/1	0.92	0.11	60,60,60,60	0
53	MG	2A	3166	1/1	0.92	0.10	53,53,53,53	0
53	MG	2A	3167	1/1	0.92	0.17	56,56,56,56	0
53	MG	1T	201	1/1	0.92	0.15	68,68,68,68	0
53	MG	2A	3169	1/1	0.92	0.25	48,48,48,48	0
53	MG	1A	3455	1/1	0.92	0.18	65,65,65,65	0
53	MG	2A	3366	1/1	0.92	0.10	37,37,37,37	0
53	MG	2a	1630	1/1	0.92	0.21	66,66,66,66	0
53	MG	2A	3035	1/1	0.92	0.16	65,65,65,65	0
53	MG	1A	3695	1/1	0.92	0.10	57,57,57,57	0
53	MG	2A	3037	1/1	0.92	0.30	67,67,67,67	0
53	MG	1a	3071	1/1	0.92	0.08	68,68,68,68	0
53	MG	2a	1635	1/1	0.92	0.19	59,59,59,59	0
53	MG	1A	3263	1/1	0.92	0.14	61,61,61,61	0
53	MG	2a	1637	1/1	0.92	0.17	65,65,65,65	0
53	MG	1A	3224	1/1	0.92	0.22	30,30,30,30	0
53	MG	2A	3044	1/1	0.92	0.07	57,57,57,57	0
53	MG	1a	3077	1/1	0.92	0.27	69,69,69,69	0
53	MG	2A	3196	1/1	0.92	0.34	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1V	3002	1/1	0.92	0.09	62,62,62,62	0
53	MG	1A	3047	1/1	0.92	0.22	59,59,59,59	0
53	MG	2a	1644	1/1	0.92	0.10	91,91,91,91	0
53	MG	2A	3204	1/1	0.92	0.35	64,64,64,64	0
53	MG	1A	3193	1/1	0.92	0.23	43,43,43,43	0
53	MG	2A	3391	1/1	0.92	0.11	51,51,51,51	0
53	MG	10	101	1/1	0.92	0.15	67,67,67,67	0
53	MG	2a	1649	1/1	0.92	0.10	55,55,55,55	0
53	MG	2A	3051	1/1	0.92	0.44	69,69,69,69	0
53	MG	1A	3103	1/1	0.92	0.07	81,81,81,81	0
53	MG	1A	3122	1/1	0.92	0.14	61,61,61,61	0
53	MG	1A	3237	1/1	0.92	0.32	41,41,41,41	0
53	MG	2A	3218	1/1	0.92	0.21	44,44,44,44	0
53	MG	2A	3408	1/1	0.92	0.14	43,43,43,43	0
53	MG	2a	1657	1/1	0.92	0.18	68,68,68,68	0
53	MG	1A	3018	1/1	0.92	0.18	64,64,64,64	0
53	MG	2A	3410	1/1	0.92	0.10	44,44,44,44	0
53	MG	2A	3221	1/1	0.92	0.13	59,59,59,59	0
53	MG	2A	3059	1/1	0.92	0.14	42,42,42,42	0
53	MG	2A	3416	1/1	0.92	0.25	45,45,45,45	0
53	MG	2A	3225	1/1	0.92	0.31	57,57,57,57	0
53	MG	2a	1664	1/1	0.92	0.10	68,68,68,68	0
53	MG	2A	3421	1/1	0.92	0.08	56,56,56,56	0
53	MG	1A	3478	1/1	0.92	0.12	56,56,56,56	0
53	MG	1A	3318	1/1	0.92	0.20	51,51,51,51	0
53	MG	1A	3480	1/1	0.92	0.14	61,61,61,61	0
53	MG	1A	3482	1/1	0.92	0.07	55,55,55,55	0
53	MG	1A	3381	1/1	0.92	0.27	48,48,48,48	0
53	MG	1A	3202	1/1	0.92	0.40	33,33,33,33	0
53	MG	1a	3094	1/1	0.92	0.12	88,88,88,88	0
53	MG	1a	3095	1/1	0.92	0.12	66,66,66,66	0
53	MG	2a	1681	1/1	0.92	0.16	64,64,64,64	0
53	MG	1A	3590	1/1	0.92	0.19	54,54,54,54	0
53	MG	1A	3320	1/1	0.92	0.19	46,46,46,46	0
53	MG	1A	3276	1/1	0.92	0.24	43,43,43,43	0
53	MG	2A	3241	1/1	0.92	0.12	53,53,53,53	0
53	MG	2A	3438	1/1	0.92	0.09	47,47,47,47	0
53	MG	1A	3277	1/1	0.92	0.24	39,39,39,39	0
53	MG	1a	3105	1/1	0.92	0.10	60,60,60,60	0
53	MG	1A	3726	1/1	0.92	0.15	56,56,56,56	0
53	MG	1A	3492	1/1	0.92	0.09	80,80,80,80	0
53	MG	1a	3007	1/1	0.92	0.08	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3278	1/1	0.92	0.15	51,51,51,51	0
53	MG	1A	3730	1/1	0.92	0.14	52,52,52,52	0
53	MG	1A	3497	1/1	0.92	0.12	35,35,35,35	0
53	MG	2A	3254	1/1	0.92	0.20	47,47,47,47	0
53	MG	1A	3503	1/1	0.92	0.17	43,43,43,43	0
53	MG	2A	3461	1/1	0.92	0.08	65,65,65,65	0
53	MG	2a	1703	1/1	0.92	0.12	91,91,91,91	0
53	MG	1A	3734	1/1	0.92	0.29	69,69,69,69	0
53	MG	2A	3477	1/1	0.92	0.13	64,64,64,64	0
53	MG	1A	3508	1/1	0.92	0.20	77,77,77,77	0
53	MG	2A	3258	1/1	0.92	0.15	53,53,53,53	0
53	MG	2A	3259	1/1	0.92	0.28	45,45,45,45	0
53	MG	1A	3022	1/1	0.92	0.21	58,58,58,58	0
53	MG	1A	3742	1/1	0.92	0.15	36,36,36,36	0
53	MG	1A	3397	1/1	0.92	0.17	35,35,35,35	0
53	MG	2A	3096	1/1	0.92	0.15	67,67,67,67	0
53	MG	2a	1718	1/1	0.92	0.15	93,93,93,93	0
53	MG	1A	3280	1/1	0.92	0.28	55,55,55,55	0
53	MG	1a	3127	1/1	0.92	0.13	73,73,73,73	0
53	MG	1A	3401	1/1	0.92	0.22	71,71,71,71	0
53	MG	2A	3277	1/1	0.92	0.21	61,61,61,61	0
53	MG	2A	3100	1/1	0.92	0.14	59,59,59,59	0
53	MG	1A	3107	1/1	0.92	0.17	63,63,63,63	0
53	MG	1A	3023	1/1	0.92	0.22	60,60,60,60	0
53	MG	1A	3750	1/1	0.92	0.10	73,73,73,73	0
53	MG	2A	3106	1/1	0.92	0.20	54,54,54,54	0
53	MG	2A	3289	1/1	0.92	0.34	50,50,50,50	0
53	MG	1A	3756	1/1	0.92	0.10	47,47,47,47	0
54	HGR	1A	3749	36/36	0.92	0.15	24,38,52,65	0
53	MG	1A	3336	1/1	0.92	0.39	34,34,34,34	0
53	MG	2A	3293	1/1	0.92	0.12	37,37,37,37	0
53	MG	1A	3246	1/1	0.93	0.09	40,40,40,40	0
53	MG	2a	1604	1/1	0.93	0.27	59,59,59,59	0
53	MG	1A	3663	1/1	0.93	0.20	47,47,47,47	0
53	MG	1A	3407	1/1	0.93	0.18	57,57,57,57	0
53	MG	1A	3166	1/1	0.93	0.12	42,42,42,42	0
53	MG	2A	3380	1/1	0.93	0.09	52,52,52,52	0
53	MG	1A	3520	1/1	0.93	0.11	74,74,74,74	0
53	MG	1A	3410	1/1	0.93	0.16	43,43,43,43	0
53	MG	1A	3154	1/1	0.93	0.10	50,50,50,50	0
53	MG	2A	3110	1/1	0.93	0.07	45,45,45,45	0
53	MG	1A	3524	1/1	0.93	0.26	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3243	1/1	0.93	0.21	35,35,35,35	0
53	MG	1A	3340	1/1	0.93	0.21	50,50,50,50	0
53	MG	2A	3388	1/1	0.93	0.14	61,61,61,61	0
53	MG	2A	3113	1/1	0.93	0.26	62,62,62,62	0
53	MG	1A	3071	1/1	0.93	0.46	37,37,37,37	0
53	MG	1A	3474	1/1	0.93	0.09	57,57,57,57	0
53	MG	2A	3397	1/1	0.93	0.07	54,54,54,54	0
53	MG	1a	3013	1/1	0.93	0.09	54,54,54,54	0
53	MG	2A	3024	1/1	0.93	0.11	57,57,57,57	0
53	MG	1A	3596	1/1	0.93	0.09	58,58,58,58	0
53	MG	2A	3026	1/1	0.93	0.25	57,57,57,57	0
53	MG	2A	3121	1/1	0.93	0.15	62,62,62,62	0
53	MG	1A	3418	1/1	0.93	0.08	65,65,65,65	0
53	MG	1B	3014	1/1	0.93	0.24	43,43,43,43	0
53	MG	1A	3288	1/1	0.93	0.25	47,47,47,47	0
53	MG	1B	3016	1/1	0.93	0.15	38,38,38,38	0
53	MG	1A	3532	1/1	0.93	0.14	73,73,73,73	0
53	MG	1a	3093	1/1	0.93	0.11	71,71,71,71	0
53	MG	1A	3134	1/1	0.93	0.10	63,63,63,63	0
53	MG	1A	3604	1/1	0.93	0.10	64,64,64,64	0
53	MG	1a	3024	1/1	0.93	0.14	68,68,68,68	0
53	MG	1D	302	1/1	0.93	0.29	49,49,49,49	0
53	MG	2A	3275	1/1	0.93	0.10	37,37,37,37	0
53	MG	2A	3140	1/1	0.93	0.15	68,68,68,68	0
53	MG	2A	3141	1/1	0.93	0.22	68,68,68,68	0
53	MG	2A	3279	1/1	0.93	0.20	32,32,32,32	0
53	MG	1A	3605	1/1	0.93	0.24	63,63,63,63	0
53	MG	2A	3283	1/1	0.93	0.19	46,46,46,46	0
53	MG	1A	3423	1/1	0.93	0.14	63,63,63,63	0
53	MG	2A	3040	1/1	0.93	0.44	66,66,66,66	0
53	MG	1A	3481	1/1	0.93	0.16	55,55,55,55	0
53	MG	1A	3608	1/1	0.93	0.07	55,55,55,55	0
53	MG	1A	3229	1/1	0.93	0.19	57,57,57,57	0
53	MG	1A	3484	1/1	0.93	0.09	54,54,54,54	0
53	MG	1A	3080	1/1	0.93	0.11	67,67,67,67	0
53	MG	1A	3616	1/1	0.93	0.16	87,87,87,87	0
53	MG	2A	3294	1/1	0.93	0.14	53,53,53,53	0
53	MG	1F	306	1/1	0.93	0.20	48,48,48,48	0
53	MG	2A	3296	1/1	0.93	0.27	39,39,39,39	0
53	MG	2A	3299	1/1	0.93	0.15	56,56,56,56	0
53	MG	2a	1656	1/1	0.93	0.11	52,52,52,52	0
53	MG	2A	3450	1/1	0.93	0.24	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1G	8001	1/1	0.93	0.10	77,77,77,77	0
53	MG	1A	3349	1/1	0.93	0.11	32,32,32,32	0
53	MG	2A	3459	1/1	0.93	0.14	53,53,53,53	0
53	MG	2A	3303	1/1	0.93	0.17	39,39,39,39	0
53	MG	1a	3038	1/1	0.93	0.15	52,52,52,52	0
53	MG	1A	3619	1/1	0.93	0.09	55,55,55,55	0
53	MG	2A	3057	1/1	0.93	0.13	65,65,65,65	0
53	MG	1a	3118	1/1	0.93	0.14	92,92,92,92	0
53	MG	2A	3310	1/1	0.93	0.13	52,52,52,52	0
53	MG	2A	3311	1/1	0.93	0.09	50,50,50,50	0
53	MG	1A	3382	1/1	0.93	0.13	56,56,56,56	0
53	MG	1A	3233	1/1	0.93	0.14	58,58,58,58	0
53	MG	2a	1673	1/1	0.93	0.19	55,55,55,55	0
53	MG	1A	3299	1/1	0.93	0.14	37,37,37,37	0
53	MG	2A	3062	1/1	0.93	0.08	58,58,58,58	0
53	MG	1A	3352	1/1	0.93	0.20	68,68,68,68	0
53	MG	1A	3440	1/1	0.93	0.17	65,65,65,65	0
53	MG	1Q	204	1/1	0.93	0.17	53,53,53,53	0
53	MG	2A	3505	1/1	0.93	0.16	77,77,77,77	0
53	MG	2A	3066	1/1	0.93	0.17	51,51,51,51	0
53	MG	1R	204	1/1	0.93	0.46	47,47,47,47	0
53	MG	1A	3056	1/1	0.93	0.10	40,40,40,40	0
53	MG	2A	3181	1/1	0.93	0.20	58,58,58,58	0
53	MG	1A	3499	1/1	0.93	0.13	63,63,63,63	0
53	MG	1A	3500	1/1	0.93	0.14	68,68,68,68	0
53	MG	1A	3501	1/1	0.93	0.12	59,59,59,59	0
53	MG	1A	3637	1/1	0.93	0.17	42,42,42,42	0
53	MG	1A	3733	1/1	0.93	0.13	42,42,42,42	0
53	MG	1A	3108	1/1	0.93	0.15	45,45,45,45	0
53	MG	2A	3077	1/1	0.93	0.14	53,53,53,53	0
53	MG	2a	1696	1/1	0.93	0.17	67,67,67,67	0
53	MG	1A	3110	1/1	0.93	0.15	51,51,51,51	0
53	MG	2A	3335	1/1	0.93	0.18	48,48,48,48	0
53	MG	2A	3199	1/1	0.93	0.21	26,26,26,26	0
53	MG	2A	3200	1/1	0.93	0.12	54,54,54,54	0
53	MG	1W	202	1/1	0.93	0.24	52,52,52,52	0
53	MG	2A	3339	1/1	0.93	0.15	40,40,40,40	0
53	MG	2A	3202	1/1	0.93	0.10	48,48,48,48	0
53	MG	2A	3203	1/1	0.93	0.19	28,28,28,28	0
53	MG	1a	3058	1/1	0.93	0.10	68,68,68,68	0
53	MG	1A	3183	1/1	0.93	0.16	29,29,29,29	0
53	MG	2A	3084	1/1	0.93	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3212	1/1	0.93	0.23	37,37,37,37	0
53	MG	2E	303	1/1	0.93	0.08	57,57,57,57	0
53	MG	2E	305	1/1	0.93	0.18	52,52,52,52	0
53	MG	2E	306	1/1	0.93	0.25	68,68,68,68	0
53	MG	2A	3086	1/1	0.93	0.18	70,70,70,70	0
53	MG	1A	3740	1/1	0.93	0.26	48,48,48,48	0
53	MG	1A	3220	1/1	0.93	0.12	38,38,38,38	0
53	MG	1A	3400	1/1	0.93	0.10	58,58,58,58	0
53	MG	1k	3001	1/1	0.93	0.13	66,66,66,66	0
53	MG	1A	3204	1/1	0.93	0.20	57,57,57,57	0
53	MG	1A	3331	1/1	0.93	0.08	56,56,56,56	0
53	MG	2A	3222	1/1	0.93	0.34	58,58,58,58	0
53	MG	1A	3746	1/1	0.93	0.31	55,55,55,55	0
53	MG	1A	3652	1/1	0.93	0.14	59,59,59,59	0
53	MG	2A	3001	1/1	0.93	0.07	48,48,48,48	0
53	MG	1A	3568	1/1	0.93	0.30	51,51,51,51	0
53	MG	1A	3456	1/1	0.93	0.08	43,43,43,43	0
55	ZN	24	501	1/1	0.93	0.12	173,173,173,173	0
53	MG	1A	3570	1/1	0.93	0.27	62,62,62,62	0
53	MG	1A	3049	1/1	0.94	0.06	51,51,51,51	0
53	MG	1A	3222	1/1	0.94	0.30	47,47,47,47	0
53	MG	2A	3172	1/1	0.94	0.20	52,52,52,52	0
53	MG	2A	3173	1/1	0.94	0.14	32,32,32,32	0
53	MG	2A	3175	1/1	0.94	0.23	48,48,48,48	0
53	MG	1a	3100	1/1	0.94	0.14	92,92,92,92	0
53	MG	1A	3539	1/1	0.94	0.12	69,69,69,69	0
53	MG	1A	3375	1/1	0.94	0.10	69,69,69,69	0
53	MG	2A	3328	1/1	0.94	0.07	45,45,45,45	0
53	MG	2D	303	1/1	0.94	0.09	60,60,60,60	0
53	MG	1a	3011	1/1	0.94	0.07	64,64,64,64	0
53	MG	2E	302	1/1	0.94	0.34	49,49,49,49	0
53	MG	2A	3185	1/1	0.94	0.11	35,35,35,35	0
53	MG	2A	3186	1/1	0.94	0.21	31,31,31,31	0
53	MG	1A	3182	1/1	0.94	0.12	39,39,39,39	0
53	MG	1A	3150	1/1	0.94	0.13	38,38,38,38	0
53	MG	1A	3379	1/1	0.94	0.10	71,71,71,71	0
53	MG	1A	3039	1/1	0.94	0.21	67,67,67,67	0
53	MG	2A	3194	1/1	0.94	0.28	33,33,33,33	0
53	MG	2A	3195	1/1	0.94	0.14	57,57,57,57	0
53	MG	1A	3109	1/1	0.94	0.11	69,69,69,69	0
53	MG	1A	3325	1/1	0.94	0.11	50,50,50,50	0
53	MG	1B	3009	1/1	0.94	0.09	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2T	201	1/1	0.94	0.10	56,56,56,56	0
53	MG	2T	202	1/1	0.94	0.08	58,58,58,58	0
53	MG	1a	3114	1/1	0.94	0.10	100,100,100,100	0
53	MG	1A	3326	1/1	0.94	0.19	44,44,44,44	0
53	MG	1a	3022	1/1	0.94	0.07	77,77,77,77	0
53	MG	28	8001	1/1	0.94	0.13	64,64,64,64	0
53	MG	2A	3347	1/1	0.94	0.22	56,56,56,56	0
53	MG	1A	3327	1/1	0.94	0.14	62,62,62,62	0
53	MG	1A	3187	1/1	0.94	0.17	31,31,31,31	0
53	MG	1a	3119	1/1	0.94	0.50	79,79,79,79	0
53	MG	2A	3207	1/1	0.94	0.18	54,54,54,54	0
53	MG	2A	3208	1/1	0.94	0.15	27,27,27,27	0
53	MG	2A	3209	1/1	0.94	0.09	50,50,50,50	0
53	MG	1A	3188	1/1	0.94	0.38	39,39,39,39	0
53	MG	2A	3361	1/1	0.94	0.10	64,64,64,64	0
53	MG	1a	3122	1/1	0.94	0.11	60,60,60,60	0
53	MG	2A	3074	1/1	0.94	0.11	64,64,64,64	0
53	MG	1A	3395	1/1	0.94	0.09	54,54,54,54	0
53	MG	2A	3365	1/1	0.94	0.09	75,75,75,75	0
53	MG	1a	3124	1/1	0.94	0.14	100,100,100,100	0
53	MG	1A	3037	1/1	0.94	0.07	57,57,57,57	0
53	MG	1A	3190	1/1	0.94	0.17	31,31,31,31	0
53	MG	2A	3370	1/1	0.94	0.10	59,59,59,59	0
53	MG	1a	3129	1/1	0.94	0.10	61,61,61,61	0
53	MG	2a	1618	1/1	0.94	0.13	63,63,63,63	0
53	MG	1A	3097	1/1	0.94	0.23	50,50,50,50	0
53	MG	1B	3020	1/1	0.94	0.11	42,42,42,42	0
53	MG	2A	3085	1/1	0.94	0.16	70,70,70,70	0
53	MG	2A	3224	1/1	0.94	0.27	64,64,64,64	0
53	MG	1A	3192	1/1	0.94	0.30	26,26,26,26	0
53	MG	1A	3032	1/1	0.94	0.12	30,30,30,30	0
53	MG	1A	3339	1/1	0.94	0.19	46,46,46,46	0
53	MG	1D	306	1/1	0.94	0.08	52,52,52,52	0
53	MG	1A	3566	1/1	0.94	0.10	58,58,58,58	0
53	MG	1A	3159	1/1	0.94	0.10	49,49,49,49	0
53	MG	1A	3341	1/1	0.94	0.14	61,61,61,61	0
53	MG	1A	3244	1/1	0.94	0.11	53,53,53,53	0
53	MG	1E	306	1/1	0.94	0.10	46,46,46,46	0
53	MG	1A	3495	1/1	0.94	0.16	49,49,49,49	0
53	MG	2A	3238	1/1	0.94	0.11	57,57,57,57	0
53	MG	1A	3344	1/1	0.94	0.15	60,60,60,60	0
53	MG	1A	3700	1/1	0.94	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3400	1/1	0.94	0.08	65,65,65,65	0
53	MG	1A	3195	1/1	0.94	0.14	54,54,54,54	0
53	MG	1A	3576	1/1	0.94	0.16	19,19,19,19	0
53	MG	1A	3577	1/1	0.94	0.11	42,42,42,42	0
53	MG	1A	3581	1/1	0.94	0.27	64,64,64,64	0
53	MG	1A	3412	1/1	0.94	0.12	56,56,56,56	0
53	MG	2A	3246	1/1	0.94	0.09	38,38,38,38	0
53	MG	2A	3247	1/1	0.94	0.12	58,58,58,58	0
53	MG	1N	3002	1/1	0.94	0.12	92,92,92,92	0
53	MG	2A	3415	1/1	0.94	0.11	61,61,61,61	0
53	MG	2A	3107	1/1	0.94	0.25	62,62,62,62	0
53	MG	2A	3417	1/1	0.94	0.12	60,60,60,60	0
53	MG	1o	102	1/1	0.94	0.12	67,67,67,67	0
53	MG	1a	3051	1/1	0.94	0.22	54,54,54,54	0
53	MG	1A	3196	1/1	0.94	0.10	31,31,31,31	0
53	MG	1A	3415	1/1	0.94	0.10	31,31,31,31	0
53	MG	2A	3003	1/1	0.94	0.12	68,68,68,68	0
53	MG	1A	3416	1/1	0.94	0.12	41,41,41,41	0
53	MG	1A	3504	1/1	0.94	0.09	53,53,53,53	0
53	MG	2A	3007	1/1	0.94	0.09	56,56,56,56	0
53	MG	1A	3506	1/1	0.94	0.16	50,50,50,50	0
53	MG	2A	3260	1/1	0.94	0.20	41,41,41,41	0
53	MG	2A	3263	1/1	0.94	0.19	50,50,50,50	0
53	MG	2A	3265	1/1	0.94	0.15	60,60,60,60	0
53	MG	1A	3507	1/1	0.94	0.09	43,43,43,43	0
53	MG	1A	3594	1/1	0.94	0.08	48,48,48,48	0
53	MG	1A	3075	1/1	0.94	0.44	57,57,57,57	0
53	MG	2A	3439	1/1	0.94	0.12	49,49,49,49	0
53	MG	2A	3012	1/1	0.94	0.07	51,51,51,51	0
53	MG	2A	3442	1/1	0.94	0.13	37,37,37,37	0
53	MG	1A	3053	1/1	0.94	0.12	49,49,49,49	0
53	MG	1A	3101	1/1	0.94	0.12	73,73,73,73	0
53	MG	2A	3126	1/1	0.94	0.33	51,51,51,51	0
53	MG	1A	3061	1/1	0.94	0.24	46,46,46,46	0
53	MG	1A	3138	1/1	0.94	0.12	56,56,56,56	0
53	MG	2A	3278	1/1	0.94	0.16	56,56,56,56	0
53	MG	2a	1677	1/1	0.94	0.07	82,82,82,82	0
53	MG	2A	3017	1/1	0.94	0.12	58,58,58,58	0
53	MG	2A	3281	1/1	0.94	0.17	48,48,48,48	0
53	MG	1U	203	1/1	0.94	0.31	73,73,73,73	0
53	MG	2A	3134	1/1	0.94	0.17	67,67,67,67	0
53	MG	1V	3001	1/1	0.94	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3460	1/1	0.94	0.16	69,69,69,69	0
53	MG	1A	3513	1/1	0.94	0.12	56,56,56,56	0
53	MG	2A	3464	1/1	0.94	0.08	47,47,47,47	0
53	MG	2A	3469	1/1	0.94	0.10	56,56,56,56	0
53	MG	2A	3470	1/1	0.94	0.10	71,71,71,71	0
53	MG	2A	3472	1/1	0.94	0.09	57,57,57,57	0
53	MG	2A	3473	1/1	0.94	0.11	57,57,57,57	0
53	MG	2A	3475	1/1	0.94	0.08	57,57,57,57	0
53	MG	1A	3165	1/1	0.94	0.26	29,29,29,29	0
53	MG	1A	3353	1/1	0.94	0.08	60,60,60,60	0
53	MG	1A	3054	1/1	0.94	0.18	64,64,64,64	0
53	MG	2a	1698	1/1	0.94	0.09	79,79,79,79	0
53	MG	1A	3167	1/1	0.94	0.05	20,20,20,20	0
53	MG	1A	3090	1/1	0.94	0.08	64,64,64,64	0
53	MG	2A	3487	1/1	0.94	0.13	59,59,59,59	0
53	MG	1A	3142	1/1	0.94	0.10	45,45,45,45	0
53	MG	1A	3611	1/1	0.94	0.22	51,51,51,51	0
53	MG	1A	3212	1/1	0.94	0.09	48,48,48,48	0
53	MG	1A	3123	1/1	0.94	0.16	56,56,56,56	0
53	MG	1A	3311	1/1	0.94	0.20	53,53,53,53	0
53	MG	2A	3496	1/1	0.94	0.08	68,68,68,68	0
53	MG	13	101	1/1	0.94	0.25	41,41,41,41	0
53	MG	15	101	1/1	0.94	0.28	54,54,54,54	0
53	MG	1A	3617	1/1	0.94	0.09	93,93,93,93	0
53	MG	1a	3084	1/1	0.94	0.11	60,60,60,60	0
53	MG	1A	3444	1/1	0.94	0.20	54,54,54,54	0
53	MG	1A	3079	1/1	0.94	0.11	74,74,74,74	0
53	MG	17	102	1/1	0.94	0.15	50,50,50,50	0
53	MG	2A	3510	1/1	0.94	0.14	38,38,38,38	0
53	MG	2A	3511	1/1	0.94	0.08	39,39,39,39	0
53	MG	1A	3365	1/1	0.94	0.11	38,38,38,38	0
53	MG	2A	3041	1/1	0.94	0.09	65,65,65,65	0
53	MG	2B	201	1/1	0.94	0.08	75,75,75,75	0
53	MG	2a	1728	1/1	0.94	0.15	85,85,85,85	0
53	MG	1A	3146	1/1	0.94	0.34	47,47,47,47	0
53	MG	1A	3530	1/1	0.94	0.13	37,37,37,37	0
53	MG	1a	3001	1/1	0.94	0.07	60,60,60,60	0
53	MG	2A	3046	1/1	0.94	0.06	45,45,45,45	0
53	MG	1A	3218	1/1	0.94	0.23	57,57,57,57	0
53	MG	1A	3451	1/1	0.94	0.19	51,51,51,51	0
53	MG	1A	3148	1/1	0.94	0.29	35,35,35,35	0
53	MG	1A	3269	1/1	0.94	0.11	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2B	210	1/1	0.94	0.39	55,55,55,55	0
53	MG	1A	3641	1/1	0.95	0.10	78,78,78,78	0
53	MG	2V	3001	1/1	0.95	0.14	46,46,46,46	0
53	MG	2A	3399	1/1	0.95	0.09	63,63,63,63	0
53	MG	1A	3390	1/1	0.95	0.08	27,27,27,27	0
53	MG	2A	3401	1/1	0.95	0.08	52,52,52,52	0
53	MG	1a	3126	1/1	0.95	0.07	104,104,104,104	0
53	MG	1A	3432	1/1	0.95	0.15	58,58,58,58	0
53	MG	1A	3580	1/1	0.95	0.19	38,38,38,38	0
53	MG	1a	3130	1/1	0.95	0.14	63,63,63,63	0
53	MG	1T	203	1/1	0.95	0.11	58,58,58,58	0
53	MG	1A	3738	1/1	0.95	0.13	43,43,43,43	0
53	MG	2A	3412	1/1	0.95	0.15	58,58,58,58	0
53	MG	1A	3391	1/1	0.95	0.10	42,42,42,42	0
53	MG	1A	3035	1/1	0.95	0.12	52,52,52,52	0
53	MG	1A	3584	1/1	0.95	0.16	61,61,61,61	0
53	MG	1a	3050	1/1	0.95	0.07	67,67,67,67	0
53	MG	1A	3284	1/1	0.95	0.23	28,28,28,28	0
53	MG	2A	3418	1/1	0.95	0.11	63,63,63,63	0
53	MG	2A	3419	1/1	0.95	0.07	36,36,36,36	0
53	MG	1A	3437	1/1	0.95	0.09	36,36,36,36	0
53	MG	1a	3139	1/1	0.95	0.09	70,70,70,70	0
53	MG	1A	3334	1/1	0.95	0.15	37,37,37,37	0
53	MG	2A	3424	1/1	0.95	0.06	63,63,63,63	0
53	MG	1A	3656	1/1	0.95	0.08	56,56,56,56	0
53	MG	2A	3177	1/1	0.95	0.17	54,54,54,54	0
53	MG	2A	3179	1/1	0.95	0.07	39,39,39,39	0
53	MG	1A	3127	1/1	0.95	0.08	60,60,60,60	0
53	MG	1A	3443	1/1	0.95	0.11	69,69,69,69	0
53	MG	2A	3431	1/1	0.95	0.16	63,63,63,63	0
53	MG	2A	3076	1/1	0.95	0.17	59,59,59,59	0
53	MG	2A	3183	1/1	0.95	0.26	32,32,32,32	0
53	MG	1A	3398	1/1	0.95	0.07	55,55,55,55	0
53	MG	2A	3298	1/1	0.95	0.07	47,47,47,47	0
53	MG	1A	3313	1/1	0.95	0.24	52,52,52,52	0
53	MG	1A	3665	1/1	0.95	0.12	61,61,61,61	0
53	MG	1A	3498	1/1	0.95	0.21	65,65,65,65	0
53	MG	2A	3302	1/1	0.95	0.09	38,38,38,38	0
53	MG	1A	3540	1/1	0.95	0.12	48,48,48,48	0
53	MG	2A	3083	1/1	0.95	0.11	50,50,50,50	0
53	MG	2A	3190	1/1	0.95	0.17	34,34,34,34	0
53	MG	1A	3338	1/1	0.95	0.31	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1l	201	1/1	0.95	0.09	73,73,73,73	0
53	MG	1A	3082	1/1	0.95	0.39	42,42,42,42	0
53	MG	13	103	1/1	0.95	0.14	50,50,50,50	0
53	MG	1A	3677	1/1	0.95	0.11	46,46,46,46	0
53	MG	1B	3004	1/1	0.95	0.06	66,66,66,66	0
53	MG	15	105	1/1	0.95	0.08	47,47,47,47	0
53	MG	1A	3600	1/1	0.95	0.42	46,46,46,46	0
53	MG	1A	3029	1/1	0.95	0.14	52,52,52,52	0
53	MG	2A	3458	1/1	0.95	0.14	44,44,44,44	0
53	MG	1A	3684	1/1	0.95	0.11	76,76,76,76	0
53	MG	1A	3685	1/1	0.95	0.10	56,56,56,56	0
53	MG	1a	3074	1/1	0.95	0.09	67,67,67,67	0
53	MG	2A	3462	1/1	0.95	0.10	73,73,73,73	0
53	MG	1a	3075	1/1	0.95	0.11	43,43,43,43	0
53	MG	2A	3466	1/1	0.95	0.13	63,63,63,63	0
53	MG	18	102	1/1	0.95	0.23	51,51,51,51	0
53	MG	19	101	1/1	0.95	0.08	40,40,40,40	0
53	MG	2A	3471	1/1	0.95	0.11	52,52,52,52	0
53	MG	1A	3502	1/1	0.95	0.15	52,52,52,52	0
53	MG	2A	3101	1/1	0.95	0.14	50,50,50,50	0
53	MG	1A	3603	1/1	0.95	0.25	44,44,44,44	0
53	MG	1A	3691	1/1	0.95	0.17	84,84,84,84	0
53	MG	2A	3215	1/1	0.95	0.17	32,32,32,32	0
53	MG	1A	3140	1/1	0.95	0.10	53,53,53,53	0
53	MG	1A	3693	1/1	0.95	0.18	41,41,41,41	0
53	MG	1A	3043	1/1	0.95	0.12	54,54,54,54	0
53	MG	2A	3486	1/1	0.95	0.19	63,63,63,63	0
53	MG	2A	3219	1/1	0.95	0.28	54,54,54,54	0
53	MG	2A	3334	1/1	0.95	0.11	55,55,55,55	0
53	MG	2A	3490	1/1	0.95	0.10	51,51,51,51	0
53	MG	1a	3005	1/1	0.95	0.13	53,53,53,53	0
53	MG	2a	1668	1/1	0.95	0.08	76,76,76,76	0
53	MG	1A	3547	1/1	0.95	0.09	62,62,62,62	0
53	MG	1A	3505	1/1	0.95	0.12	51,51,51,51	0
53	MG	2a	1672	1/1	0.95	0.18	61,61,61,61	0
53	MG	1A	3701	1/1	0.95	0.19	58,58,58,58	0
53	MG	2a	1674	1/1	0.95	0.10	68,68,68,68	0
53	MG	1A	3291	1/1	0.95	0.12	49,49,49,49	0
53	MG	2A	3499	1/1	0.95	0.08	54,54,54,54	0
53	MG	2A	3500	1/1	0.95	0.08	64,64,64,64	0
53	MG	2A	3501	1/1	0.95	0.09	56,56,56,56	0
53	MG	1A	3046	1/1	0.95	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3209	1/1	0.95	0.07	35,35,35,35	0
53	MG	1a	3012	1/1	0.95	0.07	75,75,75,75	0
53	MG	2A	3228	1/1	0.95	0.27	49,49,49,49	0
53	MG	1A	3612	1/1	0.95	0.23	51,51,51,51	0
53	MG	1D	305	1/1	0.95	0.15	66,66,66,66	0
53	MG	1A	3296	1/1	0.95	0.15	24,24,24,24	0
53	MG	1A	3155	1/1	0.95	0.18	53,53,53,53	0
53	MG	1A	3156	1/1	0.95	0.30	43,43,43,43	0
53	MG	1E	301	1/1	0.95	0.09	38,38,38,38	0
53	MG	2A	3032	1/1	0.95	0.30	42,42,42,42	0
53	MG	2A	3237	1/1	0.95	0.14	56,56,56,56	0
53	MG	1A	3157	1/1	0.95	0.12	38,38,38,38	0
53	MG	1A	3380	1/1	0.95	0.09	47,47,47,47	0
53	MG	2A	3357	1/1	0.95	0.14	73,73,73,73	0
53	MG	2A	3130	1/1	0.95	0.14	57,57,57,57	0
53	MG	2A	3360	1/1	0.95	0.10	72,72,72,72	0
53	MG	1A	3092	1/1	0.95	0.13	74,74,74,74	0
53	MG	1A	3124	1/1	0.95	0.10	40,40,40,40	0
53	MG	1A	3240	1/1	0.95	0.26	28,28,28,28	0
53	MG	1A	3565	1/1	0.95	0.10	69,69,69,69	0
53	MG	1F	304	1/1	0.95	0.07	39,39,39,39	0
53	MG	1A	3475	1/1	0.95	0.24	65,65,65,65	0
53	MG	1A	3626	1/1	0.95	0.08	26,26,26,26	0
53	MG	2a	1708	1/1	0.95	0.09	73,73,73,73	0
53	MG	1A	3106	1/1	0.95	0.09	55,55,55,55	0
53	MG	1a	3112	1/1	0.95	0.09	91,91,91,91	0
53	MG	2A	3372	1/1	0.95	0.12	34,34,34,34	0
53	MG	1A	3147	1/1	0.95	0.09	32,32,32,32	0
53	MG	2A	3251	1/1	0.95	0.09	41,41,41,41	0
53	MG	1A	3358	1/1	0.95	0.16	58,58,58,58	0
53	MG	2a	1717	1/1	0.95	0.25	94,94,94,94	0
53	MG	1A	3725	1/1	0.95	0.23	71,71,71,71	0
53	MG	2a	1719	1/1	0.95	0.10	93,93,93,93	0
53	MG	2A	3379	1/1	0.95	0.12	47,47,47,47	0
53	MG	2a	1721	1/1	0.95	0.19	80,80,80,80	0
53	MG	1P	201	1/1	0.95	0.15	57,57,57,57	0
53	MG	1A	3389	1/1	0.95	0.08	47,47,47,47	0
53	MG	2E	304	1/1	0.95	0.21	36,36,36,36	0
53	MG	1A	3523	1/1	0.95	0.14	73,73,73,73	0
53	MG	1A	3636	1/1	0.95	0.07	31,31,31,31	0
53	MG	1A	3430	1/1	0.95	0.08	49,49,49,49	0
53	MG	1A	3638	1/1	0.95	0.08	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3054	1/1	0.95	0.06	63,63,63,63	0
53	MG	2A	3261	1/1	0.95	0.12	43,43,43,43	0
53	MG	2A	3262	1/1	0.95	0.26	30,30,30,30	0
53	MG	2A	3389	1/1	0.95	0.13	64,64,64,64	0
53	MG	1R	203	1/1	0.95	0.10	49,49,49,49	0
53	MG	2A	3155	1/1	0.95	0.04	50,50,50,50	0
53	MG	2A	3266	1/1	0.95	0.17	55,55,55,55	0
53	MG	2A	3056	1/1	0.95	0.07	60,60,60,60	0
53	MG	1A	3093	1/1	0.96	0.14	67,67,67,67	0
53	MG	2A	3297	1/1	0.96	0.13	48,48,48,48	0
53	MG	1a	3064	1/1	0.96	0.08	75,75,75,75	0
53	MG	1A	3666	1/1	0.96	0.45	41,41,41,41	0
53	MG	2A	3423	1/1	0.96	0.20	67,67,67,67	0
53	MG	1A	3593	1/1	0.96	0.09	34,34,34,34	0
53	MG	1o	101	1/1	0.96	0.07	82,82,82,82	0
53	MG	2A	3191	1/1	0.96	0.25	54,54,54,54	0
53	MG	1A	3414	1/1	0.96	0.12	57,57,57,57	0
53	MG	1A	3265	1/1	0.96	0.45	66,66,66,66	0
53	MG	2A	3305	1/1	0.96	0.13	40,40,40,40	0
53	MG	1A	3333	1/1	0.96	0.14	39,39,39,39	0
53	MG	1A	3597	1/1	0.96	0.13	40,40,40,40	0
53	MG	2A	3197	1/1	0.96	0.17	41,41,41,41	0
53	MG	2A	3002	1/1	0.96	0.05	55,55,55,55	0
53	MG	1A	3678	1/1	0.96	0.08	33,33,33,33	0
53	MG	1A	3679	1/1	0.96	0.07	38,38,38,38	0
53	MG	2A	3005	1/1	0.96	0.11	51,51,51,51	0
53	MG	1a	3073	1/1	0.96	0.05	72,72,72,72	0
53	MG	1A	3055	1/1	0.96	0.08	58,58,58,58	0
53	MG	2A	3440	1/1	0.96	0.07	43,43,43,43	0
53	MG	1A	3335	1/1	0.96	0.33	42,42,42,42	0
53	MG	1A	3534	1/1	0.96	0.13	35,35,35,35	0
53	MG	1A	3419	1/1	0.96	0.18	40,40,40,40	0
53	MG	1A	3068	1/1	0.96	0.09	67,67,67,67	0
53	MG	2A	3102	1/1	0.96	0.06	40,40,40,40	0
53	MG	1A	3483	1/1	0.96	0.08	32,32,32,32	0
53	MG	1A	3689	1/1	0.96	0.11	75,75,75,75	0
53	MG	1A	3238	1/1	0.96	0.20	39,39,39,39	0
53	MG	1A	3089	1/1	0.96	0.07	61,61,61,61	0
53	MG	1A	3425	1/1	0.96	0.08	39,39,39,39	0
53	MG	1A	3179	1/1	0.96	0.08	37,37,37,37	0
53	MG	1A	3272	1/1	0.96	0.09	53,53,53,53	0
53	MG	2A	3456	1/1	0.96	0.07	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3697	1/1	0.96	0.11	37,37,37,37	0
53	MG	1B	3021	1/1	0.96	0.09	64,64,64,64	0
53	MG	2A	3021	1/1	0.96	0.07	46,46,46,46	0
53	MG	1B	3023	1/1	0.96	0.06	68,68,68,68	0
53	MG	2A	3333	1/1	0.96	0.13	30,30,30,30	0
53	MG	1A	3120	1/1	0.96	0.21	53,53,53,53	0
53	MG	1A	3214	1/1	0.96	0.14	41,41,41,41	0
53	MG	2A	3116	1/1	0.96	0.09	51,51,51,51	0
53	MG	1A	3494	1/1	0.96	0.10	63,63,63,63	0
53	MG	1D	304	1/1	0.96	0.10	25,25,25,25	0
53	MG	1A	3343	1/1	0.96	0.08	53,53,53,53	0
53	MG	1A	3111	1/1	0.96	0.17	66,66,66,66	0
53	MG	2A	3474	1/1	0.96	0.06	65,65,65,65	0
53	MG	1A	3001	1/1	0.96	0.05	41,41,41,41	0
53	MG	1A	3434	1/1	0.96	0.09	24,24,24,24	0
53	MG	1a	3017	1/1	0.96	0.07	71,71,71,71	0
53	MG	2A	3124	1/1	0.96	0.18	44,44,44,44	0
53	MG	2A	3233	1/1	0.96	0.13	60,60,60,60	0
53	MG	2A	3481	1/1	0.96	0.19	66,66,66,66	0
53	MG	2A	3125	1/1	0.96	0.17	33,33,33,33	0
53	MG	1A	3386	1/1	0.96	0.09	70,70,70,70	0
53	MG	1E	303	1/1	0.96	0.15	45,45,45,45	0
53	MG	2A	3488	1/1	0.96	0.10	66,66,66,66	0
53	MG	2A	3128	1/1	0.96	0.09	59,59,59,59	0
53	MG	2A	3129	1/1	0.96	0.09	55,55,55,55	0
53	MG	1A	3217	1/1	0.96	0.35	57,57,57,57	0
53	MG	2A	3352	1/1	0.96	0.08	49,49,49,49	0
53	MG	1A	3247	1/1	0.96	0.09	32,32,32,32	0
53	MG	1A	3198	1/1	0.96	0.08	38,38,38,38	0
53	MG	2A	3355	1/1	0.96	0.07	62,62,62,62	0
53	MG	2A	3497	1/1	0.96	0.07	86,86,86,86	0
53	MG	2A	3356	1/1	0.96	0.14	56,56,56,56	0
53	MG	1A	3441	1/1	0.96	0.10	52,52,52,52	0
53	MG	1A	3219	1/1	0.96	0.27	60,60,60,60	0
53	MG	1A	3199	1/1	0.96	0.09	45,45,45,45	0
53	MG	1A	3627	1/1	0.96	0.11	52,52,52,52	0
53	MG	1A	3033	1/1	0.96	0.21	37,37,37,37	0
53	MG	1A	3201	1/1	0.96	0.30	22,22,22,22	0
53	MG	2A	3506	1/1	0.96	0.08	62,62,62,62	0
53	MG	2A	3043	1/1	0.96	0.11	43,43,43,43	0
53	MG	1A	3003	1/1	0.96	0.17	59,59,59,59	0
53	MG	2a	1678	1/1	0.96	0.07	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3142	1/1	0.96	0.14	49,49,49,49	0
53	MG	2A	3367	1/1	0.96	0.11	56,56,56,56	0
53	MG	1A	3722	1/1	0.96	0.22	62,62,62,62	0
53	MG	2A	3513	1/1	0.96	0.28	60,60,60,60	0
53	MG	1A	3203	1/1	0.96	0.19	25,25,25,25	0
53	MG	2A	3517	1/1	0.96	0.09	47,47,47,47	0
53	MG	2A	3518	1/1	0.96	0.10	47,47,47,47	0
53	MG	1A	3355	1/1	0.96	0.17	39,39,39,39	0
53	MG	2A	3371	1/1	0.96	0.07	36,36,36,36	0
53	MG	1A	3449	1/1	0.96	0.08	57,57,57,57	0
53	MG	1A	3286	1/1	0.96	0.16	44,44,44,44	0
53	MG	2A	3375	1/1	0.96	0.11	51,51,51,51	0
53	MG	1a	3035	1/1	0.96	0.10	84,84,84,84	0
53	MG	1A	3225	1/1	0.96	0.18	52,52,52,52	0
53	MG	1A	3324	1/1	0.96	0.16	34,34,34,34	0
53	MG	1A	3226	1/1	0.96	0.07	40,40,40,40	0
53	MG	1A	3643	1/1	0.96	0.09	31,31,31,31	0
53	MG	1R	202	1/1	0.96	0.14	66,66,66,66	0
53	MG	1A	3169	1/1	0.96	0.15	25,25,25,25	0
53	MG	1A	3517	1/1	0.96	0.07	69,69,69,69	0
53	MG	1a	3128	1/1	0.96	0.13	93,93,93,93	0
53	MG	1A	3579	1/1	0.96	0.08	68,68,68,68	0
53	MG	1R	206	1/1	0.96	0.11	52,52,52,52	0
53	MG	1A	3404	1/1	0.96	0.09	63,63,63,63	0
53	MG	1A	3737	1/1	0.96	0.28	23,23,23,23	0
53	MG	1A	3405	1/1	0.96	0.09	45,45,45,45	0
53	MG	2B	219	1/1	0.96	0.08	79,79,79,79	0
53	MG	2a	1710	1/1	0.96	0.07	76,76,76,76	0
53	MG	2a	1711	1/1	0.96	0.10	105,105,105,105	0
53	MG	1A	3170	1/1	0.96	0.14	56,56,56,56	0
53	MG	1A	3261	1/1	0.96	0.14	59,59,59,59	0
53	MG	2A	3395	1/1	0.96	0.13	72,72,72,72	0
53	MG	1A	3653	1/1	0.96	0.06	54,54,54,54	0
53	MG	1A	3115	1/1	0.96	0.08	53,53,53,53	0
53	MG	1A	3467	1/1	0.96	0.11	57,57,57,57	0
53	MG	1A	3587	1/1	0.96	0.11	51,51,51,51	0
53	MG	1A	3172	1/1	0.96	0.16	23,23,23,23	0
53	MG	1A	3661	1/1	0.96	0.07	21,21,21,21	0
53	MG	2A	3402	1/1	0.96	0.07	53,53,53,53	0
53	MG	1W	203	1/1	0.96	0.10	51,51,51,51	0
53	MG	1b	3001	1/1	0.96	0.05	90,90,90,90	0
53	MG	2A	3176	1/1	0.96	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3366	1/1	0.96	0.07	37,37,37,37	0
53	MG	2a	1726	1/1	0.96	0.14	62,62,62,62	0
53	MG	2A	3178	1/1	0.96	0.18	36,36,36,36	0
53	MG	1d	503	1/1	0.96	0.07	99,99,99,99	0
53	MG	2Q	3002	1/1	0.96	0.15	51,51,51,51	0
53	MG	2A	3411	1/1	0.96	0.06	44,44,44,44	0
53	MG	1A	3473	1/1	0.96	0.09	48,48,48,48	0
53	MG	10	102	1/1	0.96	0.31	37,37,37,37	0
53	MG	1A	3752	1/1	0.96	0.09	47,47,47,47	0
53	MG	2A	3292	1/1	0.96	0.13	49,49,49,49	0
53	MG	2A	3079	1/1	0.96	0.12	54,54,54,54	0
53	MG	1A	3753	1/1	0.96	0.11	63,63,63,63	0
53	MG	1A	3755	1/1	0.96	0.08	75,75,75,75	0
56	SF4	1d	501	8/8	0.96	0.06	85,105,119,125	0
56	SF4	2d	501	8/8	0.96	0.06	87,107,123,125	0
53	MG	1A	3234	1/1	0.97	0.17	44,44,44,44	0
53	MG	13	102	1/1	0.97	0.08	35,35,35,35	0
53	MG	2A	3270	1/1	0.97	0.22	65,65,65,65	0
53	MG	1A	3135	1/1	0.97	0.12	49,49,49,49	0
53	MG	1A	3696	1/1	0.97	0.09	57,57,57,57	0
53	MG	2Q	3003	1/1	0.97	0.15	45,45,45,45	0
53	MG	2A	3273	1/1	0.97	0.07	55,55,55,55	0
53	MG	1A	3009	1/1	0.97	0.05	45,45,45,45	0
53	MG	2a	1669	1/1	0.97	0.11	71,71,71,71	0
53	MG	15	104	1/1	0.97	0.20	63,63,63,63	0
53	MG	2A	3485	1/1	0.97	0.13	58,58,58,58	0
53	MG	2A	3154	1/1	0.97	0.18	36,36,36,36	0
53	MG	1A	3297	1/1	0.97	0.35	40,40,40,40	0
53	MG	1A	3477	1/1	0.97	0.09	49,49,49,49	0
53	MG	1A	3702	1/1	0.97	0.10	76,76,76,76	0
53	MG	1A	3536	1/1	0.97	0.09	52,52,52,52	0
53	MG	1a	3098	1/1	0.97	0.05	75,75,75,75	0
53	MG	1F	305	1/1	0.97	0.06	41,41,41,41	0
53	MG	1A	3571	1/1	0.97	0.10	69,69,69,69	0
53	MG	1a	3102	1/1	0.97	0.05	58,58,58,58	0
53	MG	2A	3495	1/1	0.97	0.10	64,64,64,64	0
53	MG	1A	3044	1/1	0.97	0.06	55,55,55,55	0
53	MG	1A	3231	1/1	0.97	0.09	46,46,46,46	0
53	MG	2A	3498	1/1	0.97	0.08	82,82,82,82	0
53	MG	1A	3385	1/1	0.97	0.12	58,58,58,58	0
53	MG	19	105	1/1	0.97	0.16	74,74,74,74	0
53	MG	1A	3427	1/1	0.97	0.11	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3613	1/1	0.97	0.35	48,48,48,48	0
53	MG	2a	1690	1/1	0.97	0.10	82,82,82,82	0
53	MG	1A	3176	1/1	0.97	0.10	24,24,24,24	0
53	MG	1P	202	1/1	0.97	0.11	50,50,50,50	0
53	MG	1A	3658	1/1	0.97	0.07	35,35,35,35	0
53	MG	1A	3304	1/1	0.97	0.12	38,38,38,38	0
53	MG	2A	3429	1/1	0.97	0.09	71,71,71,71	0
53	MG	1A	3408	1/1	0.97	0.11	51,51,51,51	0
53	MG	2a	1697	1/1	0.97	0.06	48,48,48,48	0
53	MG	1A	3371	1/1	0.97	0.07	43,43,43,43	0
53	MG	1A	3268	1/1	0.97	0.11	23,23,23,23	0
53	MG	1A	3664	1/1	0.97	0.09	49,49,49,49	0
53	MG	2A	3512	1/1	0.97	0.10	46,46,46,46	0
53	MG	1A	3458	1/1	0.97	0.06	27,27,27,27	0
53	MG	1A	3620	1/1	0.97	0.08	58,58,58,58	0
53	MG	1A	3488	1/1	0.97	0.23	69,69,69,69	0
53	MG	1A	3489	1/1	0.97	0.08	69,69,69,69	0
53	MG	2a	1628	1/1	0.97	0.16	55,55,55,55	0
53	MG	1A	3588	1/1	0.97	0.06	61,61,61,61	0
53	MG	1B	3013	1/1	0.97	0.13	41,41,41,41	0
53	MG	1A	3624	1/1	0.97	0.07	19,19,19,19	0
53	MG	1A	3459	1/1	0.97	0.07	45,45,45,45	0
53	MG	1A	3460	1/1	0.97	0.14	50,50,50,50	0
53	MG	1A	3373	1/1	0.97	0.29	63,63,63,63	0
53	MG	1A	3729	1/1	0.97	0.06	57,57,57,57	0
53	MG	1B	3019	1/1	0.97	0.10	40,40,40,40	0
53	MG	1A	3249	1/1	0.97	0.25	54,54,54,54	0
53	MG	1A	3393	1/1	0.97	0.09	35,35,35,35	0
53	MG	2A	3193	1/1	0.97	0.10	27,27,27,27	0
53	MG	1B	3022	1/1	0.97	0.10	32,32,32,32	0
53	MG	1A	3186	1/1	0.97	0.19	21,21,21,21	0
53	MG	2A	3451	1/1	0.97	0.09	71,71,71,71	0
53	MG	1A	3376	1/1	0.97	0.07	38,38,38,38	0
53	MG	1A	3439	1/1	0.97	0.11	54,54,54,54	0
53	MG	2A	3454	1/1	0.97	0.07	61,61,61,61	0
53	MG	1A	3635	1/1	0.97	0.08	56,56,56,56	0
53	MG	2A	3139	1/1	0.97	0.24	35,35,35,35	0
53	MG	1A	3468	1/1	0.97	0.10	73,73,73,73	0
53	MG	1A	3690	1/1	0.97	0.17	46,46,46,46	0
53	MG	2A	3087	1/1	0.97	0.10	64,64,64,64	0
53	MG	1A	3242	1/1	0.97	0.20	35,35,35,35	0
53	MG	2A	3463	1/1	0.97	0.06	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3292	1/1	0.97	0.10	42,42,42,42	0
53	MG	2A	3394	1/1	0.97	0.11	54,54,54,54	0
53	MG	2A	3468	1/1	0.97	0.06	58,58,58,58	0
53	MG	2A	3264	1/1	0.97	0.14	30,30,30,30	0
55	ZN	14	501	1/1	0.97	0.06	168,168,168,168	0
55	ZN	1n	102	1/1	0.97	0.11	159,159,159,159	0
53	MG	2A	3329	1/1	0.97	0.06	58,58,58,58	0
53	MG	2A	3205	1/1	0.97	0.15	33,33,33,33	0
53	MG	1A	3741	1/1	0.97	0.14	36,36,36,36	0
53	MG	1A	3564	1/1	0.97	0.06	46,46,46,46	0
53	MG	2A	3280	1/1	0.98	0.07	43,43,43,43	0
53	MG	1A	3493	1/1	0.98	0.08	49,49,49,49	0
53	MG	1A	3230	1/1	0.98	0.10	23,23,23,23	0
53	MG	1A	3582	1/1	0.98	0.05	61,61,61,61	0
53	MG	2A	3516	1/1	0.98	0.04	34,34,34,34	0
53	MG	1A	3454	1/1	0.98	0.06	57,57,57,57	0
53	MG	2A	3285	1/1	0.98	0.16	46,46,46,46	0
53	MG	1A	3634	1/1	0.98	0.05	58,58,58,58	0
53	MG	1A	3143	1/1	0.98	0.08	20,20,20,20	0
53	MG	2A	3455	1/1	0.98	0.08	66,66,66,66	0
53	MG	2a	1685	1/1	0.98	0.18	55,55,55,55	0
53	MG	1A	3669	1/1	0.98	0.04	61,61,61,61	0
53	MG	2A	3457	1/1	0.98	0.08	78,78,78,78	0
53	MG	1A	3709	1/1	0.98	0.06	75,75,75,75	0
53	MG	1A	3671	1/1	0.98	0.05	60,60,60,60	0
53	MG	1A	3751	1/1	0.98	0.04	37,37,37,37	0
53	MG	1A	3711	1/1	0.98	0.12	57,57,57,57	0
53	MG	1A	3260	1/1	0.98	0.14	29,29,29,29	0
53	MG	2A	3404	1/1	0.98	0.10	44,44,44,44	0
53	MG	1A	3754	1/1	0.98	0.09	32,32,32,32	0
53	MG	1A	3610	1/1	0.98	0.06	40,40,40,40	0
53	MG	2A	3467	1/1	0.98	0.05	60,60,60,60	0
53	MG	2A	3407	1/1	0.98	0.11	49,49,49,49	0
53	MG	1A	3559	1/1	0.98	0.07	58,58,58,58	0
53	MG	2A	3146	1/1	0.98	0.15	49,49,49,49	0
53	MG	1a	3121	1/1	0.98	0.06	94,94,94,94	0
53	MG	1A	3640	1/1	0.98	0.05	43,43,43,43	0
53	MG	1A	3716	1/1	0.98	0.09	57,57,57,57	0
53	MG	1A	3759	1/1	0.98	0.04	23,23,23,23	0
53	MG	2D	302	1/1	0.98	0.08	49,49,49,49	0
53	MG	1A	3406	1/1	0.98	0.08	50,50,50,50	0
53	MG	1A	3392	1/1	0.98	0.09	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2a	1707	1/1	0.98	0.10	82,82,82,82	0
53	MG	1A	3762	1/1	0.98	0.15	26,26,26,26	0
53	MG	1B	3001	1/1	0.98	0.05	70,70,70,70	0
53	MG	2A	3359	1/1	0.98	0.05	54,54,54,54	0
53	MG	1A	3424	1/1	0.98	0.08	48,48,48,48	0
53	MG	1A	3293	1/1	0.98	0.20	43,43,43,43	0
53	MG	2A	3483	1/1	0.98	0.07	50,50,50,50	0
53	MG	2A	3308	1/1	0.98	0.09	36,36,36,36	0
53	MG	1A	3682	1/1	0.98	0.15	63,63,63,63	0
53	MG	1A	3683	1/1	0.98	0.04	61,61,61,61	0
53	MG	2A	3159	1/1	0.98	0.07	44,44,44,44	0
53	MG	1A	3645	1/1	0.98	0.09	39,39,39,39	0
53	MG	2A	3210	1/1	0.98	0.07	37,37,37,37	0
53	MG	1A	3646	1/1	0.98	0.04	64,64,64,64	0
53	MG	1A	3686	1/1	0.98	0.11	59,59,59,59	0
53	MG	1A	3168	1/1	0.98	0.19	26,26,26,26	0
53	MG	2R	8001	1/1	0.98	0.07	30,30,30,30	0
53	MG	1A	3121	1/1	0.98	0.04	50,50,50,50	0
53	MG	1A	3178	1/1	0.98	0.04	30,30,30,30	0
53	MG	2A	3373	1/1	0.98	0.14	38,38,38,38	0
53	MG	1A	3357	1/1	0.98	0.17	41,41,41,41	0
53	MG	1a	3140	1/1	0.98	0.14	101,101,101,101	0
53	MG	1A	3235	1/1	0.98	0.08	36,36,36,36	0
53	MG	20	8001	1/1	0.98	0.05	49,49,49,49	0
53	MG	1A	3298	1/1	0.98	0.18	22,22,22,22	0
53	MG	1A	3045	1/1	0.98	0.10	32,32,32,32	0
53	MG	1A	3572	1/1	0.98	0.04	74,74,74,74	0
53	MG	1A	3450	1/1	0.98	0.06	40,40,40,40	0
53	MG	1A	3735	1/1	0.98	0.06	54,54,54,54	0
53	MG	2A	3174	1/1	0.98	0.07	23,23,23,23	0
53	MG	1A	3529	1/1	0.98	0.13	55,55,55,55	0
55	ZN	2Y	501	1/1	0.98	0.06	92,92,92,92	0
53	MG	1A	3300	1/1	0.98	0.19	47,47,47,47	0
55	ZN	26	501	1/1	0.98	0.06	84,84,84,84	0
55	ZN	29	501	1/1	0.98	0.04	89,89,89,89	0
53	MG	1A	3699	1/1	0.98	0.09	78,78,78,78	0
53	MG	1A	3301	1/1	0.98	0.22	38,38,38,38	0
53	MG	1A	3553	1/1	0.98	0.06	36,36,36,36	0
53	MG	1A	3438	1/1	0.99	0.06	33,33,33,33	0
53	MG	1A	3420	1/1	0.99	0.16	28,28,28,28	0
53	MG	1H	201	1/1	0.99	0.05	50,50,50,50	0
53	MG	1a	3101	1/1	0.99	0.05	65,65,65,65	0

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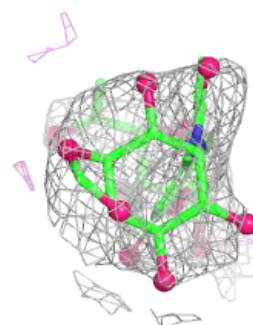
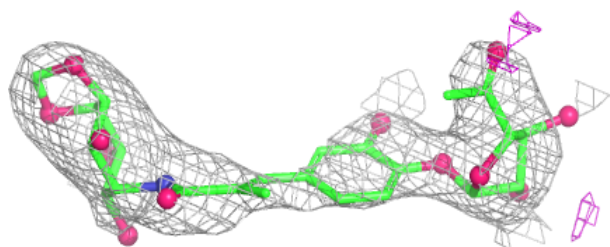
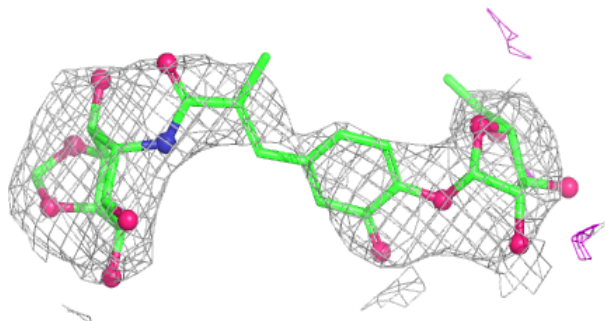
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3639	1/1	0.99	0.04	26,26,26,26	0
53	MG	1A	3575	1/1	0.99	0.10	83,83,83,83	0
53	MG	1A	3462	1/1	0.99	0.04	53,53,53,53	0
53	MG	1A	3631	1/1	0.99	0.06	53,53,53,53	0
53	MG	1E	302	1/1	0.99	0.09	43,43,43,43	0
53	MG	1A	3698	1/1	0.99	0.05	27,27,27,27	0
53	MG	2A	3390	1/1	0.99	0.06	45,45,45,45	0
53	MG	1A	3471	1/1	0.99	0.04	54,54,54,54	0
53	MG	1A	3578	1/1	0.99	0.06	30,30,30,30	0
53	MG	2A	3484	1/1	0.99	0.05	45,45,45,45	0
53	MG	1A	3670	1/1	0.99	0.05	48,48,48,48	0
55	ZN	1Y	201	1/1	0.99	0.12	80,80,80,80	0
53	MG	1A	3563	1/1	0.99	0.03	25,25,25,25	0
55	ZN	15	103	1/1	0.99	0.04	43,43,43,43	0
53	MG	1R	201	1/1	0.99	0.12	41,41,41,41	0
53	MG	1A	3672	1/1	0.99	0.03	33,33,33,33	0
53	MG	1A	3673	1/1	0.99	0.05	32,32,32,32	0
55	ZN	25	501	1/1	0.99	0.10	66,66,66,66	0
53	MG	2A	3465	1/1	0.99	0.14	41,41,41,41	0
53	MG	1A	3472	1/1	0.99	0.12	46,46,46,46	0
53	MG	1A	3006	1/1	0.99	0.13	31,31,31,31	0
53	MG	1a	3096	1/1	0.99	0.04	63,63,63,63	0
53	MG	1A	3660	1/1	0.99	0.04	50,50,50,50	0
53	MG	2A	3393	1/1	1.00	0.02	29,29,29,29	0
53	MG	1A	3668	1/1	1.00	0.03	26,26,26,26	0
53	MG	2A	3480	1/1	1.00	0.12	72,72,72,72	0
53	MG	1A	3457	1/1	1.00	0.04	30,30,30,30	0
53	MG	1A	3654	1/1	1.00	0.04	31,31,31,31	0
55	ZN	16	501	1/1	1.00	0.08	65,65,65,65	0
55	ZN	19	102	1/1	1.00	0.05	51,51,51,51	0
53	MG	1A	3550	1/1	1.00	0.03	23,23,23,23	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.

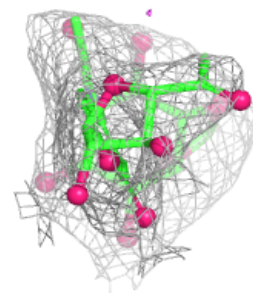
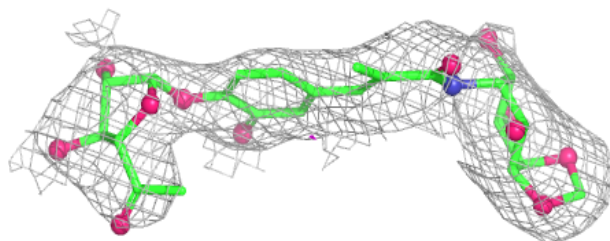
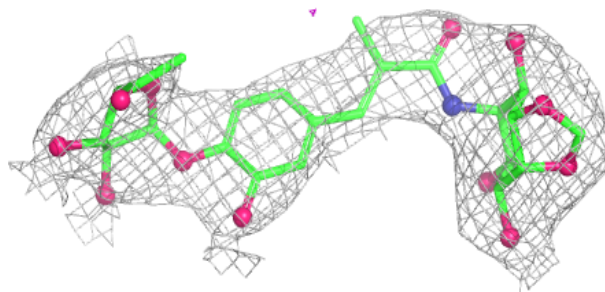


**Electron density around HGR 2A 3515:**

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

**Electron density around HGR 1A 3749:**

$2mF_o-DF_c$  (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.