



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 01:41 AM BST

PDB ID : 5DOX  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with Hygromycin-A at 3.1Å resolution  
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Deposited on : 2015-09-11  
Resolution : 3.10 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

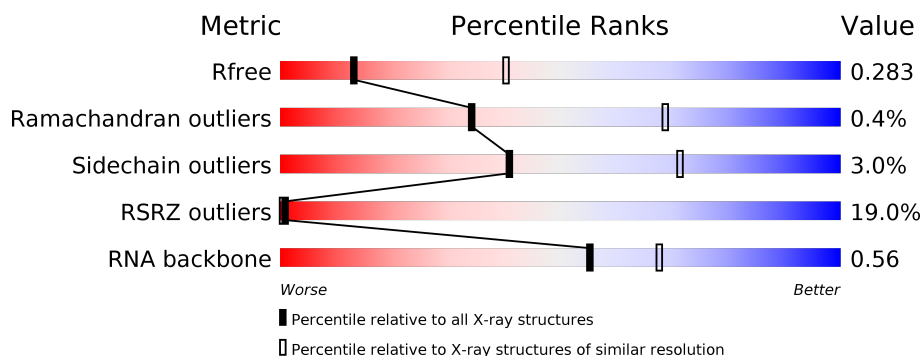
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1094 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div> </div>
1	2A	2915	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>.</div> </div> </div>
2	1B	121	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
2	2B	121	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>
3	1D	276	<div> <div>11%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
3	2D	276	<div> <div>18%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>

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

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Mol	Chain	Length	Quality of chain
16	2U	118	42% 97% ..
17	1V	101	9% 97% .
17	2V	101	17% 97% .
18	1W	113	97% ..
18	2W	113	3% 96% ..
19	1X	96	8% 99% .
19	2X	96	26% 97% ..
20	1Y	110	7% 95% ..
20	2Y	110	16% 96% ..
21	1Z	206	% 94% ..
21	2Z	206	7% 97% .
22	10	85	11% 88% 9%
22	20	85	28% 89% 9%
23	11	98	20% 98% ..
23	21	98	23% 97% ..
24	12	72	3% 96% ..
24	22	72	7% 96% ..
25	13	60	92% 7% .
25	23	60	23% 95% ..
26	14	71	23% 94% ..
26	24	71	20% 89% 8% .
27	15	60	2% 92% 7% .
27	25	60	2% 92% 7% .
28	16	54	11% 91% 7% .
28	26	54	13% 93% 6% .

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MG	19	103	-	-	-	X
53	MG	1A	3014	-	-	-	X
53	MG	1A	3035	-	-	-	X
53	MG	1A	3060	-	-	-	X
53	MG	1A	3128	-	-	-	X
53	MG	1A	3136	-	-	-	X
53	MG	1A	3250	-	-	-	X
53	MG	1A	3255	-	-	-	X
53	MG	1A	3283	-	-	-	X
53	MG	1A	3360	-	-	-	X
53	MG	1A	3516	-	-	-	X
53	MG	1A	3556	-	-	-	X
53	MG	1A	3732	-	-	-	X
53	MG	1B	3008	-	-	-	X
53	MG	1E	305	-	-	-	X
53	MG	1a	3026	-	-	-	X
53	MG	1a	3059	-	-	-	X
53	MG	1a	3142	-	-	-	X
53	MG	1e	201	-	-	-	X
53	MG	2A	3025	-	-	-	X
53	MG	2A	3123	-	-	-	X
53	MG	2A	3147	-	-	-	X
53	MG	2A	3149	-	-	-	X
53	MG	2A	3229	-	-	-	X
53	MG	2A	3323	-	-	-	X
53	MG	2A	3423	-	-	-	X
53	MG	2a	1705	-	-	-	X
53	MG	2t	201	-	-	-	X

## 2 Entry composition [i](#)

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	2E	6	Total Mg 6 6	0	0
53	17	2	Total Mg 2 2	0	0
53	1T	4	Total Mg 4 4	0	0
53	1N	2	Total Mg 2 2	0	0
53	20	1	Total Mg 1 1	0	0
53	18	1	Total Mg 1 1	0	0
53	1o	2	Total Mg 2 2	0	0
53	2W	1	Total Mg 1 1	0	0
53	2I	1	Total Mg 1 1	0	0
53	13	1	Total Mg 1 1	0	0
53	1f	1	Total Mg 1 1	0	0
53	2h	1	Total Mg 1 1	0	0
53	1P	2	Total Mg 2 2	0	0
53	2B	19	Total Mg 19 19	0	0
53	1q	1	Total Mg 1 1	0	0
53	2a	128	Total Mg 128 128	0	0
53	1k	1	Total Mg 1 1	0	0
53	1E	6	Total Mg 6 6	0	0
53	1b	1	Total Mg 1 1	0	0
53	2l	1	Total Mg 1 1	0	0
53	2F	2	Total Mg 2 2	0	0
53	28	2	Total Mg 2 2	0	0

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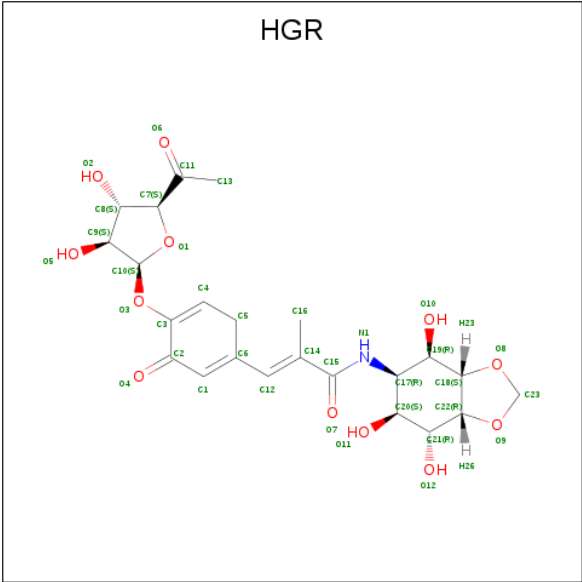
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	2e	1	Total 1	Mg 1	0	0
53	1W	2	Total 2	Mg 2	0	0
53	1A	768	Total 768	Mg 768	0	0
53	1t	1	Total 1	Mg 1	0	0
53	2P	1	Total 1	Mg 1	0	0
53	1X	1	Total 1	Mg 1	0	0
53	2T	3	Total 3	Mg 3	0	0
53	1D	7	Total 7	Mg 7	0	0
53	2N	1	Total 1	Mg 1	0	0
53	1e	1	Total 1	Mg 1	0	0
53	1V	2	Total 2	Mg 2	0	0
53	2X	1	Total 1	Mg 1	0	0
53	1a	143	Total 143	Mg 143	0	0
53	2Q	3	Total 3	Mg 3	0	0
53	15	5	Total 5	Mg 5	0	0
53	1R	5	Total 5	Mg 5	0	0
53	1G	2	Total 2	Mg 2	0	0
53	2O	2	Total 2	Mg 2	0	0
53	11	2	Total 2	Mg 2	0	0
53	1d	2	Total 2	Mg 2	0	0
53	1H	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	2Y	1	Total 1	Mg 1	0	0
53	2R	1	Total 1	Mg 1	0	0
53	1Z	1	Total 1	Mg 1	0	0
53	2D	3	Total 3	Mg 3	0	0
53	2k	1	Total 1	Mg 1	0	0
53	1U	3	Total 3	Mg 3	0	0
53	1r	1	Total 1	Mg 1	0	0
53	19	4	Total 4	Mg 4	0	0
53	1l	2	Total 2	Mg 2	0	0
53	2V	1	Total 1	Mg 1	0	0
53	1F	6	Total 6	Mg 6	0	0
53	10	6	Total 6	Mg 6	0	0
53	1g	2	Total 2	Mg 2	0	0
53	2t	1	Total 1	Mg 1	0	0
53	1Q	3	Total 3	Mg 3	0	0
53	2A	517	Total 517	Mg 517	0	0
53	1h	1	Total 1	Mg 1	0	0
53	1B	23	Total 23	Mg 23	0	0

- Molecule 54 is Hygromycin A (three-letter code: HGR) (formula: C<sub>23</sub>H<sub>29</sub>NO<sub>12</sub>).



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

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

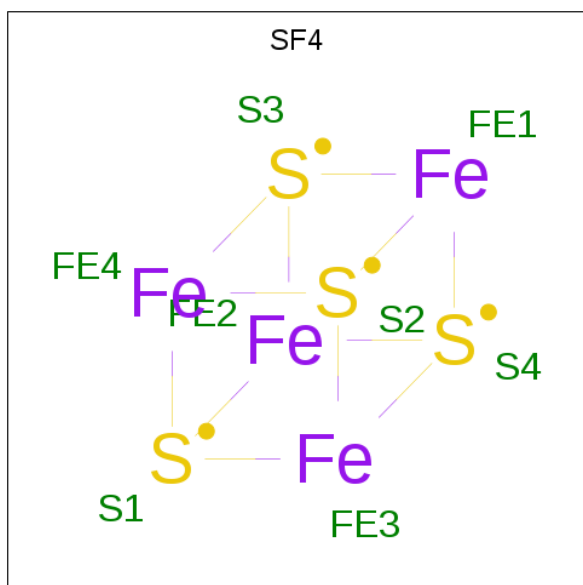
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1Y	1	Total	Zn	0	0
			1	1		
55	14	1	Total	Zn	0	0
			1	1		
55	1n	1	Total	Zn	0	0
			1	1		
55	15	1	Total	Zn	0	0
			1	1		
55	29	1	Total	Zn	0	0
			1	1		
55	19	1	Total	Zn	0	0
			1	1		
55	26	1	Total	Zn	0	0
			1	1		
55	25	1	Total	Zn	0	0
			1	1		
55	24	1	Total	Zn	0	0
			1	1		
55	2n	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2Y	1	Total	Zn	0	0
			1	1		
55	16	1	Total	Zn	0	0
			1	1		

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

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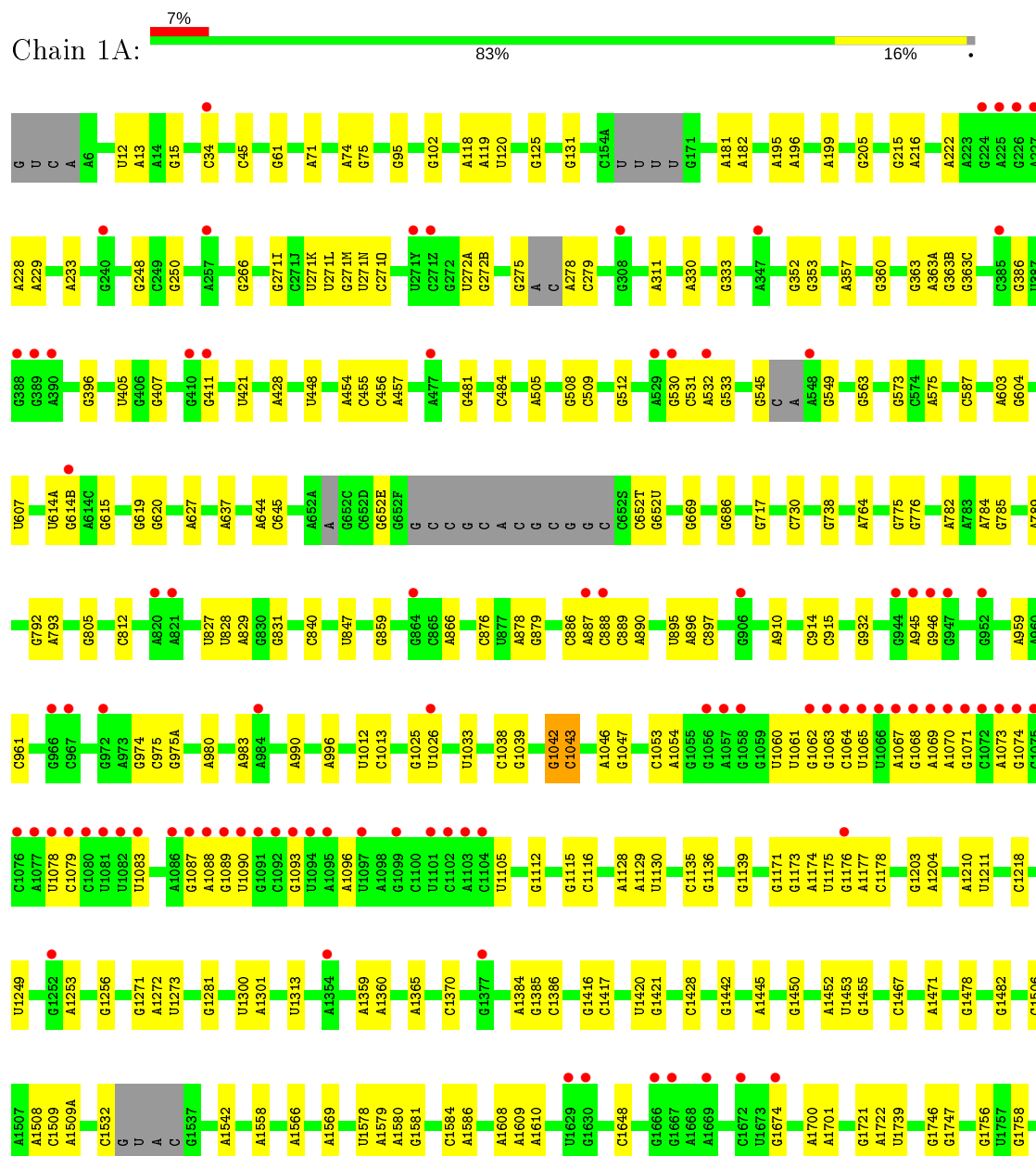
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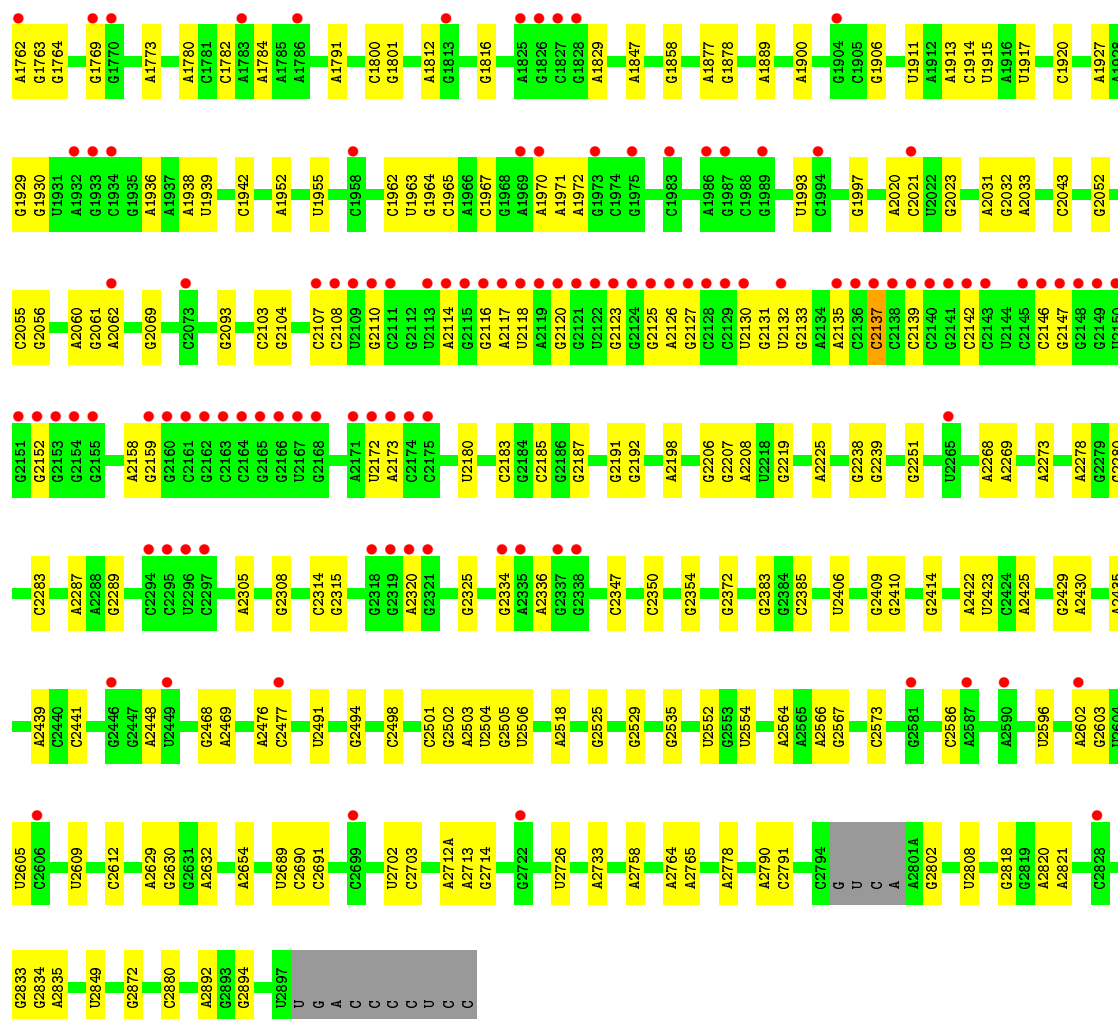
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	26	1	Total 1	O 1	0	0
57	27	2	Total 2	O 2	0	0
57	28	3	Total 3	O 3	0	0
57	2a	179	Total 179	O 179	0	0
57	2d	1	Total 1	O 1	0	0
57	2e	2	Total 2	O 2	0	0
57	2f	3	Total 3	O 3	0	0
57	2l	3	Total 3	O 3	0	0
57	2m	1	Total 1	O 1	0	0
57	2o	1	Total 1	O 1	0	0
57	2p	1	Total 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

### 3 Residue-property plots [i](#)

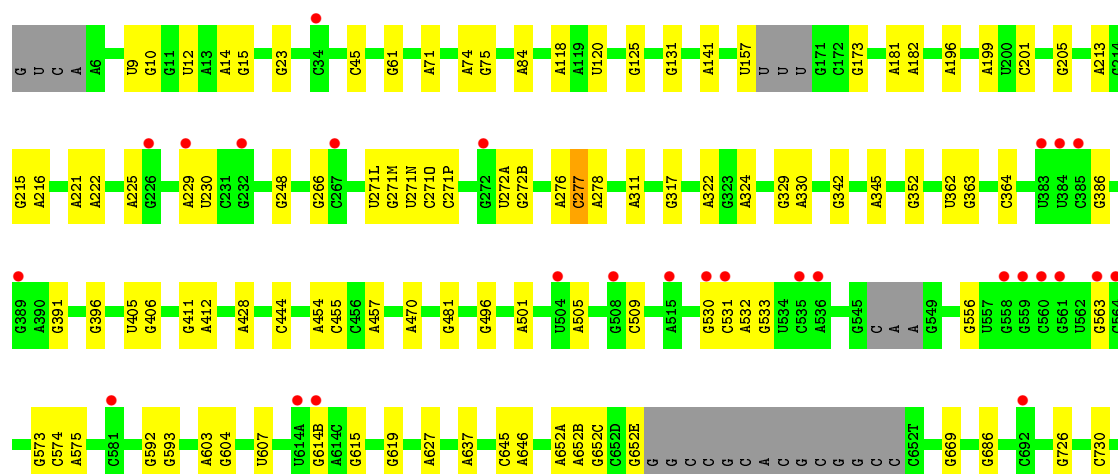
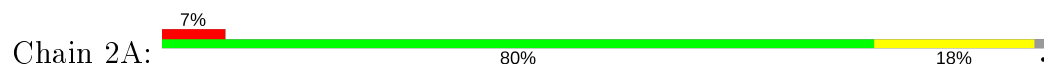
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: 23S Ribosomal RNA

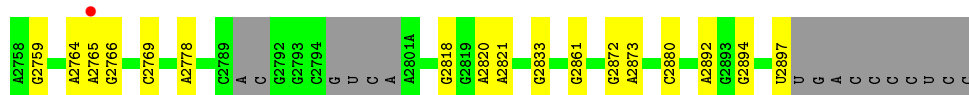




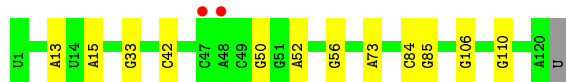
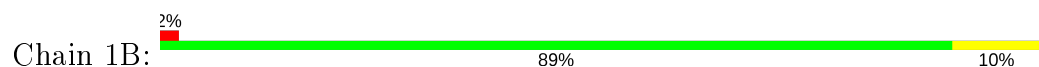
- Molecule 1: 23S Ribosomal RNA



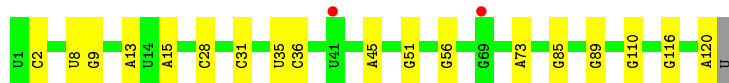
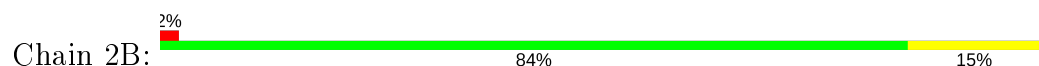




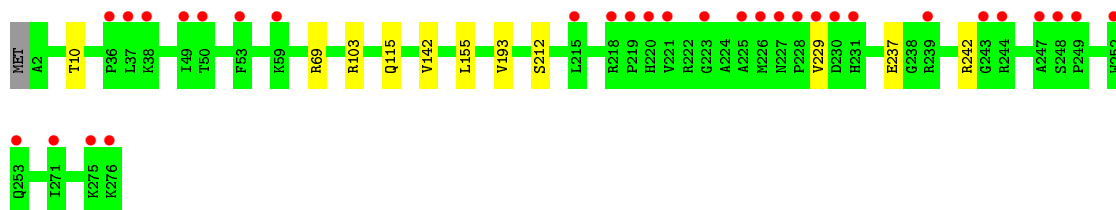
- Molecule 2: 5S Ribosomal RNA



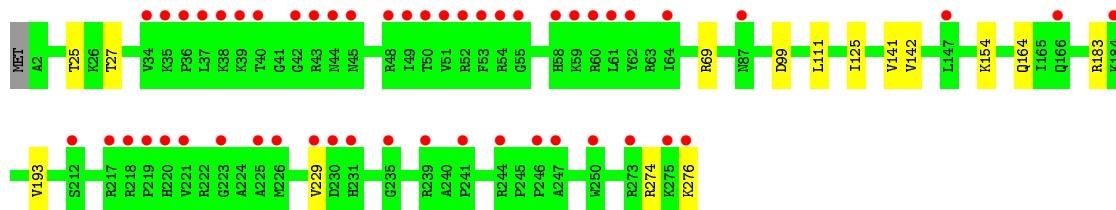
- Molecule 2: 5S Ribosomal RNA



- Molecule 3: 50S ribosomal protein L2



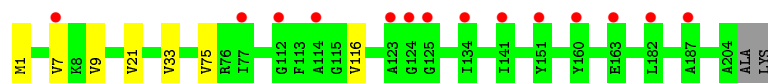
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3



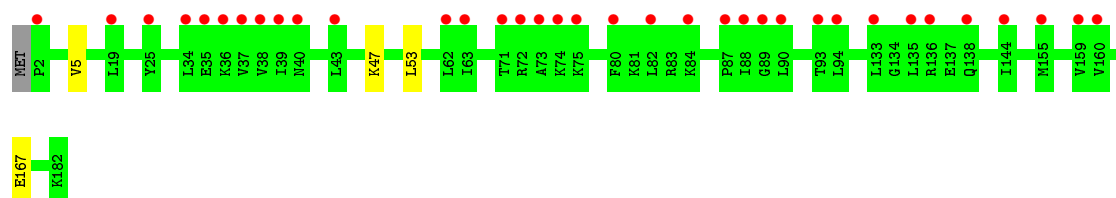
- Molecule 5: 50S ribosomal protein L4



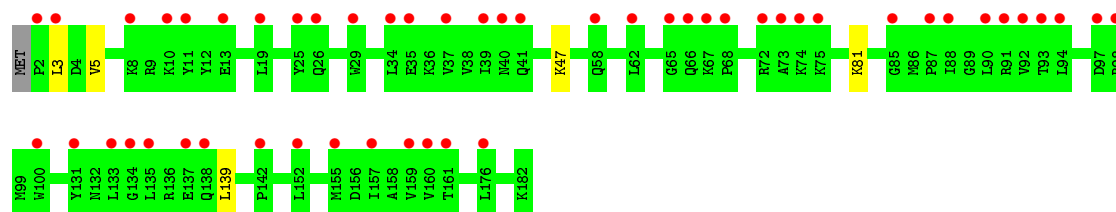
- Molecule 5: 50S ribosomal protein L4



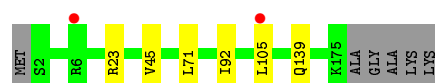
- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6



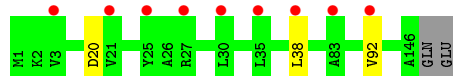
- Molecule 7: 50S ribosomal protein L6



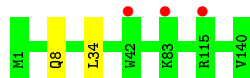
- Molecule 8: 50S ribosomal protein L9



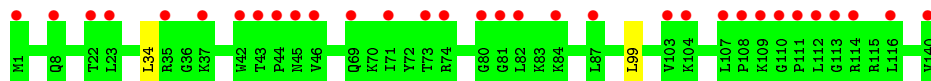
- Molecule 8: 50S ribosomal protein L9



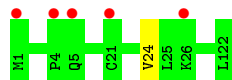
- Molecule 9: 50S ribosomal protein L13



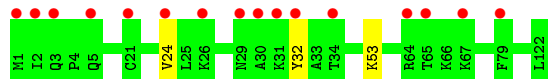
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14

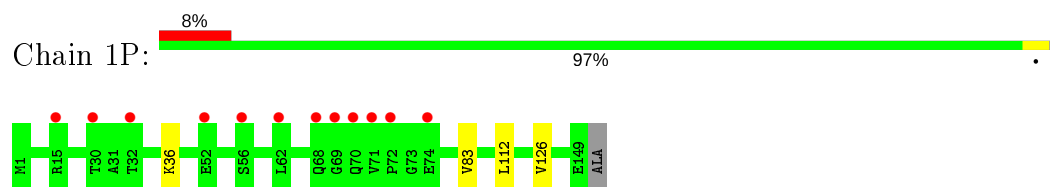


- Molecule 10: 50S ribosomal protein L14

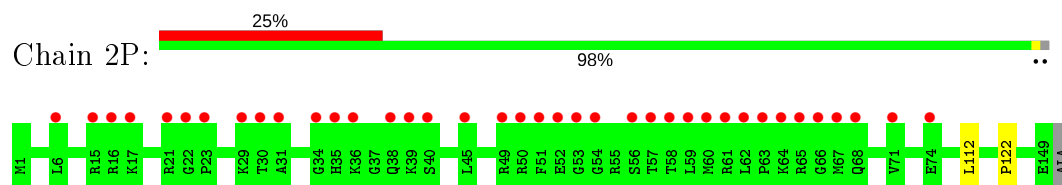




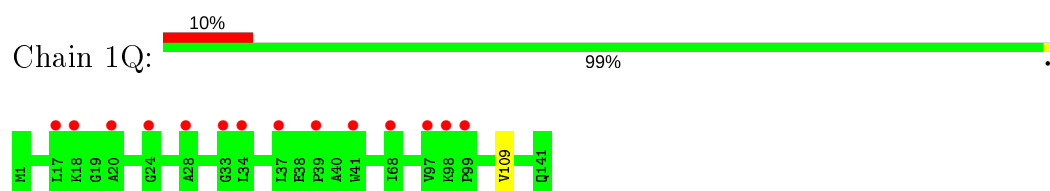
- Molecule 11: 50S ribosomal protein L15



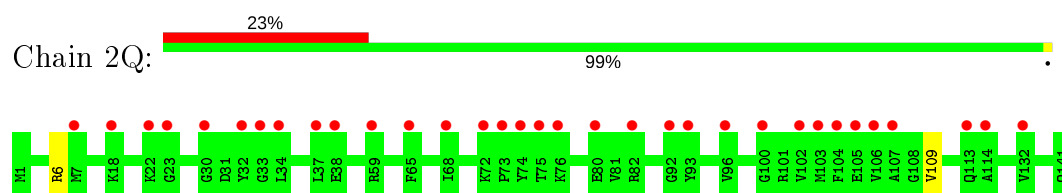
- Molecule 11: 50S ribosomal protein L15



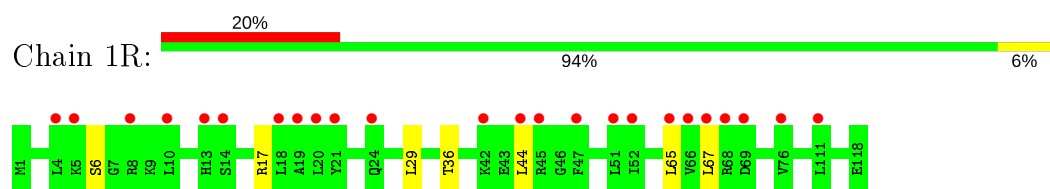
- Molecule 12: 50S ribosomal protein L16



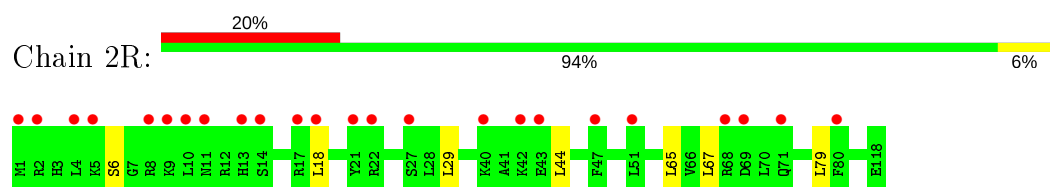
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

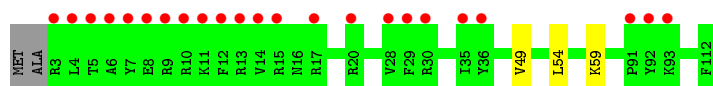


- Molecule 13: 50S ribosomal protein L17

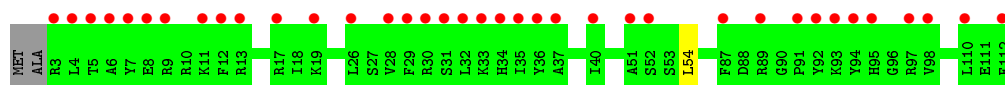


- Molecule 14: 50S ribosomal protein L18

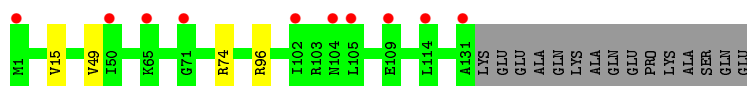
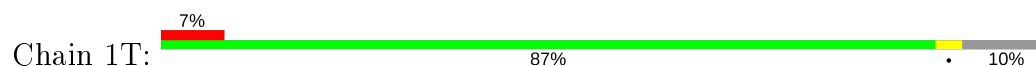




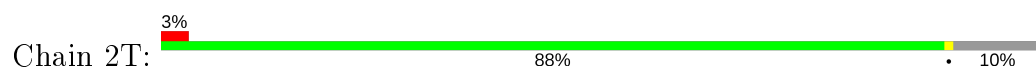
- Molecule 14: 50S ribosomal protein L18



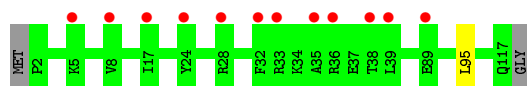
- Molecule 15: 50S ribosomal protein L19



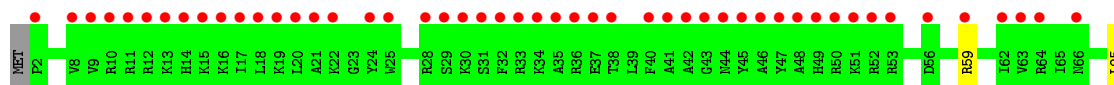
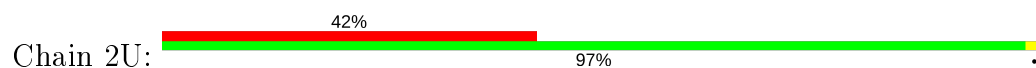
- Molecule 15: 50S ribosomal protein L19



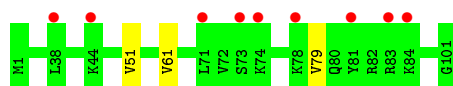
- Molecule 16: 50S ribosomal protein L20



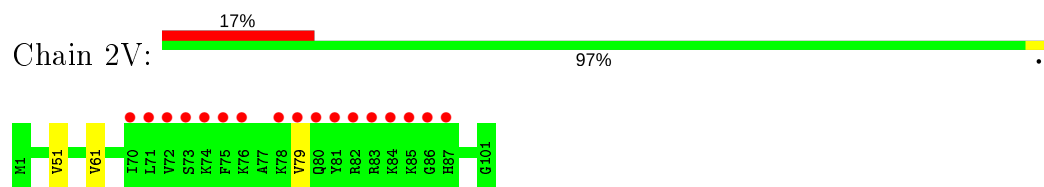
- Molecule 16: 50S ribosomal protein L20



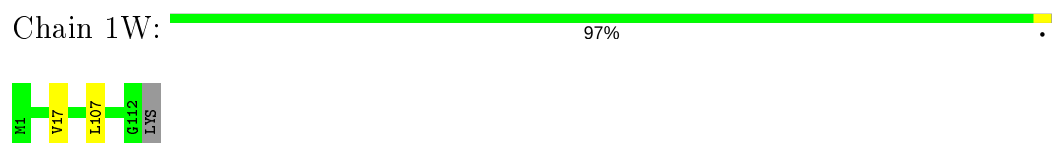
- Molecule 17: 50S ribosomal protein L21



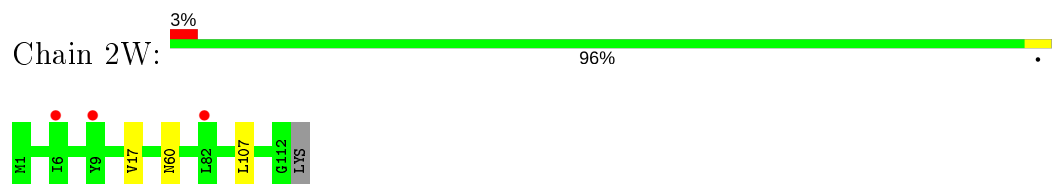
- Molecule 17: 50S ribosomal protein L21



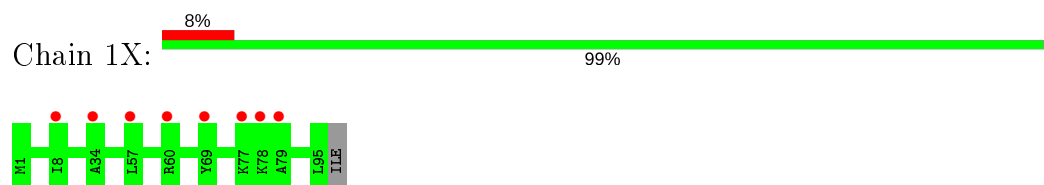
- Molecule 18: 50S ribosomal protein L22



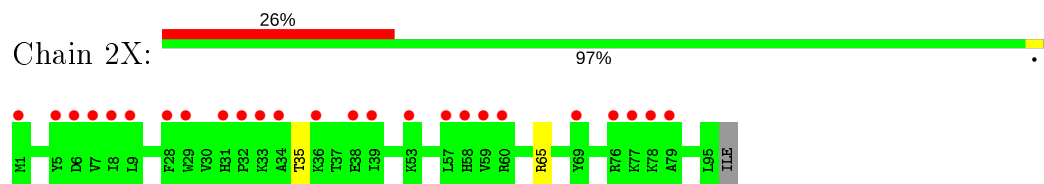
- Molecule 18: 50S ribosomal protein L22



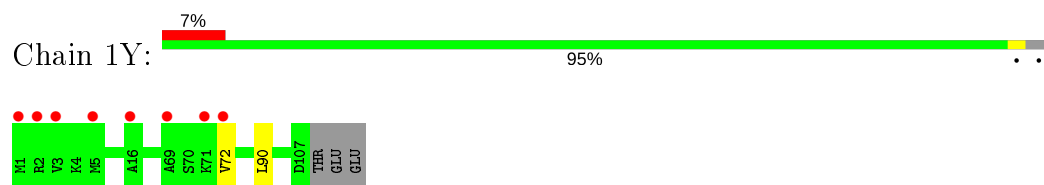
- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23

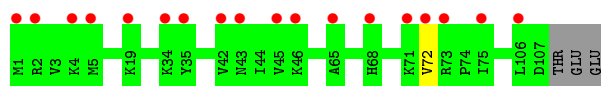


- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

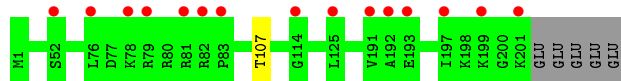




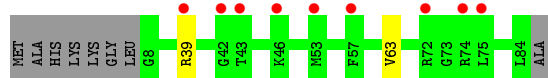
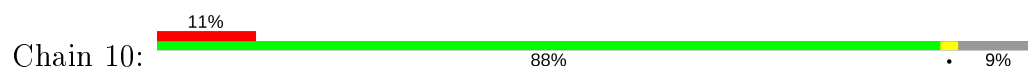
- Molecule 21: 50S ribosomal protein L25



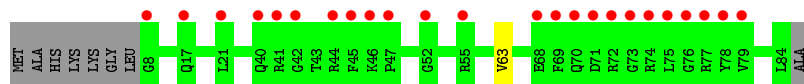
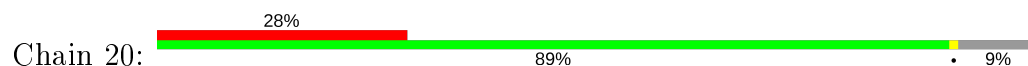
- Molecule 21: 50S ribosomal protein L25



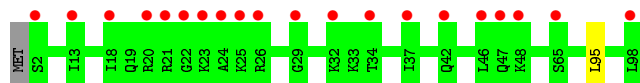
- Molecule 22: 50S ribosomal protein L27



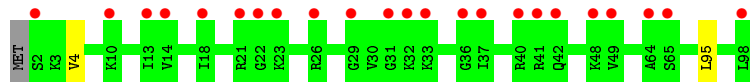
- Molecule 22: 50S ribosomal protein L27



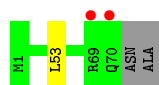
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



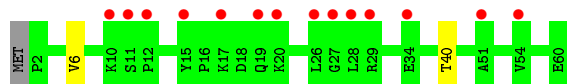
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



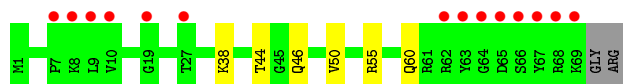
- Molecule 25: 50S ribosomal protein L30



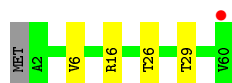
- Molecule 26: 50S ribosomal protein L31



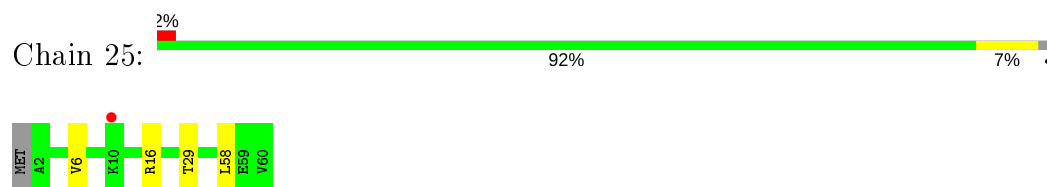
- Molecule 26: 50S ribosomal protein L31



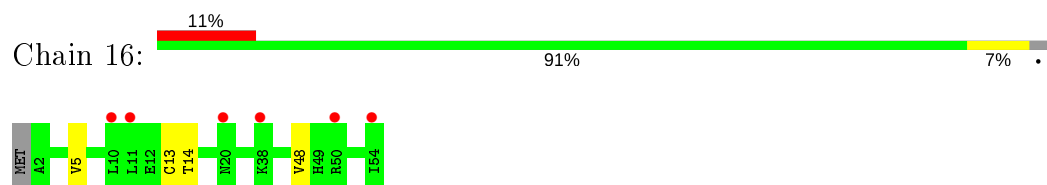
- Molecule 27: 50S ribosomal protein L32



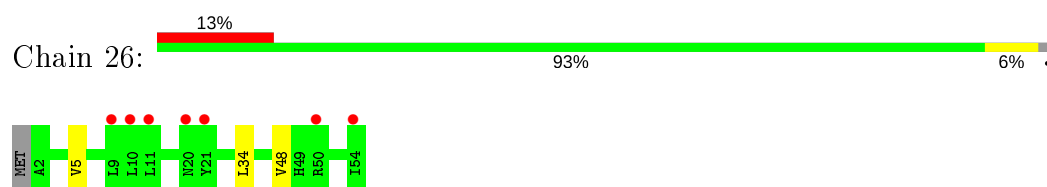
- Molecule 27: 50S ribosomal protein L32



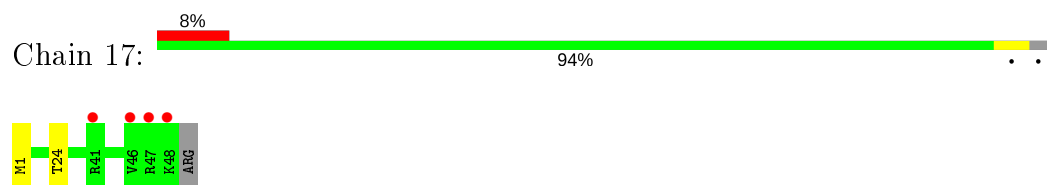
- Molecule 28: 50S ribosomal protein L33



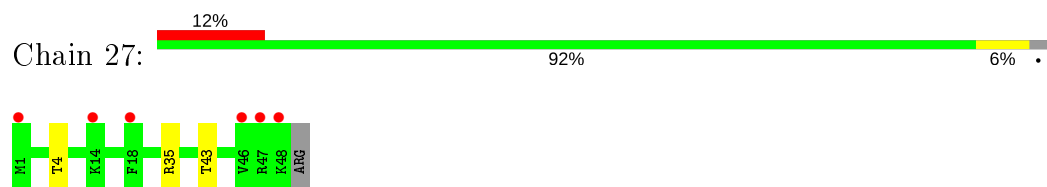
- Molecule 28: 50S ribosomal protein L33



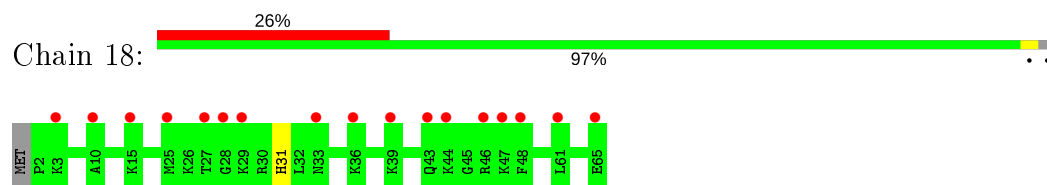
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34

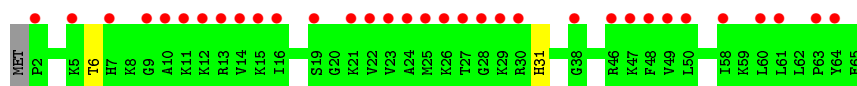


- Molecule 30: 50S ribosomal protein L35

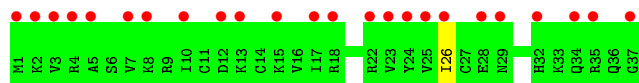


- Molecule 30: 50S ribosomal protein L35

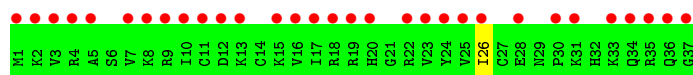
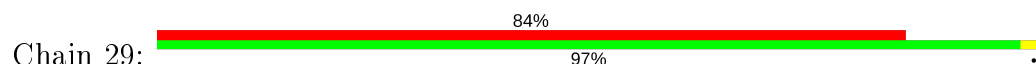




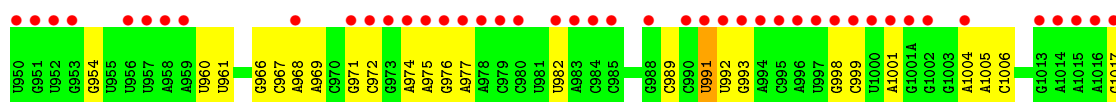
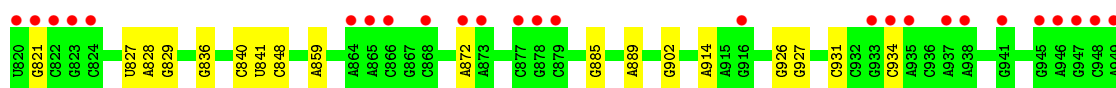
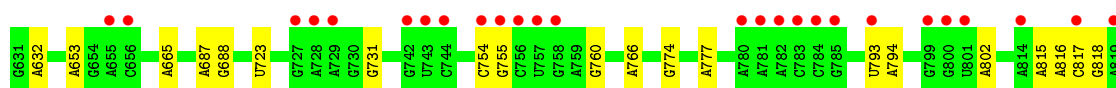
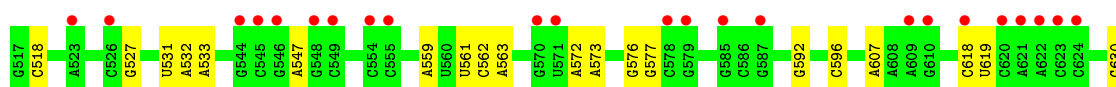
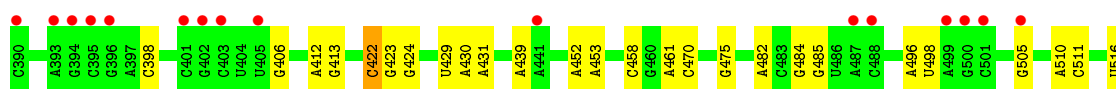
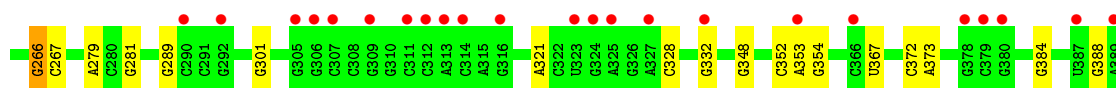
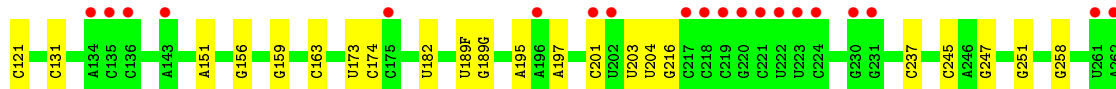
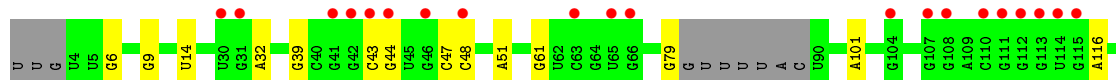
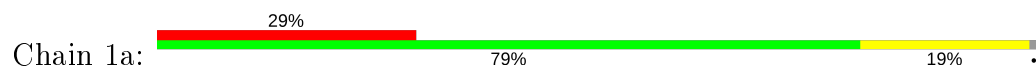
- Molecule 31: 50S ribosomal protein L36



- Molecule 31: 50S ribosomal protein L36

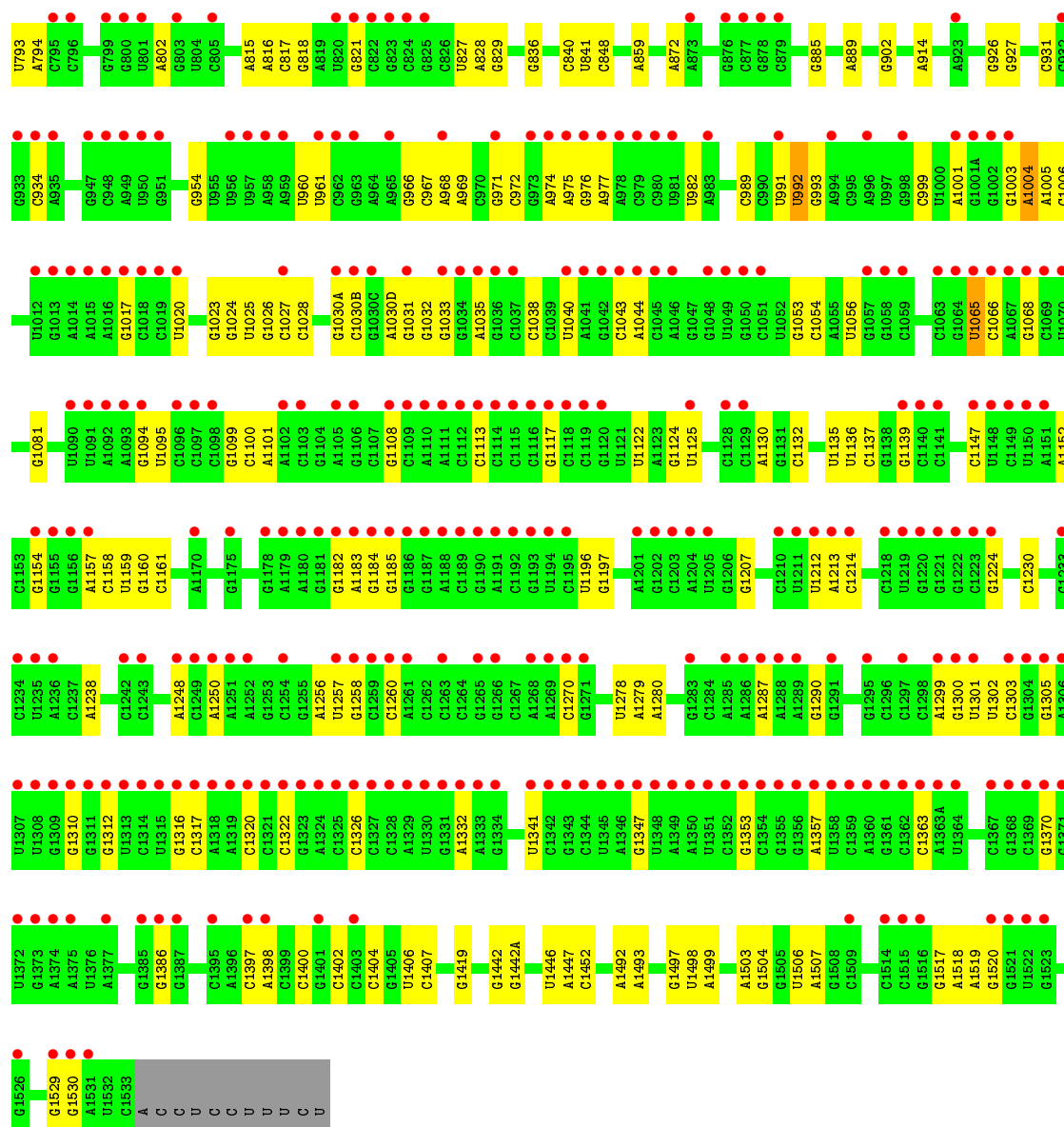


- Molecule 32: 16S Ribosomal RNA

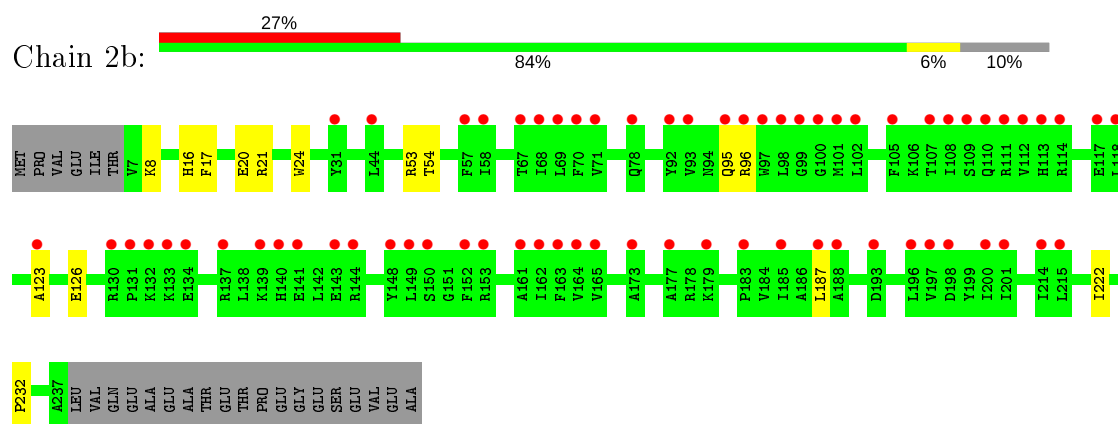




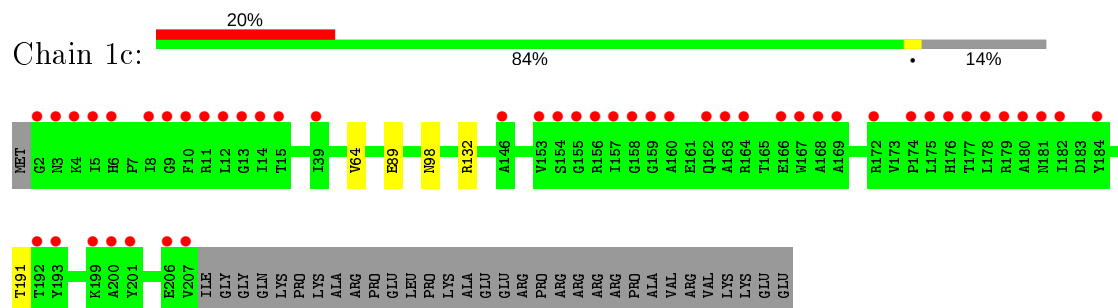




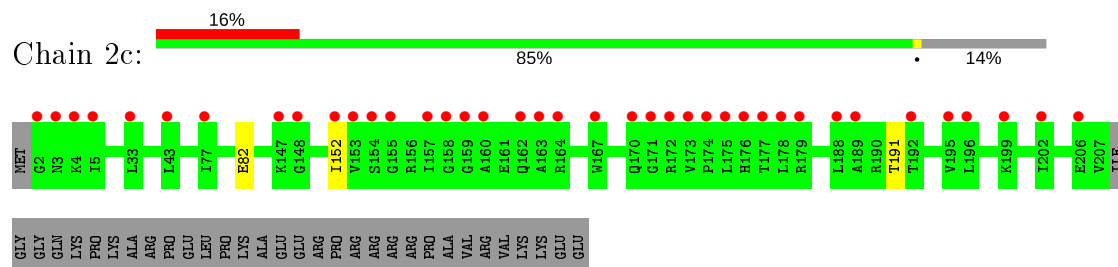
• Molecule 33: 30S ribosomal protein S2



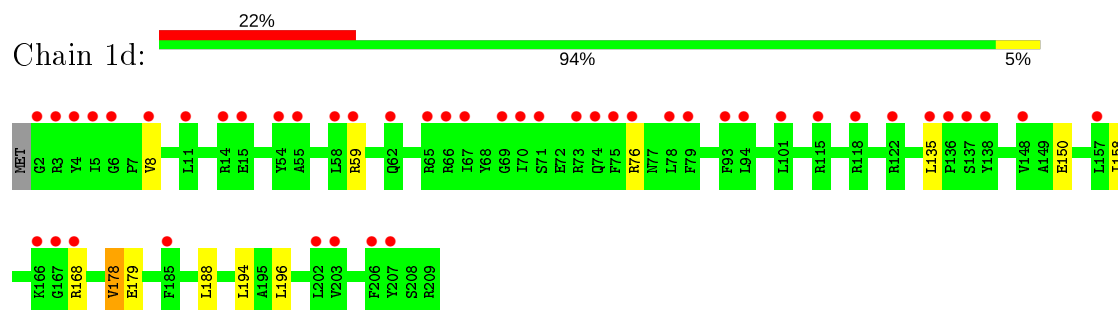
- Molecule 34: 30S ribosomal protein S3



- Molecule 34: 30S ribosomal protein S3

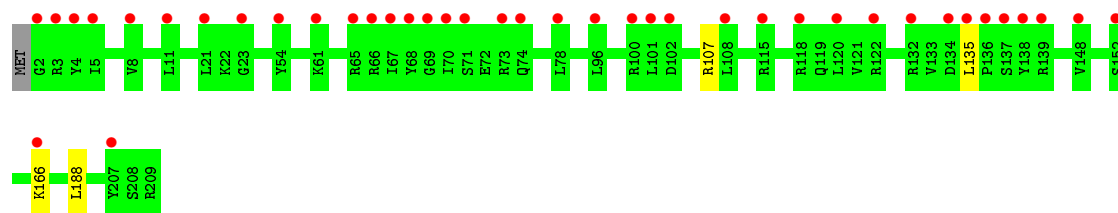


- Molecule 35: 30S ribosomal protein S4

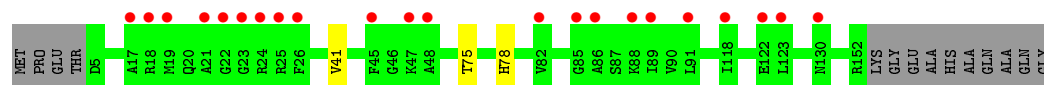
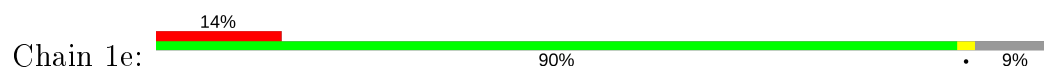


- Molecule 35: 30S ribosomal protein S4

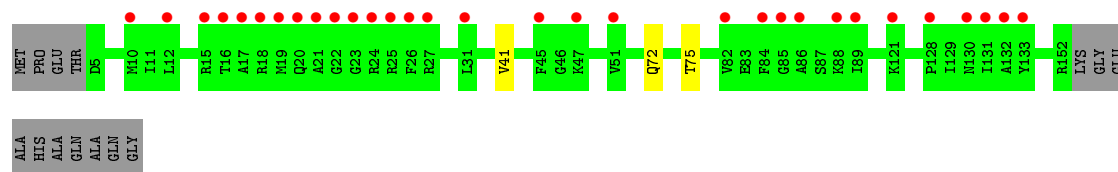
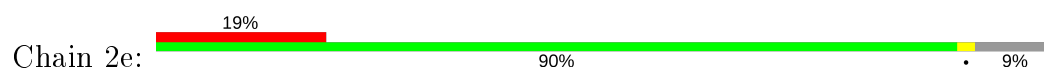




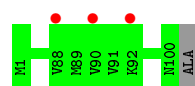
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



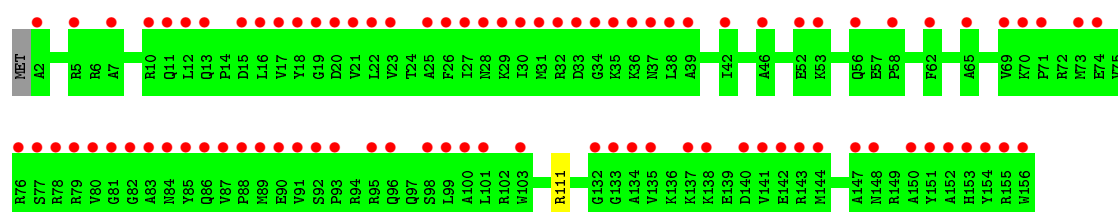
- Molecule 37: 30S ribosomal protein S6



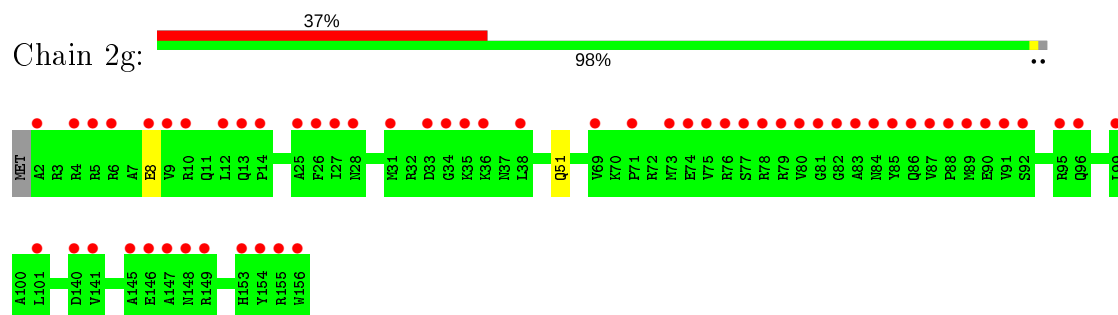
- Molecule 37: 30S ribosomal protein S6



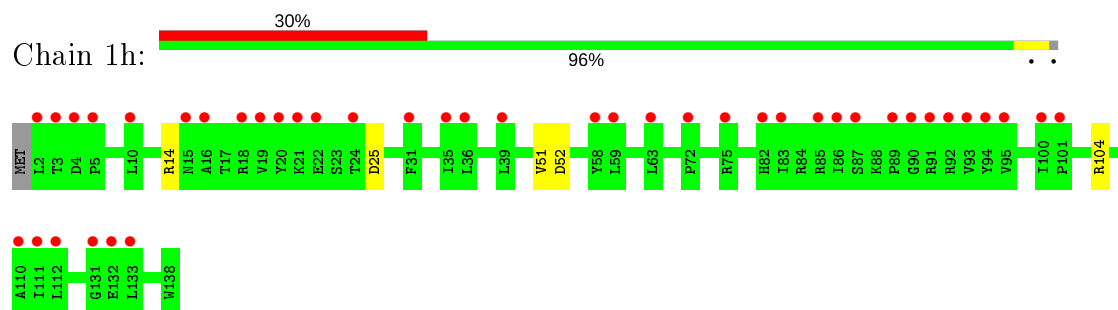
- Molecule 38: 30S ribosomal protein S7



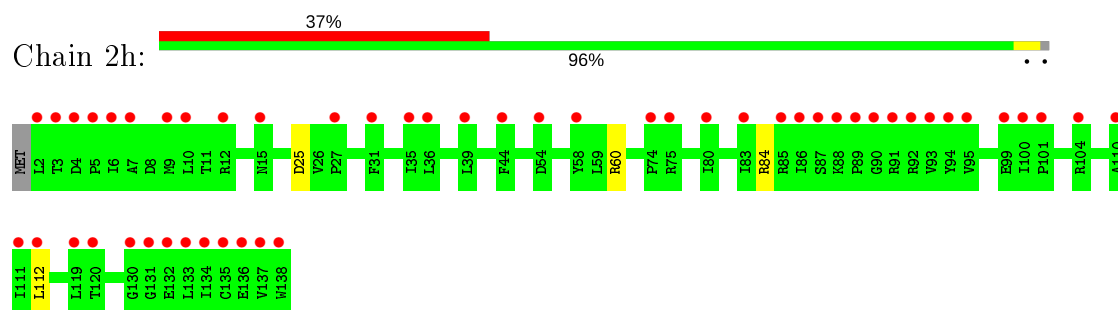
- Molecule 38: 30S ribosomal protein S7



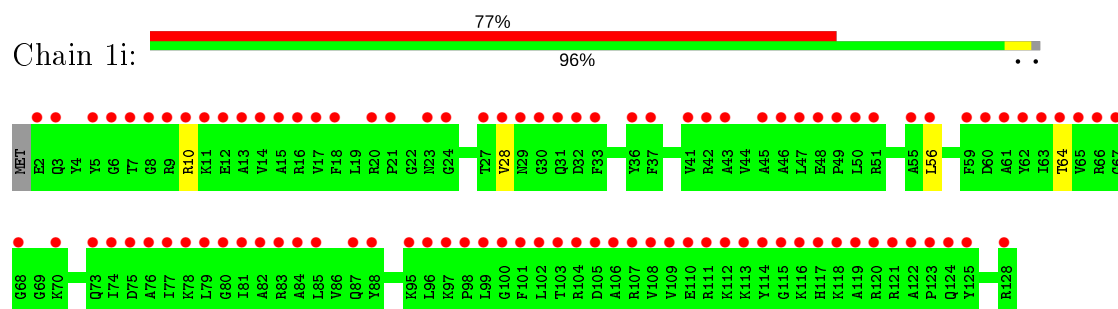
- Molecule 39: 30S ribosomal protein S8



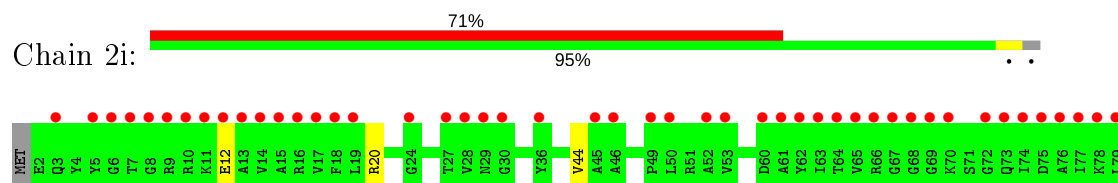
- Molecule 39: 30S ribosomal protein S8

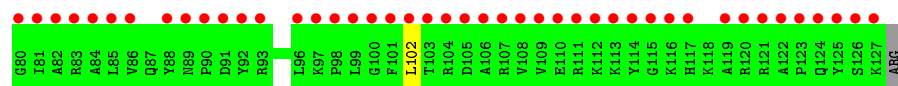


- Molecule 40: 30S ribosomal protein S9

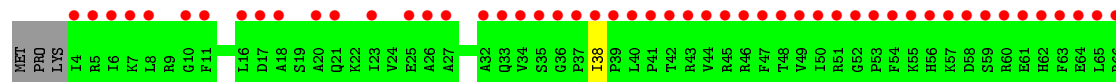
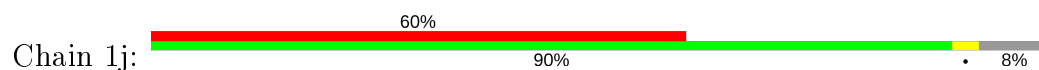


- Molecule 40: 30S ribosomal protein S9

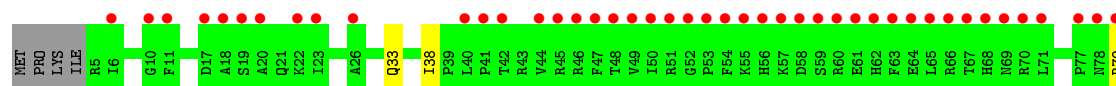
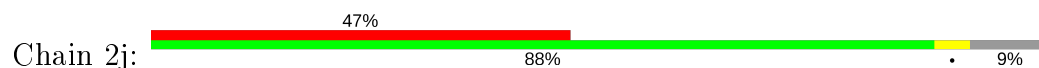




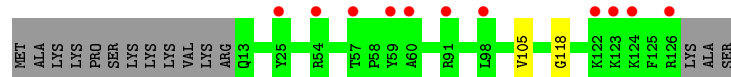
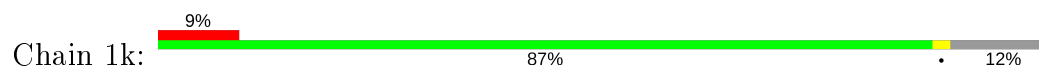
- Molecule 41: 30S ribosomal protein S10



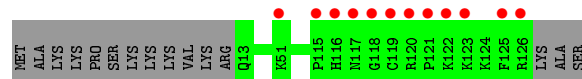
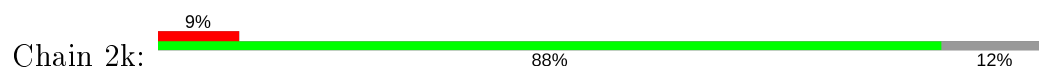
- Molecule 41: 30S ribosomal protein S10



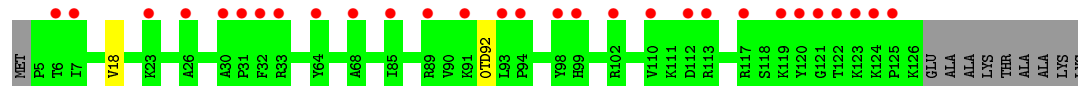
- Molecule 42: 30S ribosomal protein S11



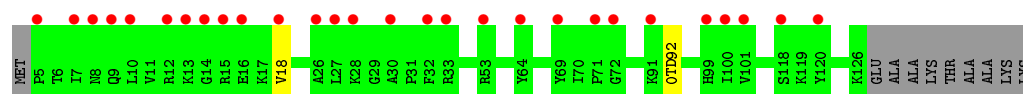
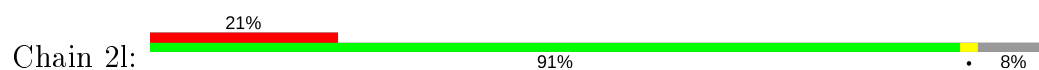
- Molecule 42: 30S ribosomal protein S11



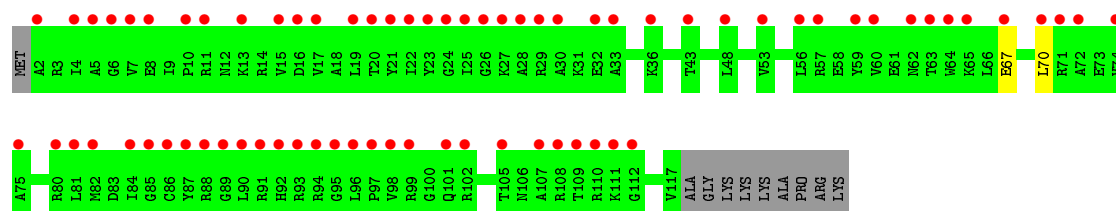
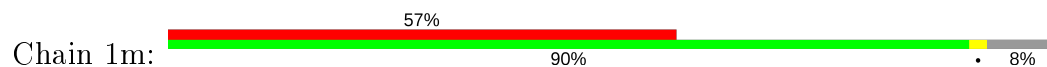
- Molecule 43: 30S ribosomal protein S12



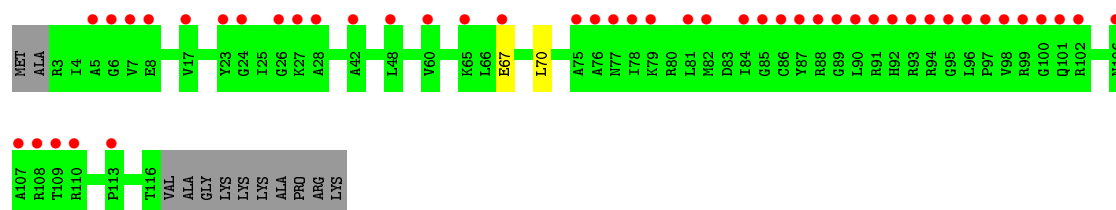
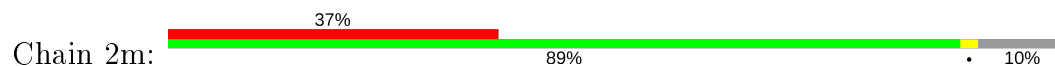
- Molecule 43: 30S ribosomal protein S12



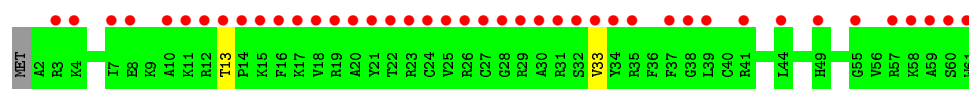
- Molecule 44: 30S ribosomal protein S13



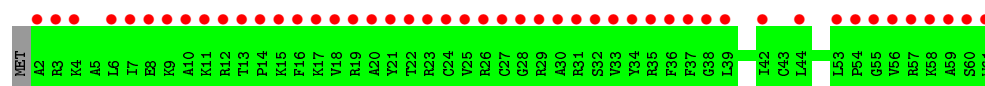
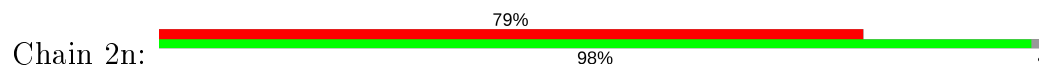
- Molecule 44: 30S ribosomal protein S13



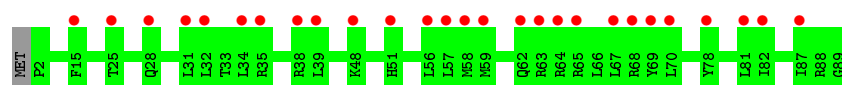
- Molecule 45: 30S ribosomal protein S14 type Z



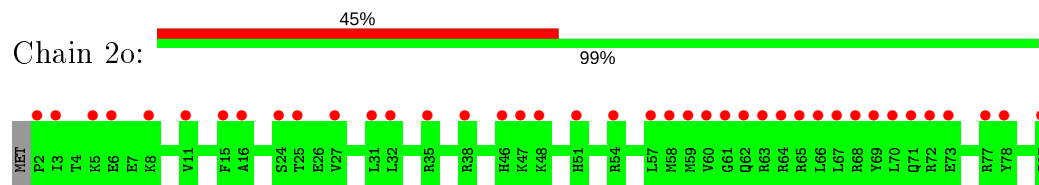
- Molecule 45: 30S ribosomal protein S14 type Z



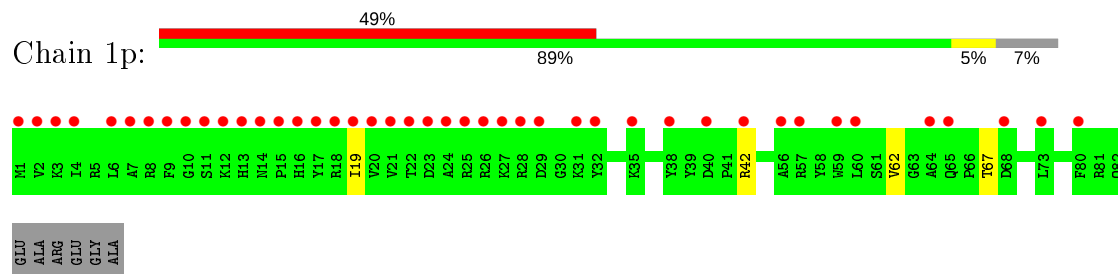
- Molecule 46: 30S ribosomal protein S15



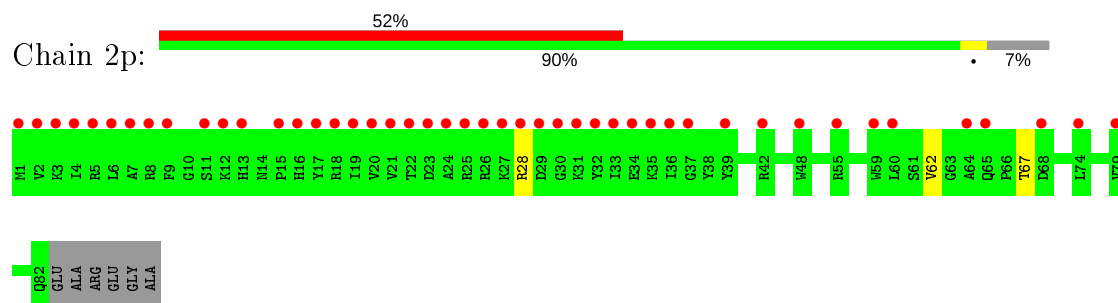
- Molecule 46: 30S ribosomal protein S15



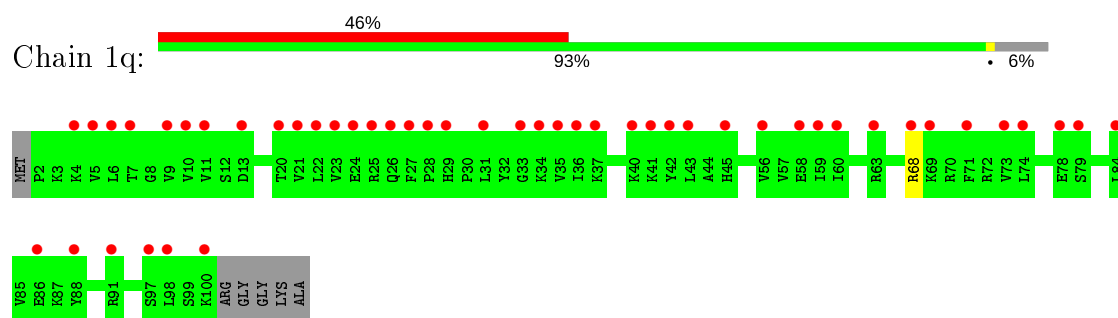
- Molecule 47: 30S ribosomal protein S16



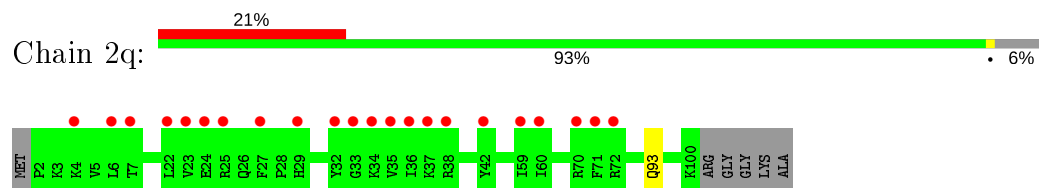
- Molecule 47: 30S ribosomal protein S16



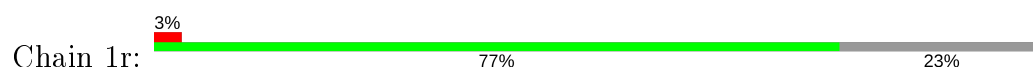
- Molecule 48: 30S ribosomal protein S17

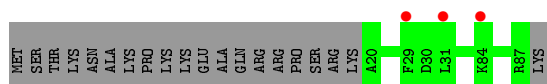


- Molecule 48: 30S ribosomal protein S17

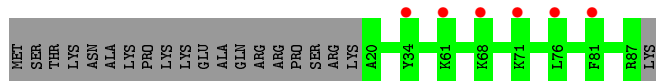
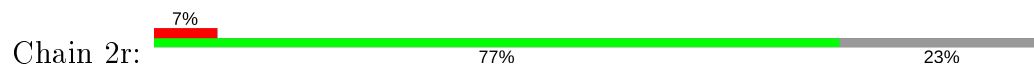


- Molecule 49: 30S ribosomal protein S18

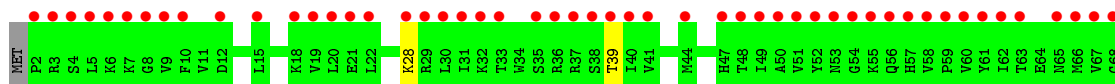
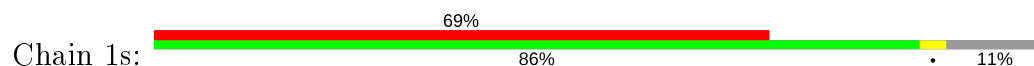




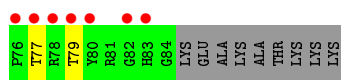
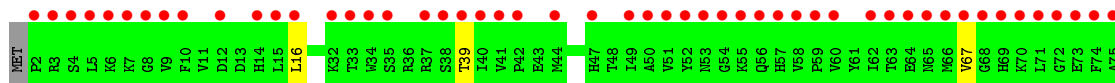
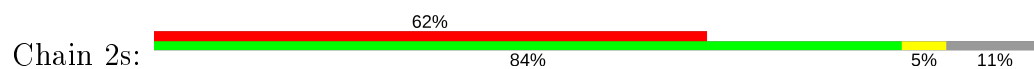
- Molecule 49: 30S ribosomal protein S18



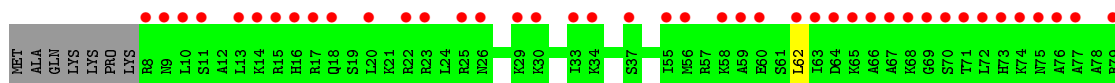
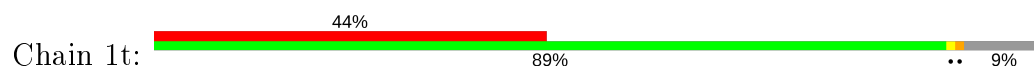
- Molecule 50: 30S ribosomal protein S19



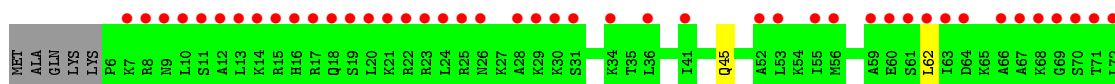
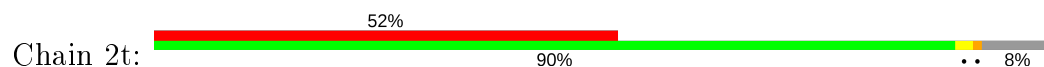
- Molecule 50: 30S ribosomal protein S19



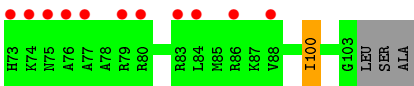
- Molecule 51: 30S ribosomal protein S20



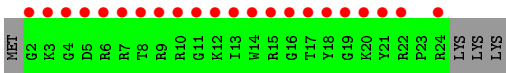
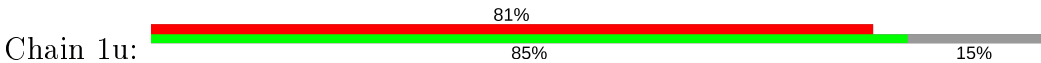
- Molecule 51: 30S ribosomal protein S20



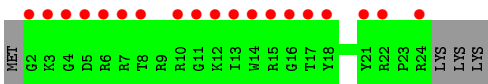
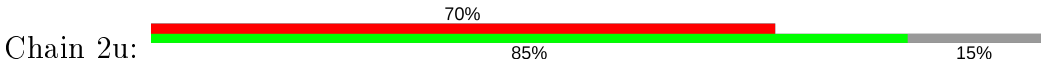




• Molecule 52: 30S ribosomal protein Thx



• 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 0.231 , 0.283	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> )	0.28 , 69.6	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	0.78	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: 5MU, ZN, OMG, MA6, SF4, 0TD, HGR, MG, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1A	0.33	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

All (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
1	2A	2104	G	C6-N1-C2	9.30	130.68	125.10
1	2A	2185	C	C2-N3-C4	9.30	124.55	119.90
1	2A	1079	C	N1-C2-O2	8.40	123.94	118.90
1	2A	2104	G	N1-C6-O6	-8.33	114.90	119.90
1	1A	1042	G	OP2-P-O3'	-8.15	87.28	105.20
1	1A	2137	C	C2-N1-C1'	7.55	127.11	118.80
1	2A	2104	G	C5-C6-N1	-7.14	107.93	111.50
1	1A	1043	C	OP1-P-OP2	7.03	130.15	119.60
1	1A	2137	C	N1-C2-O2	6.85	123.01	118.90
1	2A	2103	C	C5-C4-N4	6.76	124.93	120.20
1	2A	2185	C	C5-C6-N1	6.68	124.34	121.00
32	2a	754	C	C2-N1-C1'	6.61	126.07	118.80
32	1a	1006	C	C5-C6-N1	6.51	124.26	121.00
1	2A	1097	U	C2-N1-C1'	6.39	125.37	117.70
32	1a	754	C	C2-N1-C1'	6.38	125.81	118.80
32	2a	266	G	P-O3'-C3'	6.35	127.32	119.70
1	2A	1079	C	N3-C2-O2	-6.34	117.46	121.90
32	2a	1040	U	C5-C4-O4	6.21	129.63	125.90
1	2A	2185	C	N3-C4-N4	-6.12	113.72	118.00
1	2A	2185	C	C4-C5-C6	-6.11	114.34	117.40
1	1A	1313	U	C2-N1-C1'	6.06	124.97	117.70
32	1a	266	G	P-O3'-C3'	6.06	126.97	119.70
32	2a	1033	G	C6-N1-C2	6.04	128.72	125.10
1	2A	2185	C	N3-C2-O2	-6.02	117.68	121.90
1	1A	2501	C	C2-N1-C1'	-6.00	112.20	118.80
32	1a	754	C	N1-C2-O2	5.92	122.45	118.90
1	1A	2137	C	N3-C2-O2	-5.89	117.78	121.90
1	2A	277	C	N1-C2-O2	5.87	122.42	118.90
32	1a	1285	A	P-O3'-C3'	5.82	126.69	119.70
1	1A	2137	C	C6-N1-C2	-5.76	118.00	120.30
1	1A	512	G	O4'-C1'-N9	5.74	112.79	108.20
32	2a	1003	G	N3-C4-C5	-5.73	125.73	128.60
32	2a	1001	A	C5-C6-N6	5.72	128.28	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1082	U	C2-N1-C1'	5.70	124.54	117.70
1	2A	2105	C	C2-N3-C4	5.57	122.69	119.90
1	2A	2185	C	N1-C2-N3	-5.50	115.35	119.20
32	2a	754	C	N1-C2-O2	5.49	122.20	118.90
32	2a	748	C	P-O3'-C3'	5.47	126.27	119.70
32	2a	992	U	P-O3'-C3'	5.45	126.25	119.70
1	2A	2103	C	C2-N3-C4	5.45	122.62	119.90
32	2a	1001	A	N1-C6-N6	-5.45	115.33	118.60
1	2A	2185	C	C5-C4-N4	5.42	123.99	120.20
32	1a	422	C	O4'-C1'-N1	5.39	112.52	108.20
1	2A	1313	U	C2-N1-C1'	5.39	124.17	117.70
32	1a	266	G	OP2-P-O3'	5.38	117.05	105.20
32	1a	1201	A	P-O3'-C3'	5.36	126.13	119.70
1	2A	2321	G	C4-N9-C1'	5.29	133.37	126.50
1	1A	847	U	C2-N1-C1'	5.28	124.04	117.70
32	2a	1158	C	C2-N1-C1'	5.22	124.54	118.80
1	2A	1100	C	C2-N3-C4	5.21	122.50	119.90
32	1a	1065	U	P-O3'-C3'	5.19	125.93	119.70
32	2a	1003	G	C2-N3-C4	5.19	114.50	111.90
32	2a	1065	U	P-O3'-C3'	5.14	125.86	119.70
1	2A	2103	C	N3-C4-N4	-5.12	114.41	118.00
32	2a	687	A	P-O3'-C3'	5.11	125.83	119.70
32	2a	1004	A	O4'-C1'-N9	5.10	112.28	108.20
32	1a	991	U	P-O3'-C3'	5.09	125.81	119.70
32	1a	422	C	C2-N1-C1'	-5.08	113.22	118.80
1	2A	2105	C	N1-C2-O2	5.08	121.94	118.90
32	1a	1036	G	C4-N9-C1'	5.06	133.08	126.50
32	2a	266	G	OP2-P-O3'	5.05	116.32	105.20
32	1a	1067	A	P-O3'-C3'	5.02	125.72	119.70

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

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	34	69
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	64
4	2E	202/206 (98%)	195 (96%)	7 (4%)	0	100	100
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	29	64
5	2F	201/210 (96%)	198 (98%)	1 (0%)	2 (1%)	15	49
6	1G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	25	59
6	2G	179/182 (98%)	168 (94%)	9 (5%)	2 (1%)	14	46
7	1H	172/180 (96%)	166 (96%)	5 (3%)	1 (1%)	25	59
7	2H	171/180 (95%)	168 (98%)	3 (2%)	0	100	100
8	1I	145/148 (98%)	134 (92%)	10 (7%)	1 (1%)	22	57
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%)	22	57
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	57
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%)	17	52
14	2S	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	1T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	10	39
26	24	67/71 (94%)	55 (82%)	10 (15%)	2 (3%)	4	23
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	5	26
33	2b	229/256 (90%)	205 (90%)	13 (6%)	11 (5%)	2	14
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%)	15	49
35	2d	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29	64
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
38	1g	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
38	2g	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	22	57
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%)	19	54
40	2i	124/128 (97%)	114 (92%)	8 (6%)	2 (2%)	9	37
41	1j	95/105 (90%)	84 (88%)	9 (10%)	2 (2%)	7	30
41	2j	94/105 (90%)	87 (93%)	6 (6%)	1 (1%)	14	46
42	1k	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	8	34
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%)	17	52
44	2m	112/126 (89%)	109 (97%)	2 (2%)	1 (1%)	17	52
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
48	1q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	15	49
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%)	14	46
51	2t	96/106 (91%)	91 (95%)	4 (4%)	1 (1%)	15	49
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%)	34	69

All (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
33	1b	232	PRO
42	1k	118	GLY
48	1q	68	ARG
33	2b	16	HIS
33	2b	53	ARG
33	2b	54	THR
33	2b	232	PRO
44	2m	67	GLU
8	1I	73	GLU
14	1S	59	LYS
35	1d	178	VAL
35	1d	179	GLU
41	1j	79	ARG
26	24	55	ARG
26	24	60	GLN
33	2b	17	PHE
33	2b	21	ARG

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Mol	Chain	Res	Type
33	2b	123	ALA
33	2b	126	GLU
40	2i	12	GLU
41	2j	79	ARG
4	1E	52	LEU
3	2D	125	ILE
5	2F	130	ALA
6	2G	47	LYS
6	2G	81	LYS
38	2g	8	GLU
6	1G	47	LYS
33	1b	95	GLN
44	1m	67	GLU
5	2F	21	ALA
33	2b	8	LYS
33	2b	95	GLN
7	1H	92	ILE
11	1P	36	LYS
51	1t	100	ILE
33	2b	20	GLU
51	2t	100	ILE
33	1b	127	ILE
40	1i	56	LEU
35	2d	166	LYS
40	2i	44	VAL
41	1j	77	PRO
11	2P	122	PRO
42	1k	105	VAL

### 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%)	24	56
3	2D	215/218 (99%)	202 (94%)	13 (6%)	19	49
4	1E	164/166 (99%)	156 (95%)	8 (5%)	25	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	157 (96%)	7 (4%)	29	62
5	1F	160/166 (96%)	152 (95%)	8 (5%)	24	57
5	2F	159/166 (96%)	151 (95%)	8 (5%)	24	57
6	1G	144/156 (92%)	141 (98%)	3 (2%)	53	79
6	2G	142/156 (91%)	139 (98%)	3 (2%)	53	79
7	1H	144/148 (97%)	139 (96%)	5 (4%)	36	68
7	2H	143/148 (97%)	138 (96%)	5 (4%)	36	68
8	1I	111/124 (90%)	106 (96%)	5 (4%)	27	60
8	2I	108/124 (87%)	105 (97%)	3 (3%)	43	73
9	1N	119/119 (100%)	117 (98%)	2 (2%)	60	83
9	2N	118/119 (99%)	116 (98%)	2 (2%)	60	83
10	1O	100/100 (100%)	99 (99%)	1 (1%)	76	90
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	71
11	1P	115/116 (99%)	112 (97%)	3 (3%)	46	74
11	2P	115/116 (99%)	114 (99%)	1 (1%)	78	91
12	1Q	111/111 (100%)	110 (99%)	1 (1%)	78	91
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	59	82
13	1R	101/101 (100%)	94 (93%)	7 (7%)	15	45
13	2R	101/101 (100%)	94 (93%)	7 (7%)	15	45
14	1S	87/88 (99%)	85 (98%)	2 (2%)	50	77
14	2S	85/88 (97%)	84 (99%)	1 (1%)	71	88
15	1T	115/127 (91%)	111 (96%)	4 (4%)	36	68
15	2T	113/127 (89%)	111 (98%)	2 (2%)	59	82
16	1U	93/94 (99%)	92 (99%)	1 (1%)	73	89
16	2U	93/94 (99%)	91 (98%)	2 (2%)	52	78
17	1V	81/82 (99%)	78 (96%)	3 (4%)	34	66
17	2V	80/82 (98%)	77 (96%)	3 (4%)	33	66
18	1W	90/92 (98%)	88 (98%)	2 (2%)	52	78
18	2W	90/92 (98%)	87 (97%)	3 (3%)	38	69
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	86/91 (94%)	84 (98%)	2 (2%)	50	77
20	2Y	86/91 (94%)	85 (99%)	1 (1%)	71	88
21	1Z	169/179 (94%)	160 (95%)	9 (5%)	22	54
21	2Z	165/179 (92%)	164 (99%)	1 (1%)	86	94
22	10	61/67 (91%)	59 (97%)	2 (3%)	38	69
22	20	61/67 (91%)	60 (98%)	1 (2%)	62	84
23	11	79/83 (95%)	78 (99%)	1 (1%)	69	87
23	21	81/83 (98%)	79 (98%)	2 (2%)	47	75
24	12	65/67 (97%)	64 (98%)	1 (2%)	65	85
24	22	66/67 (98%)	65 (98%)	1 (2%)	65	85
25	13	51/52 (98%)	47 (92%)	4 (8%)	12	40
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	65
26	14	58/63 (92%)	57 (98%)	1 (2%)	60	83
26	24	54/63 (86%)	50 (93%)	4 (7%)	13	42
27	15	51/52 (98%)	47 (92%)	4 (8%)	12	40
27	25	50/52 (96%)	46 (92%)	4 (8%)	12	40
28	16	51/52 (98%)	47 (92%)	4 (8%)	12	40
28	26	50/52 (96%)	47 (94%)	3 (6%)	19	49
29	17	41/42 (98%)	39 (95%)	2 (5%)	25	57
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	43
30	18	54/55 (98%)	53 (98%)	1 (2%)	57	81
30	28	54/55 (98%)	52 (96%)	2 (4%)	34	66
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	72
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	72
33	1b	191/220 (87%)	183 (96%)	8 (4%)	30	62
33	2b	187/220 (85%)	183 (98%)	4 (2%)	53	79
34	1c	144/188 (77%)	139 (96%)	5 (4%)	36	68
34	2c	140/188 (74%)	137 (98%)	3 (2%)	53	79
35	1d	171/181 (94%)	160 (94%)	11 (6%)	17	48
35	2d	172/181 (95%)	169 (98%)	3 (2%)	60	83
36	1e	114/123 (93%)	111 (97%)	3 (3%)	46	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	114/123 (93%)	111 (97%)	3 (3%)	46	74
37	1f	85/90 (94%)	85 (100%)	0	100	100
37	2f	85/90 (94%)	83 (98%)	2 (2%)	49	76
38	1g	120/127 (94%)	119 (99%)	1 (1%)	81	92
38	2g	119/127 (94%)	118 (99%)	1 (1%)	81	92
39	1h	116/119 (98%)	111 (96%)	5 (4%)	29	62
39	2h	114/119 (96%)	110 (96%)	4 (4%)	36	68
40	1i	91/99 (92%)	88 (97%)	3 (3%)	38	69
40	2i	88/99 (89%)	86 (98%)	2 (2%)	50	77
41	1j	68/92 (74%)	67 (98%)	1 (2%)	65	85
41	2j	68/92 (74%)	65 (96%)	3 (4%)	28	61
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%)	76	90
43	2l	96/108 (89%)	95 (99%)	1 (1%)	76	90
44	1m	90/101 (89%)	89 (99%)	1 (1%)	73	89
44	2m	87/101 (86%)	86 (99%)	1 (1%)	73	89
45	1n	49/50 (98%)	47 (96%)	2 (4%)	30	64
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%)	20	51
47	2p	68/74 (92%)	65 (96%)	3 (4%)	28	61
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	93 (99%)	1 (1%)	73	89
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%)	28	61
50	2s	67/80 (84%)	62 (92%)	5 (8%)	13	42
51	1t	71/82 (87%)	69 (97%)	2 (3%)	43	73
51	2t	70/82 (85%)	67 (96%)	3 (4%)	29	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	41	71

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	10	THR
3	1D	69	ARG
3	1D	103	ARG
3	1D	115	GLN
3	1D	142	VAL
3	1D	155	LEU
3	1D	193	VAL
3	1D	212	SER
3	1D	229	VAL
3	1D	237	GLU
3	1D	242	ARG
4	1E	7	VAL
4	1E	21	VAL
4	1E	33	VAL
4	1E	49	LEU
4	1E	75	VAL
4	1E	116	VAL
4	1E	144	ARG
4	1E	184	VAL
5	1F	23	ASP
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	100	THR
5	1F	110	LEU
5	1F	125	LEU
5	1F	197	ASP
6	1G	5	VAL
6	1G	53	LEU
6	1G	167	GLU
7	1H	23	ARG
7	1H	45	VAL
7	1H	71	LEU
7	1H	105	LEU

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Mol	Chain	Res	Type
7	1H	139	GLN
8	1I	12	LEU
8	1I	38	LEU
8	1I	75	LEU
8	1I	92	VAL
8	1I	140	LEU
9	1N	8	GLN
9	1N	34	LEU
10	1O	24	VAL
11	1P	83	VAL
11	1P	112	LEU
11	1P	126	VAL
12	1Q	109	VAL
13	1R	6	SER
13	1R	17	ARG
13	1R	29	LEU
13	1R	36	THR
13	1R	44	LEU
13	1R	65	LEU
13	1R	67	LEU
14	1S	49	VAL
14	1S	54	LEU
15	1T	15	VAL
15	1T	49	VAL
15	1T	74	ARG
15	1T	96	ARG
16	1U	95	LEU
17	1V	51	VAL
17	1V	61	VAL
17	1V	79	VAL
18	1W	17	VAL
18	1W	107	LEU
20	1Y	72	VAL
20	1Y	90	LEU
21	1Z	58	VAL
21	1Z	61	LEU
21	1Z	76	LEU
21	1Z	94	GLU
21	1Z	102	LEU
21	1Z	107	THR
21	1Z	150	LEU
21	1Z	161	VAL

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Mol	Chain	Res	Type
21	1Z	203	GLU
22	10	39	ARG
22	10	63	VAL
23	11	95	LEU
24	12	53	LEU
25	13	6	VAL
25	13	8	LEU
25	13	40	THR
25	13	60	GLU
26	14	61	ARG
27	15	6	VAL
27	15	16	ARG
27	15	26	THR
27	15	29	THR
28	16	5	VAL
28	16	13	CYS
28	16	14	THR
28	16	48	VAL
29	17	1	MET
29	17	24	THR
30	18	31	HIS
31	19	26	ILE
33	1b	9	GLU
33	1b	10	LEU
33	1b	19	HIS
33	1b	51	LEU
33	1b	112	VAL
33	1b	122	PHE
33	1b	157	ARG
33	1b	185	ILE
34	1c	64	VAL
34	1c	89	GLU
34	1c	98	ASN
34	1c	132	ARG
34	1c	191	THR
35	1d	8	VAL
35	1d	59	ARG
35	1d	76	ARG
35	1d	135	LEU
35	1d	150	GLU
35	1d	158	ILE
35	1d	168	ARG

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Mol	Chain	Res	Type
35	1d	178	VAL
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
36	1e	41	VAL
36	1e	75	THR
36	1e	78	HIS
38	1g	111	ARG
39	1h	14	ARG
39	1h	25	ASP
39	1h	51	VAL
39	1h	52	ASP
39	1h	104	ARG
40	1i	10	ARG
40	1i	28	VAL
40	1i	64	THR
41	1j	38	ILE
43	1l	18	VAL
44	1m	70	LEU
45	1n	13	THR
45	1n	33	VAL
47	1p	19	ILE
47	1p	42	ARG
47	1p	62	VAL
47	1p	67	THR
50	1s	28	LYS
50	1s	39	THR
50	1s	79	THR
51	1t	62	LEU
51	1t	100	ILE
3	2D	25	THR
3	2D	27	THR
3	2D	69	ARG
3	2D	99	ASP
3	2D	111	LEU
3	2D	141	VAL
3	2D	142	VAL
3	2D	154	LYS
3	2D	164	GLN
3	2D	183	ARG
3	2D	193	VAL
3	2D	229	VAL

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Mol	Chain	Res	Type
3	2D	276	LYS
4	2E	1	MET
4	2E	7	VAL
4	2E	9	VAL
4	2E	21	VAL
4	2E	33	VAL
4	2E	75	VAL
4	2E	116	VAL
5	2F	20	LEU
5	2F	27	GLU
5	2F	53	THR
5	2F	57	VAL
5	2F	70	THR
5	2F	74	ARG
5	2F	175	THR
5	2F	197	ASP
6	2G	3	LEU
6	2G	5	VAL
6	2G	139	LEU
7	2H	33	LEU
7	2H	71	LEU
7	2H	88	LEU
7	2H	129	THR
7	2H	139	GLN
8	2I	20	ASP
8	2I	38	LEU
8	2I	92	VAL
9	2N	34	LEU
9	2N	99	LEU
10	2O	24	VAL
10	2O	32	TYR
10	2O	53	LYS
11	2P	112	LEU
12	2Q	6	ARG
12	2Q	109	VAL
13	2R	6	SER
13	2R	18	LEU
13	2R	29	LEU
13	2R	44	LEU
13	2R	65	LEU
13	2R	67	LEU
13	2R	79	LEU

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Mol	Chain	Res	Type
14	2S	54	LEU
15	2T	49	VAL
15	2T	95	ARG
16	2U	59	ARG
16	2U	95	LEU
17	2V	51	VAL
17	2V	61	VAL
17	2V	79	VAL
18	2W	17	VAL
18	2W	60	ASN
18	2W	107	LEU
19	2X	35	THR
19	2X	65	ARG
20	2Y	72	VAL
21	2Z	107	THR
22	20	63	VAL
23	21	4	VAL
23	21	95	LEU
24	22	53	LEU
25	23	6	VAL
25	23	40	THR
26	24	38	LYS
26	24	44	THR
26	24	46	GLN
26	24	50	VAL
27	25	6	VAL
27	25	16	ARG
27	25	29	THR
27	25	58	LEU
28	26	5	VAL
28	26	34	LEU
28	26	48	VAL
29	27	4	THR
29	27	35	ARG
29	27	43	THR
30	28	6	THR
30	28	31	HIS
31	29	26	ILE
33	2b	24	TRP
33	2b	96	ARG
33	2b	187	LEU
33	2b	222	ILE

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Mol	Chain	Res	Type
34	2c	82	GLU
34	2c	152	ILE
34	2c	191	THR
35	2d	107	ARG
35	2d	135	LEU
35	2d	188	LEU
36	2e	41	VAL
36	2e	72	GLN
36	2e	75	THR
37	2f	16	GLN
37	2f	72	VAL
38	2g	51	GLN
39	2h	25	ASP
39	2h	60	ARG
39	2h	84	ARG
39	2h	112	LEU
40	2i	20	ARG
40	2i	102	LEU
41	2j	33	GLN
41	2j	38	ILE
41	2j	96	ILE
43	2l	18	VAL
44	2m	70	LEU
47	2p	28	ARG
47	2p	62	VAL
47	2p	67	THR
48	2q	93	GLN
50	2s	16	LEU
50	2s	39	THR
50	2s	67	VAL
50	2s	77	THR
50	2s	79	THR
51	2t	45	GLN
51	2t	62	LEU
51	2t	100	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
4	1E	137	HIS
4	1E	143	ASN

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Mol	Chain	Res	Type
4	1E	180	ASN
5	1F	75	HIS
10	1O	5	GLN
13	1R	24	GLN
15	1T	58	ASN
16	1U	94	ASN
17	1V	80	GLN
19	1X	31	HIS
20	1Y	92	ASN
21	1Z	73	GLN
21	1Z	132	ASN
21	1Z	151	HIS
23	11	16	ASN
23	11	56	GLN
24	12	65	ASN
30	18	35	GLN
33	1b	78	GLN
33	1b	113	HIS
33	1b	212	GLN
34	1c	176	HIS
35	1d	129	ASN
35	1d	160	GLN
35	1d	161	ASN
38	1g	28	ASN
38	1g	148	ASN
38	1g	153	HIS
40	1i	3	GLN
40	1i	34	ASN
40	1i	87	GLN
41	1j	13	HIS
41	1j	84	GLN
42	1k	93	GLN
44	1m	77	ASN
46	1o	62	GLN
47	1p	16	HIS
48	1q	16	GLN
48	1q	26	GLN
50	1s	23	ASN
3	2D	45	ASN
3	2D	87	ASN
3	2D	126	GLN
3	2D	166	GLN

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Mol	Chain	Res	Type
4	2E	48	GLN
4	2E	143	ASN
4	2E	180	ASN
11	2P	35	HIS
13	2R	13	HIS
13	2R	24	GLN
15	2T	58	ASN
16	2U	94	ASN
17	2V	64	HIS
19	2X	31	HIS
19	2X	82	GLN
20	2Y	57	GLN
21	2Z	55	HIS
21	2Z	73	GLN
21	2Z	132	ASN
21	2Z	151	HIS
23	21	16	ASN
23	21	56	GLN
24	22	65	ASN
30	28	35	GLN
33	2b	40	HIS
34	2c	6	HIS
34	2c	69	HIS
35	2d	123	HIS
35	2d	129	ASN
36	2e	72	GLN
36	2e	78	HIS
38	2g	13	GLN
38	2g	28	ASN
40	2i	3	GLN
41	2j	62	HIS
41	2j	69	ASN
42	2k	93	GLN
44	2m	77	ASN
47	2p	16	HIS
50	2s	23	ASN
50	2s	47	HIS
50	2s	83	HIS
51	2t	26	ASN

### 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%)

All (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
1	1A	61	G
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	95	G
1	1A	102	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	131	G
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	250	G
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U

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Mol	Chain	Res	Type
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	330	A
1	1A	333	G
1	1A	352	G
1	1A	353	G
1	1A	357	A
1	1A	360	G
1	1A	363	G
1	1A	363(A)	A
1	1A	363(B)	G
1	1A	363(C)	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	421	U
1	1A	428	A
1	1A	448	U
1	1A	454	A
1	1A	455	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	484	C
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G

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Mol	Chain	Res	Type
1	1A	573	G
1	1A	575	A
1	1A	587	C
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	615	G
1	1A	619	G
1	1A	620	G
1	1A	627	A
1	1A	637	A
1	1A	644	A
1	1A	645	C
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	652(U)	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	738	G
1	1A	764	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	792	G
1	1A	793	A
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	829	A
1	1A	831	G
1	1A	859	G
1	1A	866	A
1	1A	876	C
1	1A	878	A

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Mol	Chain	Res	Type
1	1A	879	G
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	897	C
1	1A	910	A
1	1A	914	C
1	1A	915	C
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	975(A)	G
1	1A	980	A
1	1A	983	A
1	1A	990	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1025	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1039	G
1	1A	1042	G
1	1A	1043	C
1	1A	1046	A
1	1A	1047	G
1	1A	1053	C
1	1A	1054	A
1	1A	1060	U
1	1A	1061	U
1	1A	1062	G
1	1A	1063	G
1	1A	1064	C
1	1A	1065	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1068	G
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1078	U
1	1A	1079	C
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1093	G
1	1A	1096	A
1	1A	1105	U
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1139	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1203	G
1	1A	1204	A
1	1A	1211	U
1	1A	1218	C
1	1A	1249	U
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U

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Mol	Chain	Res	Type
1	1A	1281	G
1	1A	1300	U
1	1A	1301	A
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1452	A
1	1A	1453	U
1	1A	1455	G
1	1A	1467	C
1	1A	1471	A
1	1A	1478	G
1	1A	1482	G
1	1A	1506	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1542	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A

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Mol	Chain	Res	Type
1	1A	1648	C
1	1A	1674	G
1	1A	1700	A
1	1A	1701	A
1	1A	1721	G
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1747	G
1	1A	1756	G
1	1A	1758	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1769	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1784	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1829	A
1	1A	1847	A
1	1A	1858	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1914	C
1	1A	1927	A
1	1A	1929	G
1	1A	1930	G
1	1A	1936	A
1	1A	1938	A
1	1A	1952	A
1	1A	1955	U
1	1A	1963	U

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Mol	Chain	Res	Type
1	1A	1964	G
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2021	C
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2052	G
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2093	G
1	1A	2103	C
1	1A	2104	G
1	1A	2107	C
1	1A	2108	C
1	1A	2110	G
1	1A	2114	A
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2120	G
1	1A	2123	G
1	1A	2125	G
1	1A	2127	G
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2135	A
1	1A	2137	C

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Mol	Chain	Res	Type
1	1A	2139	C
1	1A	2142	C
1	1A	2146	C
1	1A	2147	G
1	1A	2152	G
1	1A	2158	A
1	1A	2159	G
1	1A	2172	U
1	1A	2173	A
1	1A	2180	U
1	1A	2183	C
1	1A	2185	C
1	1A	2187	G
1	1A	2191	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2278	A
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2314	C
1	1A	2315	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G

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Mol	Chain	Res	Type
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2409	G
1	1A	2410	G
1	1A	2414	G
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2469	A
1	1A	2476	A
1	1A	2477	C
1	1A	2491	U
1	1A	2494	G
1	1A	2498	C
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2525	G
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2564	A
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2586	C
1	1A	2596	U
1	1A	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2612	C

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Mol	Chain	Res	Type
1	1A	2629	A
1	1A	2630	G
1	1A	2632	A
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2808	U
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2834	G
1	1A	2835	A
1	1A	2849	U
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	13	A
2	1B	15	A
2	1B	33	G
2	1B	42	C
2	1B	50	G
2	1B	52	A
2	1B	56	G
2	1B	73	A
2	1B	84	C

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Mol	Chain	Res	Type
2	1B	85	G
2	1B	106	G
2	1B	110	G
32	1a	6	G
32	1a	9	G
32	1a	14	U
32	1a	32	A
32	1a	39	G
32	1a	43	C
32	1a	44	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	79	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	151	A
32	1a	156	G
32	1a	159	G
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	237	C
32	1a	245	C
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	279	A

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Mol	Chain	Res	Type
32	1a	281	G
32	1a	289	G
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	388	G
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	431	A
32	1a	439	A
32	1a	452	A
32	1a	453	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	475	G
32	1a	482	A
32	1a	484	G
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	531	U

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Mol	Chain	Res	Type
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	563	A
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C
32	1a	607	A
32	1a	618	C
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	653	A
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	755	G
32	1a	760	G
32	1a	766	A
32	1a	774	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	802	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	818	G
32	1a	821	G
32	1a	827	U
32	1a	828	A
32	1a	829	G
32	1a	836	G
32	1a	840	C

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Mol	Chain	Res	Type
32	1a	841	U
32	1a	848	C
32	1a	859	A
32	1a	872	A
32	1a	885	G
32	1a	889	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	931	C
32	1a	934	C
32	1a	954	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	989	C
32	1a	991	U
32	1a	992	U
32	1a	993	G
32	1a	998	G
32	1a	999	C
32	1a	1001	A
32	1a	1004	A
32	1a	1005	A
32	1a	1017	G
32	1a	1020	U
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C

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Mol	Chain	Res	Type
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(D)	A
32	1a	1031	G
32	1a	1032	G
32	1a	1033	G
32	1a	1035	A
32	1a	1036	G
32	1a	1037	C
32	1a	1038	C
32	1a	1043	C
32	1a	1044	A
32	1a	1053	G
32	1a	1054	C
32	1a	1056	U
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1099	G
32	1a	1100	C
32	1a	1101	A
32	1a	1108	G
32	1a	1113	C
32	1a	1122	U
32	1a	1124	G
32	1a	1125	U
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1135	U
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1152	A
32	1a	1154	G
32	1a	1157	A
32	1a	1159	U
32	1a	1160	G
32	1a	1161	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1166	G
32	1a	1182	G
32	1a	1183	A
32	1a	1184	G
32	1a	1185	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1224	G
32	1a	1227	A
32	1a	1230	C
32	1a	1238	A
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1261	A
32	1a	1270	C
32	1a	1278	U
32	1a	1280	A
32	1a	1281	U
32	1a	1282	C
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1301	U
32	1a	1302	U
32	1a	1305	G
32	1a	1310	G
32	1a	1312	G
32	1a	1316	G
32	1a	1317	C
32	1a	1320	C
32	1a	1322	C
32	1a	1326	C
32	1a	1332	A

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Mol	Chain	Res	Type
32	1a	1341	U
32	1a	1347	G
32	1a	1353	G
32	1a	1357	A
32	1a	1363	C
32	1a	1370	G
32	1a	1378	C
32	1a	1386	G
32	1a	1397	C
32	1a	1398	A
32	1a	1406	U
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1493	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
1	2A	9	U
1	2A	10	G
1	2A	12	U
1	2A	14	A
1	2A	15	G
1	2A	23	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	118	A
1	2A	120	U
1	2A	125	G
1	2A	131	G

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Mol	Chain	Res	Type
1	2A	141	A
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	199	A
1	2A	201	C
1	2A	205	G
1	2A	213	A
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	271(P)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	276	A
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	317	G
1	2A	322	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	345	A
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	364	C
1	2A	386	G
1	2A	391	G

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Mol	Chain	Res	Type
1	2A	396	G
1	2A	405	U
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	496	G
1	2A	501	A
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	556	G
1	2A	563	G
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	592	G
1	2A	593	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	619	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(A)	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(E)	G
1	2A	669	G

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Mol	Chain	Res	Type
1	2A	686	G
1	2A	726	G
1	2A	730	C
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	793	A
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	829	A
1	2A	831	G
1	2A	859	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	892	G
1	2A	893	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	907	U
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	926	A
1	2A	932	G
1	2A	936	C
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G

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Mol	Chain	Res	Type
1	2A	961	C
1	2A	962	G
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	989	G
1	2A	996	A
1	2A	999	U
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1023	U
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1034	G
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1058	G
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
1	2A	1065	U
1	2A	1067	A
1	2A	1068	G
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U

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Mol	Chain	Res	Type
1	2A	1079	C
1	2A	1080	C
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1089	G
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1094	U
1	2A	1102	C
1	2A	1105	U
1	2A	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1129	A
1	2A	1130	U
1	2A	1131	G
1	2A	1135	C
1	2A	1136	G
1	2A	1142(A)	A
1	2A	1170	G
1	2A	1171	G
1	2A	1188	U
1	2A	1211	U
1	2A	1237	A
1	2A	1244	G
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1274	A
1	2A	1300	U
1	2A	1301	A
1	2A	1313	U

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Mol	Chain	Res	Type
1	2A	1314	C
1	2A	1319	G
1	2A	1342	A
1	2A	1348	G
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1380	G
1	2A	1383	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1509(B)	A
1	2A	1542	A
1	2A	1543	C
1	2A	1558	A
1	2A	1560	G
1	2A	1566	A
1	2A	1569	A

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Mol	Chain	Res	Type
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1602	U
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1631(A)	A
1	2A	1640	C
1	2A	1648	C
1	2A	1667	G
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1722	A
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1774	C
1	2A	1780	A
1	2A	1781	C
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1861	G
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A

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Mol	Chain	Res	Type
1	2A	1914	C
1	2A	1917	PSU
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2052	G
1	2A	2055	C
1	2A	2056	G
1	2A	2058	A
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2093	G
1	2A	2095	C
1	2A	2099	U
1	2A	2100	G
1	2A	2101	G
1	2A	2103	C
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2111	C
1	2A	2112	G

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Mol	Chain	Res	Type
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2121	G
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2138	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2159	G
1	2A	2161	C
1	2A	2163	C
1	2A	2164	C
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2186	G
1	2A	2189	U
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2249	U
1	2A	2275	C

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Mol	Chain	Res	Type
1	2A	2279	G
1	2A	2282	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2292	C
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2311	A
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2343	C
1	2A	2345	G
1	2A	2347	C
1	2A	2348	U
1	2A	2350	C
1	2A	2366	A
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2406	U
1	2A	2409	G
1	2A	2410	G
1	2A	2414	G
1	2A	2423	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2440	C
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A

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Mol	Chain	Res	Type
1	2A	2459	A
1	2A	2474	C
1	2A	2476	A
1	2A	2480	C
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
1	2A	2492	U
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2517	C
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2532	G
1	2A	2549	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2646	C
1	2A	2654	A
1	2A	2663	G
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G

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Mol	Chain	Res	Type
1	2A	2726	U
1	2A	2733	A
1	2A	2748	A
1	2A	2757	A
1	2A	2759	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2769	C
1	2A	2778	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2861	G
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	15	A
2	2B	28	C
2	2B	31	C
2	2B	35	U
2	2B	36	C
2	2B	45	A
2	2B	51	G
2	2B	56	G
2	2B	73	A
2	2B	85	G
2	2B	89	G
2	2B	110	G
2	2B	116	G
2	2B	120	A
32	2a	5	U
32	2a	6	G
32	2a	9	G

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Mol	Chain	Res	Type
32	2a	14	U
32	2a	32	A
32	2a	39	G
32	2a	43	C
32	2a	44	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	78	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	151	A
32	2a	156	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(F)	U
32	2a	189(G)	G
32	2a	195	A
32	2a	197	A
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	237	C
32	2a	245	C
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	279	A
32	2a	281	G
32	2a	289	G
32	2a	301	G
32	2a	321	A
32	2a	328	C
32	2a	332	G

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Mol	Chain	Res	Type
32	2a	348	G
32	2a	349	A
32	2a	350	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	388	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	422	C
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	431	A
32	2a	439	A
32	2a	452	A
32	2a	453	A
32	2a	458	C
32	2a	461	A
32	2a	470	C
32	2a	475	G
32	2a	477	A
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	531	U
32	2a	532	A
32	2a	533	A

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Mol	Chain	Res	Type
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	562	C
32	2a	563	A
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	592	G
32	2a	596	C
32	2a	607	A
32	2a	618	C
32	2a	619	U
32	2a	630	G
32	2a	632	A
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	760	G
32	2a	766	A
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	802	A
32	2a	815	A
32	2a	816	A
32	2a	817	C
32	2a	818	G
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	829	G
32	2a	836	G
32	2a	840	C

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Mol	Chain	Res	Type
32	2a	841	U
32	2a	848	C
32	2a	859	A
32	2a	872	A
32	2a	885	G
32	2a	889	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	954	G
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	989	C
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	999	C
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1017	G
32	2a	1020	U
32	2a	1023	G
32	2a	1024	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1030(B)	C

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Mol	Chain	Res	Type
32	2a	1030(D)	A
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A
32	2a	1038	C
32	2a	1043	C
32	2a	1044	A
32	2a	1053	G
32	2a	1054	C
32	2a	1056	U
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1099	G
32	2a	1100	C
32	2a	1101	A
32	2a	1108	G
32	2a	1113	C
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1130	A
32	2a	1132	C
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1139	G
32	2a	1147	C
32	2a	1152	A
32	2a	1154	G
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1161	C
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1185	G

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Mol	Chain	Res	Type
32	2a	1196	U
32	2a	1197	G
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1224	G
32	2a	1230	C
32	2a	1238	A
32	2a	1248	A
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1290	G
32	2a	1299	A
32	2a	1300	G
32	2a	1301	U
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1310	G
32	2a	1312	G
32	2a	1316	G
32	2a	1317	C
32	2a	1320	C
32	2a	1322	C
32	2a	1326	C
32	2a	1332	A
32	2a	1341	U
32	2a	1347	G
32	2a	1353	G
32	2a	1357	A
32	2a	1363	C
32	2a	1370	G
32	2a	1386	G
32	2a	1397	C

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Mol	Chain	Res	Type
32	2a	1398	A
32	2a	1406	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1492	A
32	2a	1493	A
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	266	G
1	1A	278	A
1	1A	827	U
1	1A	840	C
1	1A	888	C
1	1A	895	U
1	1A	1065	U
1	1A	1067	A
1	1A	1176	G
1	1A	1210	A
1	1A	1442	G
1	1A	2126	A
1	1A	2430	A
1	1A	2689	U
1	2A	266	G
1	2A	271(M)	G
1	2A	752	A

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Mol	Chain	Res	Type
1	2A	827	U
1	2A	840	C
1	2A	900	A
1	2A	1053	C
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1210	A
1	2A	1273	U
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2288	A
1	2A	2321	G
1	2A	2602	A
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
32	MA6	2a	1519	32	19,26,27	0.96	1 (5%)	18,38,41	1.92	6 (33%)
1	PSU	2A	2605	1	17,21,22	1.61	2 (11%)	20,30,33	3.17	6 (30%)
32	M2G	2a	966	32	20,27,28	1.45	3 (15%)	22,40,43	2.19	5 (22%)
32	UR3	2a	1498	32	14,22,23	0.81	1 (7%)	15,32,35	0.72	1 (6%)
32	5MC	1a	1404	32	15,22,23	1.33	1 (6%)	19,32,35	1.33	3 (15%)
32	5MC	1a	967	32	15,22,23	1.27	1 (6%)	19,32,35	1.42	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	2MG	1a	1207	32	19,26,27	1.30	2 (10%)	21,38,41	2.32	9 (42%)
32	PSU	2a	516	32,53	17,21,22	1.59	3 (17%)	20,30,33	3.06	6 (30%)
43	0TD	2l	92	43	4,9,10	3.09	1 (25%)	3,11,13	5.10	1 (33%)
32	5MC	2a	1404	32	15,22,23	1.37	1 (6%)	19,32,35	1.24	3 (15%)
1	5MC	1A	1962	1	15,22,23	1.34	1 (6%)	19,32,35	1.32	3 (15%)
32	MA6	1a	1518	32	19,26,27	0.96	1 (5%)	18,38,41	1.70	6 (33%)
1	2MA	1A	2503	1,53	17,25,26	1.29	2 (11%)	19,37,40	2.16	3 (15%)
1	4OC	1A	1920	1	15,22,24	0.66	0	17,31,35	1.31	2 (11%)
32	MA6	1a	1519	32	19,26,27	1.01	1 (5%)	18,38,41	1.67	5 (27%)
1	2MU	1A	2552	1,53	14,22,24	0.88	0	14,31,36	0.79	1 (7%)
1	OMG	1A	2251	1	18,26,27	1.15	2 (11%)	20,38,41	2.08	6 (30%)
1	2MA	2A	2503	1,53	17,25,26	1.41	2 (11%)	19,37,40	2.10	3 (15%)
32	4OC	2a	1402	32	16,23,24	0.61	0	17,32,35	1.19	1 (5%)
32	7MG	2a	527	32	22,26,27	1.73	4 (18%)	28,39,42	2.76	9 (32%)
32	5MC	2a	1407	32	15,22,23	1.29	1 (6%)	19,32,35	1.36	3 (15%)
32	5MC	1a	1407	32	15,22,23	1.34	1 (6%)	19,32,35	1.38	2 (10%)
32	5MC	2a	967	32	15,22,23	1.36	1 (6%)	19,32,35	1.32	3 (15%)
1	5MU	2A	1915	1	15,22,23	1.05	1 (6%)	16,32,35	2.06	1 (6%)
32	5MC	2a	1400	32	15,22,23	1.35	1 (6%)	19,32,35	1.34	3 (15%)
32	M2G	1a	966	32	20,27,28	1.46	3 (15%)	22,40,43	2.19	5 (22%)
32	4OC	1a	1402	32	16,23,24	0.60	0	17,32,35	1.14	2 (11%)
1	PSU	1A	2605	1	17,21,22	1.58	4 (23%)	20,30,33	3.18	6 (30%)
1	OMG	2A	2251	1,53	18,26,27	1.20	2 (11%)	20,38,41	2.13	6 (30%)
1	PSU	2A	1917	1	17,21,22	1.57	2 (11%)	20,30,33	3.13	6 (30%)
1	5MU	1A	1939	1	15,22,23	1.11	2 (13%)	16,32,35	1.86	2 (12%)
1	PSU	1A	1917	1,53	17,21,22	1.51	2 (11%)	20,30,33	3.09	6 (30%)
1	2MU	2A	2552	1,53	14,22,24	0.92	0	14,31,36	0.79	0
1	5MC	2A	1962	1	15,22,23	1.25	1 (6%)	19,32,35	1.35	3 (15%)
1	PSU	2A	1911	1	17,21,22	1.53	2 (11%)	20,30,33	3.06	6 (30%)
1	4OC	2A	1920	1	15,22,24	0.68	0	17,31,35	1.45	2 (11%)
32	2MG	2a	1207	32	19,26,27	1.25	2 (10%)	21,38,41	2.28	8 (38%)
43	0TD	1l	92	43	4,9,10	3.06	1 (25%)	3,11,13	5.63	1 (33%)
32	PSU	1a	516	32,53	17,21,22	1.48	2 (11%)	20,30,33	3.08	6 (30%)
1	5MU	1A	1915	1,53	15,22,23	1.06	1 (6%)	16,32,35	1.98	1 (6%)
1	5MC	2A	1942	1	15,22,23	1.31	1 (6%)	19,32,35	1.35	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	UR3	1a	1498	32	14,22,23	0.77	1 (7%)	15,32,35	0.70	0
32	MA6	2a	1518	32	19,26,27	1.00	1 (5%)	18,38,41	1.67	4 (22%)
32	5MC	1a	1400	32	15,22,23	1.35	1 (6%)	19,32,35	1.31	3 (15%)
1	5MC	1A	1942	1	15,22,23	1.30	1 (6%)	19,32,35	1.28	3 (15%)
1	PSU	1A	1911	1	17,21,22	1.47	2 (11%)	20,30,33	3.09	6 (30%)
1	5MU	2A	1939	1	15,22,23	1.11	1 (6%)	16,32,35	1.82	2 (12%)
32	7MG	1a	527	32	22,26,27	1.76	4 (18%)	28,39,42	2.73	9 (32%)

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	MA6	2a	1519	32	-	7/7/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/5/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	PSU	2a	516	32,53	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
1	5MC	1A	1962	1	-	2/5/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
1	2MA	1A	2503	1,53	-	1/3/25/26	0/3/3/3
1	4OC	1A	1920	1	-	1/7/27/30	0/2/2/2
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
1	2MU	1A	2552	1,53	-	0/7/27/28	0/2/2/2
1	OMG	1A	2251	1	-	0/5/27/28	0/3/3/3
1	2MA	2A	2503	1,53	-	3/3/25/26	0/3/3/3
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	7MG	2a	527	32	-	1/7/37/38	0/3/3/3
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,53	-	0/5/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/5/25/26	0/2/2/2
1	PSU	1A	1917	1,53	-	1/7/25/26	0/2/2/2
1	2MU	2A	2552	1,53	-	1/7/27/28	0/2/2/2
1	5MC	2A	1962	1	-	2/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/7/27/30	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
43	0TD	1l	92	43	-	3/3/12/14	-
32	PSU	1a	516	32,53	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1,53	-	0/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/5/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32	-	3/7/37/38	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-5.92	1.69	1.84
43	1l	92	0TD	CB-SB	-5.86	1.70	1.84
32	1a	527	7MG	C6-C5	4.97	1.48	1.41
32	2a	967	5MC	C5-C4	4.95	1.49	1.41
32	2a	1404	5MC	C5-C4	4.89	1.48	1.41
32	1a	1400	5MC	C5-C4	4.82	1.48	1.41
32	2a	1400	5MC	C5-C4	4.81	1.48	1.41
32	2a	527	7MG	C6-C5	4.80	1.48	1.41
32	1a	1404	5MC	C5-C4	4.77	1.48	1.41
32	1a	1407	5MC	C5-C4	4.74	1.48	1.41
1	2A	2605	PSU	C5-C1'	-4.74	1.48	1.52
1	2A	2503	2MA	C6-C5	4.72	1.48	1.41
1	1A	1962	5MC	C5-C4	4.72	1.48	1.41
1	2A	1942	5MC	C5-C4	4.64	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	967	5MC	C5-C4	4.63	1.48	1.41
1	1A	1942	5MC	C5-C4	4.63	1.48	1.41
32	2a	1407	5MC	C5-C4	4.54	1.48	1.41
32	2a	516	PSU	C5-C1'	-4.43	1.48	1.52
1	2A	1962	5MC	C5-C4	4.42	1.48	1.41
1	1A	2503	2MA	C6-C5	4.38	1.48	1.41
32	1a	1207	2MG	C6-C5	4.37	1.48	1.41
32	2a	966	M2G	C6-C5	4.36	1.48	1.41
32	2a	527	7MG	C5-C4	4.36	1.47	1.39
32	1a	966	M2G	C6-C5	4.34	1.48	1.41
32	1a	527	7MG	C5-C4	4.34	1.47	1.39
1	1A	2605	PSU	C5-C1'	-4.32	1.48	1.52
32	2a	1207	2MG	C6-C5	4.25	1.48	1.41
1	2A	1917	PSU	C5-C1'	-4.21	1.48	1.52
1	2A	1911	PSU	C5-C1'	-4.08	1.48	1.52
1	2A	2251	OMG	C6-C5	3.99	1.48	1.41
1	1A	2251	OMG	C6-C5	3.74	1.47	1.41
1	1A	1917	PSU	C5-C1'	-3.74	1.49	1.52
32	1a	516	PSU	C5-C1'	-3.64	1.49	1.52
1	1A	1917	PSU	C4-C5	3.55	1.49	1.41
1	1A	1911	PSU	C4-C5	3.53	1.49	1.41
1	1A	1911	PSU	C5-C1'	-3.53	1.49	1.52
1	2A	1939	5MU	C4-C5	3.50	1.49	1.41
32	1a	966	M2G	C2-N2	3.50	1.40	1.34
1	2A	1917	PSU	C4-C5	3.48	1.48	1.41
1	1A	1939	5MU	C4-C5	3.44	1.48	1.41
32	2a	966	M2G	C2-N2	3.44	1.40	1.34
32	1a	516	PSU	C4-C5	3.42	1.48	1.41
1	2A	1911	PSU	C4-C5	3.34	1.48	1.41
32	2a	516	PSU	C4-C5	3.32	1.48	1.41
32	1a	527	7MG	C5-N7	-3.32	1.34	1.39
32	2a	527	7MG	C5-N7	-3.31	1.34	1.39
1	2A	1915	5MU	C4-C5	3.31	1.48	1.41
1	1A	1915	5MU	C4-C5	3.25	1.48	1.41
1	1A	2605	PSU	C4-C5	3.06	1.48	1.41
1	2A	2605	PSU	C4-C5	2.89	1.47	1.41
32	2a	1518	MA6	C5-C4	2.74	1.48	1.40
32	1a	966	M2G	C5-C4	2.58	1.47	1.40
32	1a	1518	MA6	C5-C4	2.57	1.47	1.40
32	1a	1519	MA6	C5-C4	2.56	1.47	1.40
1	2A	2503	2MA	C5-C4	2.54	1.47	1.40
32	2a	966	M2G	C5-C4	2.51	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1207	2MG	C5-C4	2.48	1.47	1.40
1	2A	2251	OMG	C5-C4	2.48	1.47	1.40
32	2a	1207	2MG	C5-C4	2.47	1.47	1.40
32	2a	1519	MA6	C5-C4	2.46	1.47	1.40
1	1A	2251	OMG	C5-C4	2.44	1.47	1.40
1	1A	2605	PSU	C2-N3	-2.29	1.33	1.38
32	1a	527	7MG	C4-N9	-2.29	1.34	1.38
32	2a	1498	UR3	C4-N3	2.26	1.41	1.38
32	2a	516	PSU	O4'-C1'	-2.25	1.41	1.44
1	1A	1939	5MU	C2-N3	-2.19	1.33	1.38
1	1A	2503	2MA	C5-C4	2.18	1.46	1.40
32	1a	1498	UR3	C4-N3	2.13	1.41	1.38
32	2a	527	7MG	C4-N9	-2.08	1.34	1.38
1	1A	2605	PSU	O4'-C1'	-2.01	1.41	1.44

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-9.63	82.91	101.85
32	2a	527	7MG	N3-C4-N9	9.15	138.66	126.91
32	1a	527	7MG	N3-C4-N9	8.93	138.38	126.91
1	1A	2605	PSU	N1-C2-N3	-8.88	121.37	128.43
43	2l	92	0TD	CSB-SB-CB	-8.73	84.69	101.85
32	1a	516	PSU	N1-C2-N3	-8.50	121.67	128.43
1	1A	1911	PSU	N1-C2-N3	-8.41	121.75	128.43
1	1A	1917	PSU	N1-C2-N3	-8.40	121.76	128.43
1	2A	2605	PSU	N1-C2-N3	-8.38	121.77	128.43
1	2A	1917	PSU	N1-C2-N3	-8.24	121.88	128.43
32	2a	516	PSU	N1-C2-N3	-8.16	121.94	128.43
1	2A	1911	PSU	N1-C2-N3	-8.12	121.97	128.43
1	2A	1915	5MU	C4-N3-C2	7.58	121.54	115.14
1	1A	2503	2MA	C2-N3-C4	7.31	121.47	115.52
1	1A	1915	5MU	C4-N3-C2	7.23	121.25	115.14
1	2A	2503	2MA	C2-N3-C4	6.96	121.18	115.52
1	2A	2605	PSU	C4-N3-C2	6.83	120.91	115.14
1	1A	1911	PSU	C4-N3-C2	6.81	120.89	115.14
32	1a	516	PSU	C4-N3-C2	6.77	120.86	115.14
1	1A	1917	PSU	C4-N3-C2	6.73	120.83	115.14
1	2A	1917	PSU	C4-N3-C2	6.66	120.76	115.14
32	2a	516	PSU	C4-N3-C2	6.61	120.72	115.14
1	1A	2605	PSU	C4-N3-C2	6.52	120.65	115.14
1	2A	1911	PSU	C4-N3-C2	6.47	120.61	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1939	5MU	C4-N3-C2	6.14	120.33	115.14
1	1A	1939	5MU	C4-N3-C2	5.63	119.90	115.14
32	2a	516	PSU	C5-C4-N3	-5.56	118.20	125.36
1	2A	2605	PSU	C5-C4-N3	-5.50	118.27	125.36
1	2A	1917	PSU	C5-C4-N3	-5.45	118.34	125.36
32	1a	527	7MG	N7-C8-N9	-5.43	95.62	103.38
32	2a	527	7MG	N7-C8-N9	-5.41	95.65	103.38
1	1A	1911	PSU	C5-C4-N3	-5.32	118.50	125.36
1	1A	1917	PSU	C5-C4-N3	-5.30	118.53	125.36
32	1a	516	PSU	C5-C4-N3	-5.27	118.56	125.36
1	2A	1911	PSU	C5-C4-N3	-5.24	118.61	125.36
32	1a	966	M2G	C2-N3-C4	5.23	121.22	115.28
32	2a	966	M2G	C6-N1-C2	5.23	122.41	116.18
32	2a	527	7MG	C5-C4-N3	-5.16	118.06	126.49
32	1a	966	M2G	C6-N1-C2	5.15	122.31	116.18
32	2a	966	M2G	C2-N3-C4	5.05	121.01	115.28
32	1a	1207	2MG	C2-N3-C4	5.01	120.96	115.28
32	1a	527	7MG	C5-C4-N3	-4.99	118.34	126.49
1	1A	2251	OMG	C2-N3-C4	4.93	120.99	115.36
32	2a	1207	2MG	C2-N3-C4	4.84	120.78	115.28
1	1A	2605	PSU	C5-C4-N3	-4.79	119.19	125.36
1	2A	2251	OMG	C2-N3-C4	4.75	120.78	115.36
1	2A	2503	2MA	C5-C6-N1	-4.66	118.17	123.06
1	1A	2605	PSU	C5-C6-N1	-4.48	118.94	124.44
32	1a	527	7MG	C6-N1-C2	4.47	123.03	115.93
32	2a	1207	2MG	C6-N1-C2	4.44	123.13	115.18
32	2a	527	7MG	C6-N1-C2	4.43	122.97	115.93
1	1A	2605	PSU	C6-N1-C2	4.42	122.65	115.36
1	2A	1920	4OC	C2-N3-C4	4.41	120.81	116.34
1	1A	2503	2MA	C5-C6-N1	-4.39	118.45	123.06
32	2a	1207	2MG	C5-C6-N1	-4.26	117.60	123.43
1	2A	2605	PSU	C5-C6-N1	-4.26	119.21	124.44
1	2A	1917	PSU	C5-C6-N1	-4.25	119.22	124.44
32	2a	516	PSU	C5-C6-N1	-4.23	119.24	124.44
1	2A	1911	PSU	C5-C6-N1	-4.16	119.32	124.44
32	1a	516	PSU	C6-N1-C2	4.13	122.17	115.36
32	2a	966	M2G	C5-C6-N1	-4.13	117.79	123.43
1	2A	1917	PSU	C6-N1-C2	4.10	122.12	115.36
32	2a	1207	2MG	C6-C5-C4	-4.09	116.89	120.80
1	2A	2251	OMG	C5-C6-N1	-4.09	117.84	123.43
1	1A	1917	PSU	C6-N1-C2	4.08	122.09	115.36
1	1A	1911	PSU	C6-N1-C2	4.07	122.07	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	516	PSU	C5-C6-N1	-4.06	119.44	124.44
32	1a	1207	2MG	C6-N1-C2	4.05	122.43	115.18
32	1a	1207	2MG	C5-C6-N1	-4.04	117.90	123.43
1	2A	2251	OMG	C6-N1-C2	4.04	122.34	115.93
1	2A	1911	PSU	C6-N1-C2	4.03	122.01	115.36
1	1A	1920	4OC	C2-N3-C4	4.03	120.43	116.34
1	1A	1917	PSU	C5-C6-N1	-4.02	119.50	124.44
32	1a	967	5MC	C2-N3-C4	4.02	120.87	116.02
32	1a	966	M2G	C5-C6-N1	-4.01	117.94	123.43
32	2a	516	PSU	C6-N1-C2	4.00	121.95	115.36
1	2A	2605	PSU	C6-N1-C2	3.99	121.94	115.36
1	1A	1911	PSU	C5-C6-N1	-3.97	119.56	124.44
32	2a	1518	MA6	C4-C5-N7	-3.96	105.27	109.40
32	2a	527	7MG	C6-C5-C4	3.94	119.43	115.20
1	1A	2251	OMG	C6-N1-C2	3.91	122.14	115.93
32	1a	527	7MG	C6-C5-C4	3.89	119.38	115.20
1	1A	2251	OMG	C5-C6-N1	-3.88	118.12	123.43
32	1a	1407	5MC	C2-N3-C4	3.86	120.68	116.02
32	1a	1207	2MG	C6-C5-C4	-3.85	117.13	120.80
32	1a	966	M2G	C6-C5-C4	-3.75	117.22	120.80
32	2a	1407	5MC	C2-N3-C4	3.74	120.54	116.02
1	1A	1939	5MU	C5-C6-N1	-3.74	118.17	122.19
32	2a	1402	4OC	CM4-N4-C4	-3.71	119.78	122.97
32	1a	1519	MA6	N1-C6-N6	3.70	120.94	117.06
32	2a	966	M2G	C6-C5-C4	-3.69	117.27	120.80
1	2A	1942	5MC	C2-N3-C4	3.60	120.36	116.02
32	2a	967	5MC	C2-N3-C4	3.60	120.36	116.02
32	2a	1519	MA6	C9-N6-C6	-3.59	108.63	119.51
32	1a	527	7MG	C5-C6-N1	-3.59	115.77	123.14
32	1a	1404	5MC	C2-N3-C4	3.58	120.33	116.02
32	2a	527	7MG	C5-C6-N1	-3.51	115.92	123.14
32	2a	1404	5MC	C2-N3-C4	3.50	120.24	116.02
1	2A	2251	OMG	C6-C5-C4	-3.49	117.46	120.80
32	1a	1400	5MC	C2-N3-C4	3.49	120.23	116.02
32	1a	1518	MA6	C4-C5-N7	-3.47	105.78	109.40
32	2a	1400	5MC	C2-N3-C4	3.47	120.20	116.02
1	2A	1962	5MC	C2-N3-C4	3.46	120.20	116.02
1	1A	1942	5MC	C2-N3-C4	3.46	120.19	116.02
32	2a	1518	MA6	C9-N6-C6	-3.38	109.29	119.51
1	1A	2251	OMG	C6-C5-C4	-3.34	117.61	120.80
1	2A	2605	PSU	C5-C1'-C2'	-3.31	109.42	115.32
1	1A	1962	5MC	C2-N3-C4	3.30	120.00	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1519	MA6	C10-N6-C6	-3.29	109.55	119.51
32	1a	1518	MA6	C9-N6-C6	-3.26	109.63	119.51
32	1a	1518	MA6	N3-C2-N1	-3.23	123.62	128.68
32	2a	1519	MA6	N1-C6-N6	3.23	120.46	117.06
1	1A	2251	OMG	N3-C2-N1	-3.22	122.93	127.22
1	2A	1917	PSU	C5-C1'-C2'	-3.22	109.58	115.32
1	2A	2251	OMG	N3-C2-N1	-3.19	122.97	127.22
1	2A	1911	PSU	C5-C1'-C2'	-3.19	109.63	115.32
1	1A	2605	PSU	C5-C1'-C2'	-3.19	109.64	115.32
32	1a	1207	2MG	CM2-N2-C2	-3.17	119.76	123.59
32	2a	1519	MA6	N3-C2-N1	-3.15	123.75	128.68
32	1a	1519	MA6	C9-N6-C6	-3.12	110.07	119.51
1	2A	1939	5MU	C5-C6-N1	-3.08	118.87	122.19
32	2a	1519	MA6	C10-N6-C9	-3.07	106.24	116.12
32	2a	1519	MA6	C4-C5-N7	-3.05	106.22	109.40
32	1a	1519	MA6	N3-C2-N1	-3.05	123.92	128.68
32	2a	1518	MA6	N3-C2-N1	-3.03	123.94	128.68
32	1a	1207	2MG	C4-C5-N7	-2.94	106.33	109.40
32	2a	966	M2G	C4-C5-N7	-2.91	106.36	109.40
32	1a	1519	MA6	C4-C5-N7	-2.89	106.39	109.40
32	1a	967	5MC	N4-C4-N3	2.87	121.08	117.03
1	2A	1962	5MC	N4-C4-N3	2.83	121.03	117.03
32	1a	1407	5MC	N4-C4-N3	2.80	121.00	117.03
1	1A	1962	5MC	C5-C6-N1	-2.74	119.25	122.19
32	2a	1207	2MG	CM2-N2-C2	-2.73	120.29	123.59
32	2a	527	7MG	C8-N7-C5	2.73	116.03	108.94
32	1a	527	7MG	C8-N7-C5	2.72	116.03	108.94
32	2a	1407	5MC	N4-C4-N3	2.72	120.88	117.03
1	2A	1942	5MC	N4-C4-N3	2.72	120.88	117.03
32	1a	966	M2G	C4-C5-N7	-2.71	106.57	109.40
1	2A	2251	OMG	C4-C5-N7	-2.70	106.58	109.40
32	1a	1402	4OC	CM4-N4-C4	-2.69	120.66	122.97
1	1A	2503	2MA	C4-C5-N7	-2.63	106.66	109.40
32	2a	1207	2MG	C4-C5-N7	-2.61	106.68	109.40
1	2A	2503	2MA	C4-C5-N7	-2.59	106.70	109.40
32	1a	1518	MA6	C10-N6-C9	-2.56	107.86	116.12
32	2a	1518	MA6	C10-N6-C9	-2.54	107.92	116.12
32	1a	1400	5MC	C5-C6-N1	-2.54	119.46	122.19
32	2a	1400	5MC	N4-C4-N3	2.51	120.58	117.03
32	2a	1400	5MC	C5-C6-N1	-2.50	119.50	122.19
1	1A	1917	PSU	C5-C1'-C2'	-2.49	110.87	115.32
32	1a	1404	5MC	C5-C6-N1	-2.44	119.56	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1404	5MC	N4-C4-N3	2.44	120.48	117.03
32	2a	1207	2MG	N3-C2-N1	-2.39	122.45	126.23
1	1A	1962	5MC	N4-C4-N3	2.39	120.41	117.03
1	1A	2251	OMG	C4-C5-N7	-2.35	106.95	109.40
32	2a	967	5MC	C5-C6-N1	-2.35	119.67	122.19
32	2a	967	5MC	N4-C4-N3	2.34	120.34	117.03
1	1A	1920	4OC	N4-C4-N3	2.30	120.12	116.49
1	1A	1942	5MC	C5-C6-N1	-2.29	119.73	122.19
1	2A	1942	5MC	C5-C6-N1	-2.28	119.73	122.19
32	2a	527	7MG	C5-C4-N9	-2.27	103.26	106.44
32	1a	527	7MG	C5-C4-N9	-2.27	103.26	106.44
1	1A	1942	5MC	N4-C4-N3	2.26	120.23	117.03
1	2A	1962	5MC	C5-C6-N1	-2.26	119.76	122.19
32	2a	1404	5MC	N4-C4-N3	2.26	120.22	117.03
32	1a	1400	5MC	N4-C4-N3	2.25	120.22	117.03
1	2A	1920	4OC	N4-C4-N3	2.24	120.03	116.49
32	2a	527	7MG	C2-N3-C4	2.24	120.08	113.89
32	2a	1404	5MC	C5-C6-N1	-2.23	119.79	122.19
32	1a	1518	MA6	C10-N6-C6	-2.21	112.81	119.51
32	1a	516	PSU	O4'-C1'-C2'	2.21	108.25	104.66
32	1a	527	7MG	C2-N3-C4	2.18	119.92	113.89
32	1a	1207	2MG	N3-C2-N1	-2.18	122.79	126.23
1	1A	1911	PSU	C5-C1'-C2'	-2.17	111.45	115.32
1	1A	2552	2MU	C5-C4-N3	-2.17	118.54	123.31
32	1a	1207	2MG	N2-C2-N1	2.15	119.03	116.96
32	2a	516	PSU	O4'-C1'-C2'	2.15	108.14	104.66
32	1a	1402	4OC	C5-C4-N3	-2.08	119.66	123.16
32	1a	1519	MA6	C10-N6-C6	-2.06	113.29	119.51
32	2a	1207	2MG	N2-C2-N3	2.04	118.92	116.96
32	1a	1207	2MG	O3'-C3'-C2'	2.03	118.39	111.82
32	2a	1498	UR3	C3U-N3-C4	2.01	120.78	118.12
32	1a	1518	MA6	N1-C6-N6	2.01	119.17	117.06
32	2a	1407	5MC	C5-C6-N1	-2.01	120.03	122.19

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C9
32	2a	1519	MA6	C5-C6-N6-C10
32	2a	1519	MA6	N1-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	1518	MA6	C5-C6-N6-C10
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
1	2A	1920	4OC	C2'-C1'-N1-C6
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CG-CB-SB-CSB
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
1	1A	1962	5MC	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C10
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
1	2A	2552	2MU	O4'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	2a	527	7MG	C4'-C5'-O5'-P
1	1A	1962	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
32	1a	527	7MG	C4'-C5'-O5'-P
1	1A	1920	4OC	C3'-C2'-O2'-CM2
43	1l	92	0TD	CA-CB-SB-CSB
1	2A	2503	2MA	C4'-C5'-O5'-P
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	1917	PSU	C2'-C1'-C5-C6
1	2A	2503	2MA	C3'-C4'-C5'-O5'
32	2a	1519	MA6	N1-C6-N6-C10
32	1a	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	2d	501	35	0,12,12	0.00	-	-		
56	SF4	1d	501	35	0,12,12	0.00	-	-		
54	HGR	1A	3749	-	39,39,39	2.43	9 (23%)	50,58,58	1.68	13 (26%)
54	HGR	2A	3515	-	39,39,39	2.42	9 (23%)	50,58,58	1.73	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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2A	3515	HGR	C12-C14	9.29	1.55	1.33
54	1A	3749	HGR	C12-C14	9.26	1.55	1.33
54	1A	3749	HGR	C5-C6	-5.47	1.39	1.50
54	2A	3515	HGR	C5-C6	-5.36	1.39	1.50
54	2A	3515	HGR	C5-C4	-5.28	1.39	1.49
54	1A	3749	HGR	C5-C4	-5.27	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2A	3515	HGR	C3-C2	-4.61	1.39	1.48
54	1A	3749	HGR	C3-C2	-4.58	1.39	1.48
54	1A	3749	HGR	O4-C2	4.51	1.36	1.24
54	2A	3515	HGR	O4-C2	4.49	1.36	1.24
54	1A	3749	HGR	C1-C6	2.89	1.39	1.35
54	2A	3515	HGR	C1-C6	2.84	1.39	1.35
54	1A	3749	HGR	O8-C23	2.46	1.45	1.41
54	2A	3515	HGR	O8-C23	2.44	1.45	1.41
54	2A	3515	HGR	O9-C23	2.24	1.45	1.41
54	1A	3749	HGR	O9-C23	2.19	1.45	1.41
54	1A	3749	HGR	C1-C2	-2.02	1.39	1.44
54	2A	3515	HGR	C1-C2	-2.02	1.39	1.44

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2A	3515	HGR	C10-C9-C8	-5.11	95.82	102.30
54	1A	3749	HGR	C4-C5-C6	4.21	121.43	112.36
54	2A	3515	HGR	C4-C5-C6	4.15	121.29	112.36
54	1A	3749	HGR	C10-C9-C8	-3.66	97.66	102.30
54	1A	3749	HGR	C12-C6-C1	-3.60	116.00	119.31
54	2A	3515	HGR	O1-C10-C9	-3.56	100.39	104.98
54	2A	3515	HGR	C12-C6-C1	-3.42	116.16	119.31
54	1A	3749	HGR	O8-C18-C22	-3.22	98.75	105.97
54	2A	3515	HGR	O8-C18-C22	-3.13	98.97	105.97
54	1A	3749	HGR	O9-C22-C18	-3.11	99.01	105.97
54	2A	3515	HGR	O9-C22-C18	-3.10	99.04	105.97
54	2A	3515	HGR	O4-C2-C3	-2.96	116.67	121.30
54	1A	3749	HGR	O4-C2-C3	-2.94	116.70	121.30
54	1A	3749	HGR	O1-C10-C9	-2.78	101.39	104.98
54	2A	3515	HGR	C23-O9-C22	-2.67	102.25	106.31
54	1A	3749	HGR	C23-O9-C22	-2.65	102.27	106.31
54	1A	3749	HGR	C8-C7-C11	-2.51	109.26	113.67
54	2A	3515	HGR	C8-C7-C11	-2.47	109.34	113.67
54	1A	3749	HGR	C4-C3-C2	-2.35	119.66	121.83
54	2A	3515	HGR	C1-C2-C3	2.29	120.41	115.99
54	1A	3749	HGR	C1-C2-C3	2.26	120.35	115.99
54	1A	3749	HGR	O3-C3-C2	2.14	116.63	112.56
54	1A	3749	HGR	C9-C8-C7	-2.13	99.15	101.64
54	2A	3515	HGR	C4-C3-C2	-2.09	119.91	121.83

There are no chirality outliers.

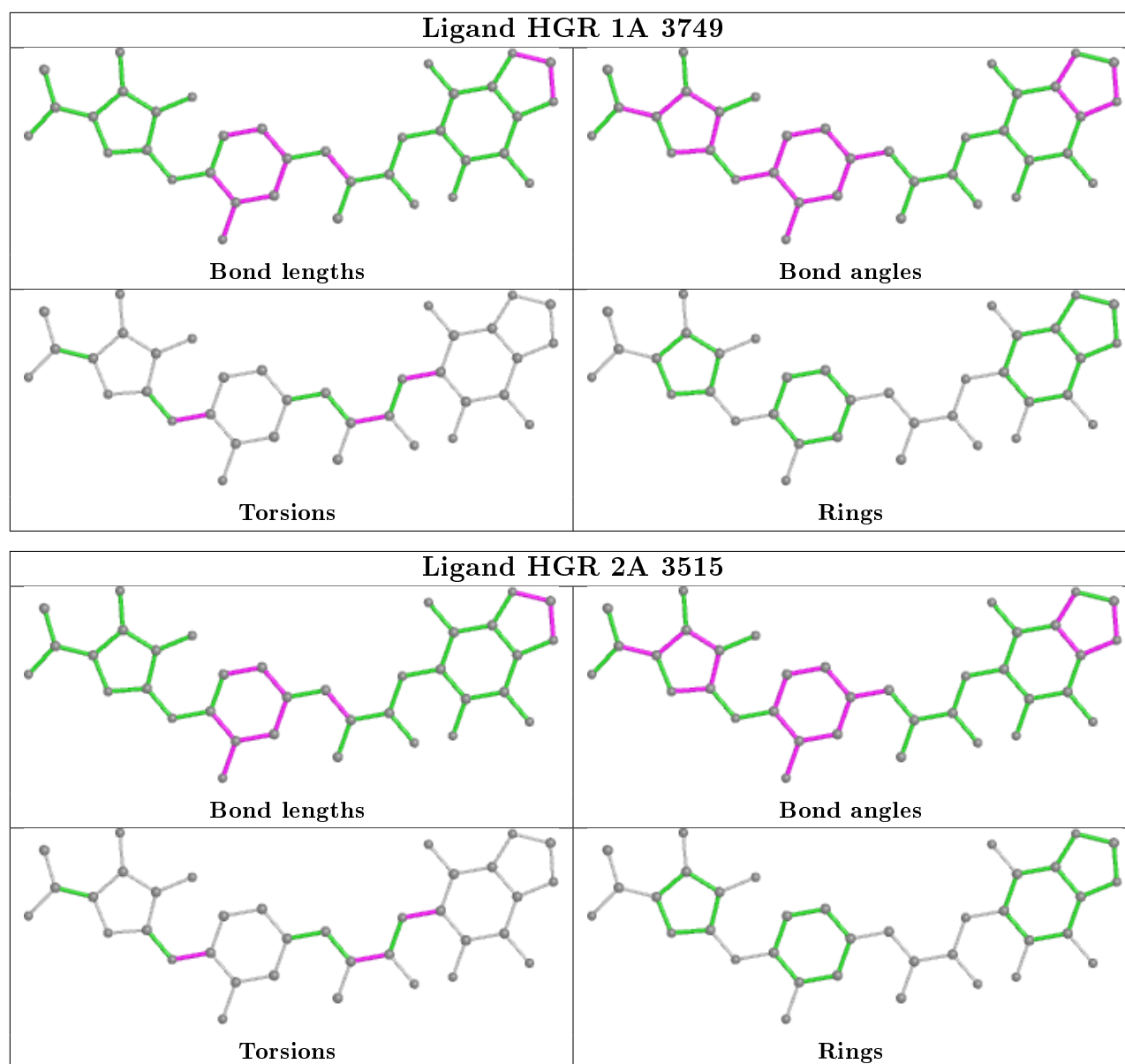
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	1A	3749	HGR	C2-C3-O3-C10
54	2A	3515	HGR	C2-C3-O3-C10
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
54	1A	3749	HGR	C16-C14-C15-O7
54	1A	3749	HGR	C16-C14-C15-N1
54	2A	3515	HGR	C16-C14-C15-O7
54	2A	3515	HGR	C16-C14-C15-N1
54	2A	3515	HGR	C19-C17-N1-C15
54	1A	3749	HGR	C19-C17-N1-C15

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	201 (7%) 16 7	28, 61, 116, 129	0
1	2A	2856/2915 (97%)	0.65	206 (7%) 15 6	34, 66, 117, 137	0
2	1B	120/121 (99%)	0.65	2 (1%) 70 49	44, 84, 99, 108	0
2	2B	120/121 (99%)	0.18	2 (1%) 70 49	51, 90, 104, 111	0
3	1D	275/276 (99%)	0.84	31 (11%) 5 2	39, 63, 82, 98	0
3	2D	275/276 (99%)	0.99	51 (18%) 1 0	40, 66, 83, 99	0
4	1E	204/206 (99%)	0.94	14 (6%) 16 7	37, 64, 84, 99	0
4	2E	204/206 (99%)	0.56	14 (6%) 16 7	38, 68, 86, 102	0
5	1F	203/210 (96%)	0.71	5 (2%) 57 34	35, 71, 95, 116	0
5	2F	203/210 (96%)	0.32	13 (6%) 19 8	38, 75, 96, 118	0
6	1G	181/182 (99%)	0.86	35 (19%) 1 0	85, 105, 113, 120	0
6	2G	181/182 (99%)	1.40	51 (28%) 0 0	85, 107, 115, 123	0
7	1H	174/180 (96%)	0.56	2 (1%) 80 64	63, 84, 97, 104	0
7	2H	173/180 (96%)	0.38	16 (9%) 9 3	69, 89, 100, 106	0
8	1I	147/148 (99%)	0.17	5 (3%) 45 24	70, 97, 107, 111	0
8	2I	146/148 (98%)	0.17	9 (6%) 20 9	67, 98, 108, 111	0
9	1N	140/140 (100%)	0.65	3 (2%) 63 43	33, 49, 75, 93	0
9	2N	140/140 (100%)	1.08	32 (22%) 0 0	67, 86, 100, 108	0
10	1O	122/122 (100%)	0.56	5 (4%) 37 18	39, 61, 81, 88	0
10	2O	122/122 (100%)	0.67	16 (13%) 3 1	59, 80, 94, 101	0
11	1P	149/150 (99%)	0.77	12 (8%) 12 5	37, 75, 96, 103	0
11	2P	149/150 (99%)	0.96	38 (25%) 0 0	41, 79, 99, 107	0
12	1Q	141/141 (100%)	0.90	14 (9%) 7 2	45, 69, 85, 93	0
12	2Q	141/141 (100%)	1.37	33 (23%) 0 0	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%)	1.36	24 (20%) 1 0	38, 55, 71, 89	0
13	2R	118/118 (100%)	1.12	24 (20%) 1 0	41, 59, 73, 91	0
14	1S	110/112 (98%)	1.10	23 (20%) 1 0	62, 83, 97, 99	0
14	2S	110/112 (98%)	1.54	37 (33%) 0 0	67, 87, 100, 103	0
15	1T	131/146 (89%)	0.70	10 (7%) 13 5	53, 74, 95, 104	0
15	2T	131/146 (89%)	0.36	4 (3%) 49 26	59, 77, 96, 106	0
16	1U	116/118 (98%)	1.14	12 (10%) 6 2	34, 58, 81, 86	0
16	2U	116/118 (98%)	1.61	49 (42%) 0 0	44, 63, 85, 90	0
17	1V	101/101 (100%)	0.79	9 (8%) 9 3	39, 68, 86, 99	0
17	2V	101/101 (100%)	0.53	17 (16%) 1 0	45, 74, 91, 102	0
18	1W	112/113 (99%)	0.59	0 100 100	34, 48, 75, 102	0
18	2W	112/113 (99%)	0.44	3 (2%) 54 31	39, 52, 80, 103	0
19	1X	95/96 (98%)	1.01	8 (8%) 11 4	40, 61, 84, 98	0
19	2X	95/96 (98%)	1.28	25 (26%) 0 0	45, 65, 87, 98	0
20	1Y	107/110 (97%)	0.85	8 (7%) 14 5	55, 75, 93, 103	0
20	2Y	107/110 (97%)	0.92	18 (16%) 1 0	63, 79, 96, 106	0
21	1Z	203/206 (98%)	0.24	3 (1%) 73 54	46, 76, 99, 114	0
21	2Z	201/206 (97%)	0.32	15 (7%) 14 5	71, 100, 110, 118	0
22	10	77/85 (90%)	1.06	9 (11%) 4 2	51, 65, 84, 88	0
22	20	77/85 (90%)	1.32	24 (31%) 0 0	57, 70, 87, 90	0
23	11	97/98 (98%)	1.29	20 (20%) 1 0	42, 70, 92, 99	0
23	21	97/98 (98%)	1.34	23 (23%) 0 0	45, 72, 94, 101	0
24	12	70/72 (97%)	0.71	2 (2%) 51 28	51, 74, 89, 103	0
24	22	70/72 (97%)	0.58	5 (7%) 16 6	56, 78, 91, 100	0
25	13	59/60 (98%)	0.49	0 100 100	45, 64, 90, 106	0
25	23	59/60 (98%)	1.11	14 (23%) 0 0	53, 70, 92, 105	0
26	14	69/71 (97%)	0.95	16 (23%) 0 0	103, 112, 118, 122	0
26	24	69/71 (97%)	0.59	14 (20%) 1 0	102, 113, 119, 122	0
27	15	59/60 (98%)	0.74	1 (1%) 70 49	33, 53, 75, 91	0
27	25	59/60 (98%)	0.40	1 (1%) 70 49	38, 57, 76, 91	0
28	16	53/54 (98%)	0.91	6 (11%) 5 2	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%)	0.69	7 (13%) 3 1	61, 73, 89, 90	0
29	17	48/49 (97%)	1.04	4 (8%) 11 4	35, 44, 81, 96	0
29	27	48/49 (97%)	1.05	6 (12%) 3 1	37, 47, 81, 98	0
30	18	64/65 (98%)	1.51	17 (26%) 0 0	48, 63, 76, 86	0
30	28	64/65 (98%)	2.33	33 (51%) 0 0	54, 67, 79, 88	0
31	19	37/37 (100%)	2.32	24 (64%) 0 0	57, 70, 86, 91	0
31	29	37/37 (100%)	3.95	31 (83%) 0 0	65, 77, 90, 94	0
32	1a	1488/1521 (97%)	1.68	440 (29%) 0 0	69, 105, 124, 132	0
32	2a	1492/1521 (98%)	1.48	437 (29%) 0 0	70, 105, 124, 132	0
33	1b	231/256 (90%)	0.87	49 (21%) 0 0	98, 108, 115, 117	0
33	2b	231/256 (90%)	1.22	68 (29%) 0 0	98, 109, 115, 119	0
34	1c	206/239 (86%)	0.88	48 (23%) 0 0	102, 112, 118, 122	0
34	2c	206/239 (86%)	0.76	39 (18%) 1 0	102, 112, 117, 122	0
35	1d	208/209 (99%)	1.12	46 (22%) 0 0	89, 102, 111, 119	0
35	2d	208/209 (99%)	1.09	40 (19%) 1 0	88, 101, 111, 119	0
36	1e	148/162 (91%)	0.59	22 (14%) 2 1	80, 100, 107, 113	0
36	2e	148/162 (91%)	0.86	31 (20%) 1 0	82, 101, 108, 114	0
37	1f	100/101 (99%)	0.08	3 (3%) 50 27	82, 97, 106, 111	0
37	2f	100/101 (99%)	0.02	5 (5%) 28 13	84, 98, 107, 110	0
38	1g	155/156 (99%)	2.95	89 (57%) 0 0	103, 112, 118, 120	0
38	2g	155/156 (99%)	1.69	57 (36%) 0 0	103, 113, 118, 121	0
39	1h	137/138 (99%)	1.38	42 (30%) 0 0	88, 101, 108, 114	0
39	2h	137/138 (99%)	1.59	51 (37%) 0 0	88, 101, 108, 115	0
40	1i	127/128 (99%)	5.25	99 (77%) 0 0	100, 114, 120, 121	0
40	2i	126/128 (98%)	4.35	91 (72%) 0 0	100, 114, 120, 124	0
41	1j	97/105 (92%)	4.30	63 (64%) 0 0	102, 113, 120, 122	0
41	2j	96/105 (91%)	2.86	49 (51%) 0 0	105, 114, 120, 121	0
42	1k	114/129 (88%)	0.51	11 (9%) 8 2	79, 100, 112, 120	0
42	2k	114/129 (88%)	0.41	12 (10%) 6 2	84, 101, 109, 112	0
43	1l	121/132 (91%)	1.22	29 (23%) 0 0	78, 94, 102, 113	0
43	2l	121/132 (91%)	1.04	28 (23%) 0 0	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%)	3.18	72 (62%)	0	0	102, 114, 119, 121	0
44	2m	114/126 (90%)	2.08	47 (41%)	0	0	105, 113, 118, 121	0
45	1n	60/61 (98%)	4.50	42 (70%)	0	0	103, 113, 119, 120	0
45	2n	60/61 (98%)	4.45	48 (80%)	0	0	104, 113, 119, 122	0
46	1o	88/89 (98%)	1.59	27 (30%)	0	0	78, 96, 106, 111	0
46	2o	88/89 (98%)	1.94	40 (45%)	0	0	81, 98, 107, 111	0
47	1p	82/88 (93%)	2.22	43 (52%)	0	0	93, 102, 111, 113	0
47	2p	82/88 (93%)	2.65	46 (56%)	0	0	92, 100, 108, 114	0
48	1q	99/105 (94%)	2.02	48 (48%)	0	0	88, 100, 108, 110	0
48	2q	99/105 (94%)	1.07	22 (22%)	0	0	87, 99, 107, 110	0
49	1r	68/88 (77%)	0.11	3 (4%)	34	17	85, 98, 107, 115	0
49	2r	68/88 (77%)	0.53	6 (8%)	10	4	91, 101, 109, 118	0
50	1s	83/93 (89%)	4.46	64 (77%)	0	0	105, 114, 119, 126	0
50	2s	83/93 (89%)	3.75	58 (69%)	0	0	100, 114, 121, 124	0
51	1t	96/106 (90%)	2.20	47 (48%)	0	0	90, 102, 110, 114	0
51	2t	98/106 (92%)	2.55	55 (56%)	0	0	77, 94, 105, 109	0
52	1u	23/27 (85%)	8.95	22 (95%)	0	0	109, 113, 117, 119	0
52	2u	23/27 (85%)	5.83	19 (82%)	0	0	108, 113, 119, 119	0
All	All	20573/21242 (96%)	1.18	3914 (19%)	1	0	28, 87, 118, 137	0

All (3914) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
40	1i	106	ALA	19.9
45	1n	61	TRP	18.0
41	2j	62	HIS	17.9
40	1i	105	ASP	17.8
1	1A	1087	G	16.9
1	1A	1091	G	16.9
52	2u	6	ARG	16.8
32	1a	1353	G	16.6
32	2a	1116	C	16.6
41	1j	48	THR	16.3
44	1m	86	CYS	16.3
52	1u	6	ARG	16.2
40	1i	107	ARG	15.7

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Mol	Chain	Res	Type	RSRZ
52	1u	14	TRP	15.4
32	1a	1286	A	15.3
35	2d	2	GLY	14.9
1	1A	1075	C	14.9
41	1j	62	HIS	14.9
45	1n	18	VAL	14.8
32	1a	1349	A	14.7
41	1j	63	PHE	14.5
52	1u	5	ASP	14.4
1	1A	1089	G	14.1
50	1s	56	GLN	13.8
41	1j	42	THR	13.8
32	1a	1287	A	13.7
50	1s	57	HIS	13.6
50	2s	5	LEU	13.6
40	1i	46	ALA	13.6
35	1d	2	GLY	13.5
38	1g	86	GLN	13.5
50	1s	4	SER	13.4
40	2i	105	ASP	13.3
40	1i	110	GLU	13.3
40	2i	110	GLU	13.3
1	1A	1090	U	12.9
40	2i	120	ARG	12.8
40	1i	109	VAL	12.7
50	2s	8	GLY	12.7
32	1a	1318	A	12.7
41	2j	59	SER	12.7
32	1a	1036	G	12.6
32	1a	1348	U	12.6
40	1i	121	ARG	12.4
40	1i	111	ARG	12.3
32	1a	1308	U	12.3
1	1A	1093	G	12.2
50	2s	3	ARG	12.2
45	1n	16	PHE	12.2
1	2A	2162	G	12.1
40	1i	119	ALA	12.1
52	1u	3	LYS	12.1
40	2i	109	VAL	11.9
40	1i	108	VAL	11.8
41	1j	61	GLU	11.8

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Mol	Chain	Res	Type	RSRZ
32	1a	1115	C	11.7
32	1a	1149	C	11.7
40	2i	106	ALA	11.7
45	2n	61	TRP	11.7
51	1t	9	ASN	11.7
32	1a	1188	A	11.7
32	1a	1186	G	11.6
38	1g	156	TRP	11.6
32	1a	1138	G	11.5
45	2n	18	VAL	11.5
45	1n	17	LYS	11.4
40	1i	15	ALA	11.4
32	1a	1317	C	11.4
52	1u	18	TYR	11.4
52	1u	12	LYS	11.3
52	1u	13	ILE	11.3
52	1u	4	GLY	11.3
32	1a	1137	C	11.3
32	1a	1367	C	11.3
45	1n	19	ARG	11.3
50	1s	71	LEU	11.3
52	2u	14	TRP	11.3
41	1j	64	GLU	11.2
32	1a	1288	A	11.2
32	2a	1312	G	11.1
34	2c	3	ASN	11.1
32	1a	1354	C	11.1
32	1a	1187	G	11.0
33	2b	101	MET	11.0
35	1d	3	ARG	11.0
40	1i	9	ARG	11.0
50	2s	4	SER	10.9
45	2n	16	PHE	10.9
50	1s	74	PHE	10.9
41	1j	50	ILE	10.9
45	1n	59	ALA	10.9
50	2s	9	VAL	10.9
32	2a	1348	U	10.9
40	1i	120	ARG	10.8
41	1j	60	ARG	10.8
40	1i	104	ARG	10.7
41	1j	57	LYS	10.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
45	2n	19	ARG	10.7
32	1a	1352	C	10.7
41	1j	46	ARG	10.6
41	2j	60	ARG	10.6
52	1u	11	GLY	10.6
40	1i	30	GLY	10.5
45	1n	22	THR	10.5
1	1A	1072	C	10.4
40	1i	113	LYS	10.4
38	1g	12	LEU	10.4
32	1a	1148	U	10.3
32	1a	1364	U	10.3
32	2a	1349	A	10.3
52	2u	5	ASP	10.3
35	2d	3	ARG	10.2
32	1a	1347	G	10.2
40	2i	14	VAL	10.2
52	1u	8	THR	10.2
38	2g	78	ARG	10.1
44	1m	98	VAL	10.1
6	2G	3	LEU	10.1
36	2e	20	GLN	10.0
40	2i	114	TYR	10.0
38	1g	20	ASP	10.0
6	2G	2	PRO	10.0
32	1a	1327	C	10.0
44	1m	110	ARG	10.0
40	1i	62	TYR	9.9
32	1a	1307	U	9.9
45	2n	15	LYS	9.9
32	1a	979	C	9.9
40	2i	115	GLY	9.9
45	2n	59	ALA	9.9
50	2s	7	LYS	9.8
32	1a	1370	G	9.8
40	2i	66	ARG	9.8
26	14	66	SER	9.8
41	2j	48	THR	9.8
32	2a	1193	G	9.8
38	1g	31	MET	9.8
52	1u	7	ARG	9.8
40	2i	108	VAL	9.8

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Mol	Chain	Res	Type	RSRZ
41	1j	47	PHE	9.8
32	2a	1149	C	9.7
32	2a	1353	G	9.7
39	2h	2	LEU	9.7
1	1A	1076	C	9.6
39	2h	4	ASP	9.6
40	1i	122	ALA	9.6
50	1s	69	HIS	9.6
40	1i	116	LYS	9.5
32	2a	1326	C	9.5
41	2j	63	PHE	9.5
32	1a	1371	G	9.5
32	1a	1248	A	9.5
52	2u	17	THR	9.4
52	1u	15	ARG	9.4
23	2l	2	SER	9.4
40	1i	66	ARG	9.3
32	2a	1064	G	9.3
41	1j	58	ASP	9.3
1	1A	1088	A	9.3
32	1a	1289	A	9.3
35	2d	70	ILE	9.3
32	2a	1286	A	9.3
45	1n	60	SER	9.3
44	1m	109	THR	9.2
40	2i	7	THR	9.2
40	1i	14	VAL	9.2
40	1i	78	LYS	9.2
52	1u	17	THR	9.2
32	2a	1186	G	9.2
45	1n	58	LYS	9.1
32	1a	1373	G	9.1
44	1m	85	GLY	9.1
40	2i	111	ARG	9.1
45	1n	20	ALA	9.1
45	1n	14	PRO	9.1
52	1u	16	GLY	9.1
32	1a	1366	C	9.1
40	1i	114	TYR	9.0
51	2t	73	HIS	9.0
34	2c	4	LYS	9.0
41	2j	64	GLU	9.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
38	1g	99	LEU	9.0
40	1i	115	GLY	8.9
32	1a	1360	A	8.9
32	2a	1117	G	8.9
40	2i	116	LYS	8.9
35	2d	137	SER	8.9
45	2n	39	LEU	8.9
20	1Y	1	MET	8.9
32	1a	1332	A	8.8
1	1A	2117	A	8.8
32	2a	1248	A	8.8
38	2g	86	GLN	8.8
52	2u	11	GLY	8.8
50	1s	50	ALA	8.8
40	1i	101	PHE	8.8
35	1d	4	TYR	8.8
50	1s	66	MET	8.8
41	1j	65	LEU	8.8
1	1A	2173	A	8.8
40	1i	7	THR	8.8
35	2d	69	GLY	8.8
44	1m	87	TYR	8.8
32	2a	1036	G	8.7
44	2m	87	TYR	8.7
32	2a	1324	A	8.7
45	1n	15	LYS	8.7
33	2b	99	GLY	8.7
32	1a	1361	G	8.7
41	1j	51	ARG	8.7
38	1g	77	SER	8.6
50	1s	5	LEU	8.6
40	1i	117	HIS	8.6
32	2a	1150	U	8.6
32	2a	1092	A	8.6
40	2i	10	ARG	8.6
32	1a	1326	C	8.6
32	1a	1179	A	8.6
32	1a	1290	G	8.5
32	1a	1249	C	8.5
38	2g	2	ALA	8.5
41	1j	41	PRO	8.5
1	1A	2116	G	8.5

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Mol	Chain	Res	Type	RSRZ
40	1i	42	ARG	8.5
1	1A	1092	C	8.5
44	2m	110	ARG	8.5
52	2u	16	GLY	8.5
50	2s	10	PHE	8.5
52	1u	10	ARG	8.5
32	2a	1354	C	8.4
50	2s	69	HIS	8.4
38	1g	36	LYS	8.4
45	2n	14	PRO	8.4
40	2i	113	LYS	8.4
32	1a	1365	G	8.4
35	1d	70	ILE	8.4
41	1j	66	ARG	8.4
38	1g	78	ARG	8.3
32	2a	1347	G	8.3
40	2i	62	TYR	8.3
35	1d	5	ILE	8.3
1	1A	1063	G	8.3
41	2j	66	ARG	8.3
51	1t	72	LEU	8.3
40	2i	64	THR	8.3
32	1a	1350	A	8.2
32	1a	1117	G	8.2
40	2i	126	SER	8.2
32	1a	1111	A	8.2
40	1i	75	ASP	8.2
32	2a	1373	G	8.2
32	2a	1191	A	8.2
44	1m	107	ALA	8.2
36	2e	22	GLY	8.2
1	1A	1074	G	8.2
32	2a	1287	A	8.2
31	29	37	GLY	8.1
40	2i	125	TYR	8.1
42	2k	117	ASN	8.1
40	2i	63	ILE	8.1
47	2p	1	MET	8.1
32	1a	975	A	8.1
38	2g	82	GLY	8.1
41	1j	49	VAL	8.1
44	2m	88	ARG	8.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1249	C	8.1
32	2a	1194	U	8.1
40	2i	107	ARG	8.1
52	2u	7	ARG	8.0
40	1i	10	ARG	8.0
38	2g	154	TYR	8.0
48	1q	7	THR	8.0
1	2A	2127	G	8.0
32	1a	1316	G	8.0
32	2a	1190	G	8.0
32	1a	974	A	7.9
32	2a	1001(A)	G	7.9
40	2i	103	THR	7.9
41	1j	71	LEU	7.9
26	14	64	GLY	7.9
40	1i	17	VAL	7.9
32	2a	1115	C	7.9
47	2p	33	ILE	7.8
41	1j	67	THR	7.8
38	1g	85	TYR	7.8
44	2m	99	ARG	7.8
32	1a	1180	A	7.8
6	2G	90	LEU	7.8
12	2Q	104	PHE	7.8
40	1i	112	LYS	7.8
32	1a	1092	A	7.8
32	2a	1319	A	7.8
32	2a	1148	U	7.7
34	2c	160	ALA	7.7
34	1c	176	HIS	7.7
41	1j	43	ARG	7.7
44	1m	90	LEU	7.7
33	2b	96	ARG	7.7
6	2G	34	LEU	7.7
32	1a	1359	C	7.7
40	2i	121	ARG	7.7
40	2i	65	VAL	7.7
32	1a	1030	C	7.6
32	2a	1310	G	7.6
1	1A	1071	G	7.6
32	2a	1202	G	7.6
32	1a	1037	C	7.6

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Mol	Chain	Res	Type	RSRZ
44	1m	97	PRO	7.6
32	1a	1034	G	7.6
40	1i	118	LYS	7.6
20	2Y	1	MET	7.6
32	1a	1185	G	7.6
31	29	12	ASP	7.6
38	1g	100	ALA	7.6
41	2j	65	LEU	7.6
40	2i	69	GLY	7.6
36	2e	21	ALA	7.5
34	1c	178	LEU	7.5
1	1A	1080	C	7.5
33	1b	101	MET	7.5
41	1j	44	VAL	7.5
50	2s	6	LYS	7.5
1	1A	2172	U	7.5
51	1t	73	HIS	7.5
29	27	48	LYS	7.5
41	2j	44	VAL	7.5
1	1A	1102	C	7.5
32	1a	1247	U	7.4
41	1j	52	GLY	7.4
40	1i	77	ILE	7.4
41	1j	35	SER	7.4
32	2a	1269	A	7.4
52	1u	2	GLY	7.4
38	2g	156	TRP	7.4
32	2a	824	C	7.4
12	2Q	33	GLY	7.4
32	2a	1327	C	7.4
38	1g	79	ARG	7.3
32	1a	976	G	7.3
1	2A	2174	C	7.3
45	2n	44	LEU	7.3
32	2a	1066	C	7.2
44	2m	97	PRO	7.2
32	1a	950	U	7.2
14	2S	5	THR	7.2
45	1n	12	ARG	7.2
40	1i	41	VAL	7.2
44	2m	24	GLY	7.2
32	1a	1368	G	7.2

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Mol	Chain	Res	Type	RSRZ
32	1a	1363(A)	A	7.2
51	2t	15	ARG	7.2
51	1t	71	THR	7.2
45	2n	12	ARG	7.1
52	2u	2	GLY	7.1
32	2a	1192	C	7.1
40	2i	78	LYS	7.1
45	2n	17	LYS	7.1
38	2g	33	ASP	7.1
39	2h	3	THR	7.1
41	1j	72	VAL	7.1
40	2i	13	ALA	7.1
32	1a	1306	A	7.1
44	2m	90	LEU	7.0
41	1j	59	SER	7.0
6	2G	41	GLN	7.0
32	1a	1314	C	7.0
44	2m	100	GLY	7.0
32	1a	1369	C	7.0
50	2s	53	ASN	7.0
32	1a	1116	C	7.0
43	1l	94	PRO	7.0
32	2a	1065	U	7.0
51	1t	66	ALA	7.0
40	1i	123	PRO	7.0
32	2a	1314	C	6.9
38	2g	25	ALA	6.9
33	2b	98	LEU	6.9
45	2n	34	TYR	6.9
50	1s	3	ARG	6.9
38	1g	34	GLY	6.9
31	29	24	TYR	6.9
38	1g	5	ARG	6.9
52	2u	8	THR	6.9
38	2g	79	ARG	6.9
40	2i	104	ARG	6.9
1	1A	2174	C	6.9
52	2u	13	ILE	6.9
23	11	2	SER	6.9
1	2A	2125	G	6.9
34	1c	160	ALA	6.8
51	2t	70	SER	6.8

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Mol	Chain	Res	Type	RSRZ
40	2i	117	HIS	6.8
1	1A	1081	U	6.8
50	2s	33	THR	6.8
32	2a	1325	C	6.8
32	1a	1304	G	6.8
40	2i	127	LYS	6.8
32	2a	1313	U	6.8
34	2c	167	TRP	6.8
6	1G	38	VAL	6.8
40	1i	76	ALA	6.8
1	2A	2126	A	6.8
36	2e	25	ARG	6.8
32	1a	1246	C	6.8
32	2a	1372	U	6.8
47	1p	12	LYS	6.8
34	1c	12	LEU	6.8
44	1m	23	TYR	6.7
6	2G	73	ALA	6.7
45	1n	30	ALA	6.7
32	1a	1112	C	6.7
1	2A	2147	G	6.7
32	1a	1309	G	6.7
32	1a	1285	A	6.7
1	1A	1103	A	6.7
1	1A	2161	C	6.7
32	1a	958	A	6.7
38	1g	141	VAL	6.7
50	1s	51	VAL	6.7
50	2s	34	TRP	6.7
31	29	13	LYS	6.7
32	1a	1189	C	6.7
40	1i	81	ILE	6.7
38	1g	152	ALA	6.7
35	2d	4	TYR	6.6
45	2n	2	ALA	6.6
40	1i	29	ASN	6.6
1	1A	2160	G	6.6
52	2u	15	ARG	6.6
32	2a	1371	G	6.6
46	2o	62	GLN	6.6
39	2h	5	PRO	6.6
38	1g	154	TYR	6.6

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Mol	Chain	Res	Type	RSRZ
41	2j	67	THR	6.6
32	1a	1325	C	6.6
45	2n	35	ARG	6.6
32	1a	1235	U	6.6
50	1s	55	LYS	6.6
32	1a	1271	G	6.6
45	2n	33	VAL	6.5
47	1p	14	ASN	6.5
40	2i	79	LEU	6.5
46	1o	65	ARG	6.5
35	1d	71	SER	6.5
38	1g	17	VAL	6.5
34	2c	176	HIS	6.5
32	1a	971	G	6.5
52	1u	19	GLY	6.5
40	2i	49	PRO	6.5
40	2i	89	ASN	6.5
51	2t	62	LEU	6.5
32	1a	1046	A	6.5
40	2i	70	LYS	6.5
47	2p	29	ASP	6.5
40	1i	47	LEU	6.5
1	2A	1076	C	6.5
32	1a	1150	U	6.5
41	2j	20	ALA	6.4
47	1p	11	SER	6.4
47	2p	21	VAL	6.4
35	2d	118	ARG	6.4
50	1s	58	VAL	6.4
44	1m	94	ARG	6.4
44	1m	25	ILE	6.4
32	2a	1224	G	6.4
32	2a	1374	A	6.4
33	1b	196	LEU	6.4
44	1m	21	TYR	6.4
34	1c	10	PHE	6.4
40	1i	88	TYR	6.4
50	1s	40	ILE	6.4
47	2p	12	LYS	6.4
14	2S	92	TYR	6.3
45	1n	13	THR	6.3
40	1i	100	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
33	1b	197	VAL	6.3
50	1s	6	LYS	6.3
1	1A	1079	C	6.3
38	1g	35	LYS	6.3
47	2p	32	TYR	6.3
45	1n	57	ARG	6.3
50	1s	30	LEU	6.3
45	2n	58	LYS	6.3
6	1G	62	LEU	6.3
6	2G	133	LEU	6.3
50	2s	79	THR	6.3
38	1g	16	LEU	6.3
44	1m	81	LEU	6.3
32	1a	1035	A	6.3
40	1i	16	ARG	6.3
33	1b	131	PRO	6.3
6	2G	92	VAL	6.3
17	2V	73	SER	6.3
50	1s	10	PHE	6.3
1	1A	1104	C	6.3
45	1n	11	LYS	6.3
50	1s	77	THR	6.3
38	1g	84	ASN	6.3
50	2s	71	LEU	6.3
40	1i	8	GLY	6.3
47	1p	59	TRP	6.3
32	1a	949	A	6.2
32	1a	1323	G	6.2
32	2a	1318	A	6.2
40	2i	73	GLN	6.2
17	2V	74	LYS	6.2
32	1a	1114	C	6.2
32	1a	1183	A	6.2
41	2j	46	ARG	6.2
44	2m	75	ALA	6.2
1	2A	2118	U	6.2
51	2t	25	ARG	6.2
51	2t	75	ASN	6.2
1	1A	2166	G	6.2
1	2A	2173	A	6.2
50	1s	68	GLY	6.2
44	2m	98	VAL	6.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	2a	1323	G	6.2
32	1a	1243	C	6.2
14	2S	4	LEU	6.2
44	1m	24	GLY	6.2
32	1a	1234	C	6.1
3	2D	38	LYS	6.1
11	2P	68	GLN	6.1
32	2a	1288	A	6.1
32	2a	1346	A	6.1
31	19	37	GLY	6.1
32	2a	1030(B)	C	6.1
32	2a	1352	C	6.1
32	1a	1385	G	6.1
52	1u	9	ARG	6.1
32	1a	1157	A	6.1
36	1e	25	ARG	6.1
45	2n	31	ARG	6.1
46	2o	65	ARG	6.1
50	2s	73	GLU	6.1
1	2A	614(B)	G	6.1
32	1a	1181	G	6.1
32	1a	978	A	6.1
32	2a	1001	A	6.1
40	1i	70	LYS	6.1
41	1j	5	ARG	6.1
52	2u	10	ARG	6.1
40	2i	17	VAL	6.1
38	1g	153	HIS	6.1
50	1s	2	PRO	6.1
1	1A	2119	A	6.1
44	2m	86	CYS	6.1
38	1g	98	SER	6.1
40	1i	5	TYR	6.1
50	1s	49	ILE	6.1
32	2a	1370	G	6.1
33	2b	108	ILE	6.1
1	1A	1082	U	6.1
26	14	68	ARG	6.0
51	1t	80	ARG	6.0
48	2q	37	LYS	6.0
50	1s	7	LYS	6.0
32	1a	1331	G	6.0

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Mol	Chain	Res	Type	RSRZ
29	17	48	LYS	6.0
34	2c	164	ARG	6.0
33	1b	95	GLN	6.0
40	2i	85	LEU	6.0
50	1s	73	GLU	6.0
34	1c	13	GLY	6.0
40	2i	18	PHE	6.0
33	2b	152	PHE	6.0
32	1a	570	G	6.0
32	1a	933	G	6.0
51	2t	23	ARG	6.0
1	1A	2139	C	5.9
32	2a	1119	C	5.9
33	2b	163	PHE	5.9
45	2n	11	LYS	5.9
34	2c	154	SER	5.9
34	2c	155	GLY	5.9
33	2b	97	TRP	5.9
44	1m	22	ILE	5.9
32	2a	1188	A	5.9
32	1a	1195	C	5.9
14	2S	93	LYS	5.9
32	2a	1308	U	5.9
32	2a	1362	C	5.9
38	1g	28	ASN	5.9
44	2m	89	GLY	5.9
47	2p	28	ARG	5.9
38	2g	74	GLU	5.9
40	1i	99	LEU	5.9
50	1s	29	ARG	5.9
38	1g	80	VAL	5.8
47	2p	31	LYS	5.8
40	2i	11	LYS	5.8
38	2g	34	GLY	5.8
32	1a	1139	G	5.8
41	2j	45	ARG	5.8
32	1a	1293	G	5.8
32	1a	1333	A	5.8
1	2A	1090	U	5.8
17	2V	81	TYR	5.8
32	2a	1222	G	5.8
45	1n	34	TYR	5.8

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Mol	Chain	Res	Type	RSRZ
32	1a	1305	G	5.8
48	1q	24	GLU	5.8
38	1g	74	GLU	5.8
32	2a	1114	C	5.8
35	1d	73	ARG	5.8
50	2s	2	PRO	5.8
32	1a	1194	U	5.8
32	1a	1257	U	5.8
41	1j	45	ARG	5.8
44	1m	71	ARG	5.8
32	2a	1235	U	5.8
50	1s	53	ASN	5.8
40	1i	67	GLY	5.8
50	1s	9	VAL	5.8
38	1g	25	ALA	5.8
32	2a	1185	G	5.7
26	14	67	TYR	5.7
38	1g	82	GLY	5.7
41	1j	34	VAL	5.7
1	2A	2145	C	5.7
32	1a	1372	U	5.7
31	29	1	MET	5.7
34	1c	155	GLY	5.7
32	2a	1017	G	5.7
6	2G	157	ILE	5.7
35	2d	71	SER	5.7
1	2A	2161	C	5.7
50	2s	74	PHE	5.7
40	1i	2	GLU	5.7
26	24	9	LEU	5.7
16	2U	43	GLY	5.7
6	1G	35	GLU	5.7
33	2b	110	GLN	5.7
31	29	35	ARG	5.7
32	1a	980	C	5.7
44	1m	99	ARG	5.7
45	1n	31	ARG	5.7
40	2i	15	ALA	5.7
32	1a	1174	G	5.7
51	2t	18	GLN	5.7
31	29	17	ILE	5.7
50	1s	32	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
44	1m	89	GLY	5.7
32	1a	946	A	5.6
32	2a	1183	A	5.6
32	2a	1250	A	5.6
32	1a	1190	G	5.6
38	2g	28	ASN	5.6
44	2m	101	GLN	5.6
11	2P	66	GLY	5.6
44	1m	74	VAL	5.6
32	2a	1368	G	5.6
38	1g	155	ARG	5.6
32	1a	1330	U	5.6
41	2j	23	ILE	5.6
32	1a	220	G	5.6
32	2a	1309	G	5.6
32	1a	218	C	5.6
32	2a	1320	C	5.6
32	1a	1119	C	5.6
32	1a	1351	U	5.6
17	2V	72	VAL	5.6
52	1u	22	ARG	5.6
40	1i	49	PRO	5.6
3	2D	50	THR	5.6
32	2a	1270	C	5.6
40	1i	28	VAL	5.6
50	1s	76	PRO	5.6
14	2S	7	TYR	5.6
40	2i	88	TYR	5.6
51	2t	69	GLY	5.6
34	1c	3	ASN	5.6
10	2O	31	LYS	5.5
44	1m	29	ARG	5.5
51	2t	74	LYS	5.5
33	2b	200	ILE	5.5
41	1j	98	ILE	5.5
19	2X	33	LYS	5.5
42	2k	123	LYS	5.5
40	2i	8	GLY	5.5
29	27	47	ARG	5.5
40	2i	83	ARG	5.5
1	1A	2147	G	5.5
1	1A	2171	A	5.5

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Mol	Chain	Res	Type	RSRZ
38	1g	134	ALA	5.5
45	1n	39	LEU	5.5
32	2a	978	A	5.5
32	2a	1316	G	5.5
33	1b	165	VAL	5.5
1	1A	1064	C	5.5
32	2a	1317	C	5.5
30	28	29	LYS	5.5
35	2d	67	ILE	5.5
32	2a	823	G	5.5
26	24	63	TYR	5.5
41	1j	38	ILE	5.4
50	2s	83	HIS	5.4
32	2a	1305	G	5.4
38	1g	91	VAL	5.4
6	2G	35	GLU	5.4
6	2G	39	ILE	5.4
32	1a	1343	G	5.4
35	2d	122	ARG	5.4
38	1g	81	GLY	5.4
32	2a	1311	G	5.4
41	2j	47	PHE	5.4
38	1g	69	VAL	5.4
32	2a	108	G	5.4
35	2d	5	ILE	5.4
32	1a	935	A	5.4
32	1a	1319	A	5.4
43	1l	91	LYS	5.4
50	1s	60	VAL	5.4
42	2k	118	GLY	5.4
46	1o	57	LEU	5.4
32	1a	1065	U	5.4
32	2a	1361	G	5.4
45	1n	25	VAL	5.4
32	1a	401	C	5.4
32	1a	1344	C	5.4
32	2a	1111	A	5.4
33	2b	197	VAL	5.4
44	2m	106	ASN	5.4
50	1s	67	VAL	5.3
48	1q	26	GLN	5.3
32	1a	951	G	5.3

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Mol	Chain	Res	Type	RSRZ
32	1a	1310	G	5.3
44	2m	109	THR	5.3
46	1o	31	LEU	5.3
50	2s	44	MET	5.3
33	1b	175	ARG	5.3
1	1A	1073	A	5.3
41	2j	56	HIS	5.3
40	2i	75	ASP	5.3
1	2A	2148	G	5.3
38	1g	38	LEU	5.3
34	2c	2	GLY	5.3
28	26	54	ILE	5.3
32	1a	1362	C	5.3
1	1A	2125	G	5.3
34	2c	152	ILE	5.3
32	1a	1291	G	5.3
32	2a	1042	G	5.3
44	2m	81	LEU	5.3
9	2N	44	PRO	5.3
1	1A	2137	C	5.3
32	1a	622	A	5.3
50	1s	72	GLY	5.3
32	2a	587	G	5.3
29	17	47	ARG	5.3
35	1d	135	LEU	5.3
32	1a	1250	A	5.3
34	1c	2	GLY	5.3
34	2c	159	GLY	5.3
42	1k	60	ALA	5.3
44	2m	7	VAL	5.3
48	1q	23	VAL	5.3
32	1a	135	C	5.3
32	1a	1320	C	5.3
48	1q	28	PRO	5.3
36	2e	26	PHE	5.3
41	1j	69	ASN	5.3
31	29	10	ILE	5.3
32	2a	755	G	5.3
40	1i	84	ALA	5.3
50	1s	47	HIS	5.3
50	1s	62	ILE	5.3
16	2U	31	SER	5.3

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Mol	Chain	Res	Type	RSRZ
11	2P	57	THR	5.2
31	29	22	ARG	5.2
50	2s	72	GLY	5.2
32	1a	136	C	5.2
14	1S	13	ARG	5.2
46	2o	25	THR	5.2
11	2P	59	LEU	5.2
32	1a	1128	C	5.2
14	1S	7	TYR	5.2
34	1c	206	GLU	5.2
35	1d	69	GLY	5.2
51	2t	66	ALA	5.2
32	2a	1118	C	5.2
47	1p	35	LYS	5.2
9	2N	43	THR	5.2
32	1a	1136	U	5.2
50	2s	52	TYR	5.2
45	1n	7	ILE	5.2
32	1a	1184	G	5.2
32	1a	1312	G	5.2
32	2a	1151	A	5.2
38	2g	77	SER	5.2
50	2s	35	SER	5.2
32	2a	933	G	5.2
14	2S	32	LEU	5.2
35	2d	136	PRO	5.2
47	2p	59	TRP	5.2
34	2c	163	ALA	5.2
47	2p	7	ALA	5.2
32	2a	654	G	5.2
50	2s	58	VAL	5.2
32	1a	63	C	5.2
34	1c	159	GLY	5.1
1	1A	2162	G	5.1
38	1g	83	ALA	5.1
16	2U	44	ASN	5.1
50	2s	54	GLY	5.1
32	1a	1113	C	5.1
32	1a	1118	C	5.1
33	2b	148	TYR	5.1
44	1m	88	ARG	5.1
1	1A	1057	A	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2169	A	5.1
14	1S	4	LEU	5.1
32	2a	1187	G	5.1
40	1i	98	PRO	5.1
50	1s	37	ARG	5.1
1	2A	2142	C	5.1
32	2a	879	C	5.1
47	2p	19	ILE	5.1
40	1i	45	ALA	5.1
3	2D	37	LEU	5.1
47	2p	9	PHE	5.1
1	2A	2151	G	5.1
1	2A	2163	C	5.1
33	2b	140	HIS	5.1
34	1c	179	ARG	5.1
47	2p	8	ARG	5.1
51	2t	20	LEU	5.1
51	1t	74	LYS	5.1
44	1m	92	HIS	5.1
32	1a	822	C	5.1
32	1a	1384	C	5.1
38	2g	27	ILE	5.1
1	2A	2165	G	5.1
17	2V	83	ARG	5.1
23	2I	36	GLY	5.1
38	2g	84	ASN	5.1
1	1A	1078	U	5.1
48	2q	71	PHE	5.1
42	2k	120	ARG	5.1
26	14	65	ASP	5.1
32	1a	500	G	5.1
51	2t	22	ARG	5.1
14	2S	33	LYS	5.1
39	1h	90	GLY	5.1
32	1a	1129	C	5.1
43	1l	113	ARG	5.1
44	1m	67	GLU	5.1
40	2i	16	ARG	5.1
41	1j	37	PRO	5.0
32	1a	1222	G	5.0
32	2a	1184	G	5.0
51	2t	26	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
35	1d	93	PHE	5.0
51	2t	72	LEU	5.0
14	2S	29	PHE	5.0
34	1c	174	PRO	5.0
45	2n	38	GLY	5.0
47	1p	4	ILE	5.0
32	2a	1094	G	5.0
50	1s	31	ILE	5.0
1	1A	2136	C	5.0
1	2A	1933	G	5.0
39	2h	92	ARG	5.0
38	1g	27	ILE	5.0
36	2e	88	LYS	5.0
51	1t	14	LYS	5.0
35	1d	66	ARG	5.0
42	2k	126	ARG	5.0
47	1p	29	ASP	5.0
32	1a	1001(A)	G	5.0
47	1p	21	VAL	5.0
32	1a	43	C	5.0
51	1t	69	GLY	5.0
11	1P	71	VAL	5.0
40	2i	124	GLN	5.0
1	2A	2164	C	5.0
38	2g	9	VAL	5.0
51	2t	10	LEU	5.0
32	2a	1315	U	5.0
51	2t	71	THR	4.9
32	1a	1358	U	4.9
30	28	24	ALA	4.9
47	2p	20	VAL	4.9
51	2t	11	SER	4.9
34	1c	4	LYS	4.9
3	2D	35	LYS	4.9
32	1a	823	G	4.9
31	29	16	VAL	4.9
40	2i	90	PRO	4.9
52	2u	12	LYS	4.9
1	1A	2118	U	4.9
32	1a	1212	U	4.9
32	1a	1313	U	4.9
35	2d	11	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
40	2i	50	LEU	4.9
46	1o	62	GLN	4.9
40	2i	5	TYR	4.9
47	1p	32	TYR	4.9
32	1a	1324	A	4.9
32	2a	1306	A	4.9
32	2a	1516	G	4.9
38	1g	142	GLU	4.9
30	28	26	LYS	4.9
1	2A	2141	G	4.9
33	1b	98	LEU	4.9
40	2i	101	PHE	4.9
40	2i	112	LYS	4.9
36	1e	18	ARG	4.9
40	1i	3	GLN	4.9
26	14	50	VAL	4.9
47	1p	42	ARG	4.9
42	1k	123	LYS	4.9
51	1t	26	ASN	4.9
32	1a	1029	C	4.9
32	1a	1233	G	4.9
32	2a	742	G	4.9
40	2i	92	TYR	4.9
1	1A	1086	A	4.9
32	2a	1035	A	4.9
51	1t	68	LYS	4.9
14	2S	8	GLU	4.9
32	2a	1068	G	4.9
40	2i	123	PRO	4.9
47	2p	27	LYS	4.9
51	2t	9	ASN	4.9
51	1t	83	ARG	4.9
3	1D	276	LYS	4.8
32	1a	947	G	4.8
32	2a	378	G	4.8
45	2n	29	ARG	4.8
51	2t	21	LYS	4.8
31	29	36	GLN	4.8
32	2a	950	U	4.8
32	1a	1017	G	4.8
32	1a	1266	G	4.8
32	1a	202	U	4.8

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Mol	Chain	Res	Type	RSRZ
41	1j	4	ILE	4.8
30	28	10	ALA	4.8
32	1a	782	A	4.8
38	2g	83	ALA	4.8
40	2i	119	ALA	4.8
45	2n	10	ALA	4.8
1	2A	2111	C	4.8
38	2g	80	VAL	4.8
32	1a	1334	G	4.8
21	2Z	192	ALA	4.8
1	1A	888	C	4.8
50	1s	81	ARG	4.8
44	1m	32	GLU	4.8
32	1a	1251	A	4.8
6	2G	11	TYR	4.8
39	1h	3	THR	4.8
47	2p	17	TYR	4.8
33	1b	194	PRO	4.8
46	1o	68	ARG	4.8
29	27	46	VAL	4.8
40	1i	74	ILE	4.8
51	1t	17	ARG	4.8
1	2A	2320	A	4.8
32	1a	1242	C	4.8
32	2a	1268	A	4.8
45	2n	13	THR	4.8
34	2c	172	ARG	4.8
38	1g	26	PHE	4.8
52	2u	3	LYS	4.8
41	1j	36	GLY	4.8
1	2A	2153	G	4.8
34	2c	153	VAL	4.8
14	2S	52	SER	4.7
40	2i	97	LYS	4.7
39	1h	2	LEU	4.7
36	1e	82	VAL	4.7
45	1n	35	ARG	4.7
20	2Y	4	LYS	4.7
34	1c	201	TYR	4.7
36	2e	23	GLY	4.7
14	2S	37	ALA	4.7
40	1i	79	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
44	1m	72	ALA	4.7
45	2n	25	VAL	4.7
46	2o	68	ARG	4.7
50	2s	57	HIS	4.7
1	1A	2149	G	4.7
1	1A	2165	G	4.7
32	1a	945	G	4.7
48	1q	40	LYS	4.7
34	2c	177	THR	4.7
40	2i	68	GLY	4.7
44	1m	93	ARG	4.7
50	1s	8	GLY	4.7
32	2a	1243	C	4.7
41	1j	17	ASP	4.7
51	1t	67	ALA	4.7
51	1t	16	HIS	4.7
50	2s	59	PRO	4.7
33	2b	111	ARG	4.7
33	1b	187	LEU	4.7
23	11	26	ARG	4.7
38	1g	11	GLN	4.7
1	2A	2319	G	4.7
25	23	11	SER	4.7
32	2a	1257	U	4.7
32	1a	1110	A	4.7
32	2a	325	A	4.7
32	2a	1110	A	4.7
40	1i	63	ILE	4.7
38	2g	85	TYR	4.7
40	1i	50	LEU	4.7
32	2a	1181	G	4.7
20	2Y	5	MET	4.7
48	1q	20	THR	4.7
39	2h	112	LEU	4.7
31	29	25	VAL	4.7
38	2g	145	ALA	4.7
50	1s	39	THR	4.7
3	1D	37	LEU	4.7
32	2a	1322	C	4.7
31	29	9	ARG	4.7
50	2s	15	LEU	4.7
43	1l	123	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
41	1j	68	HIS	4.7
40	2i	84	ALA	4.7
32	1a	1311	G	4.6
45	2n	37	PHE	4.6
1	1A	1077	A	4.6
31	29	18	ARG	4.6
44	2m	78	ILE	4.6
32	1a	998	G	4.6
38	2g	36	LYS	4.6
41	2j	41	PRO	4.6
23	21	22	GLY	4.6
33	1b	148	TYR	4.6
48	2q	24	GLU	4.6
38	2g	92	SER	4.6
44	1m	5	ALA	4.6
51	2t	83	ARG	4.6
30	28	25	MET	4.6
31	29	34	GLN	4.6
1	2A	2168	G	4.6
50	2s	51	VAL	4.6
48	1q	78	GLU	4.6
40	1i	96	LEU	4.6
45	2n	7	ILE	4.6
32	1a	1140	C	4.6
32	2a	655	A	4.6
44	1m	56	LEU	4.6
50	1s	75	ALA	4.6
32	1a	1383	C	4.6
44	1m	28	ALA	4.6
47	2p	23	ASP	4.6
11	2P	30	THR	4.6
32	1a	623	C	4.6
29	17	46	VAL	4.6
32	1a	1374	A	4.6
34	2c	162	GLN	4.6
1	2A	2160	G	4.6
32	1a	1030(C)	G	4.6
46	2o	15	PHE	4.6
23	21	26	ARG	4.6
38	1g	42	ILE	4.6
38	2g	73	MET	4.6
41	1j	74	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
50	2s	40	ILE	4.6
1	2A	1087	G	4.6
32	1a	1300	G	4.6
11	2P	35	HIS	4.6
41	1j	53	PRO	4.6
32	2a	1223	C	4.6
32	2a	621	A	4.6
31	29	33	LYS	4.6
32	1a	219	C	4.5
32	2a	403	C	4.5
33	2b	187	LEU	4.5
40	2i	6	GLY	4.5
44	2m	82	MET	4.5
1	1A	2110	G	4.5
32	1a	1178	G	4.5
32	1a	1182	G	4.5
41	1j	10	GLY	4.5
1	2A	2172	U	4.5
51	2t	80	ARG	4.5
17	2V	82	ARG	4.5
1	1A	2109	U	4.5
14	2S	31	SER	4.5
25	23	28	LEU	4.5
47	2p	35	LYS	4.5
6	2G	72	ARG	4.5
32	2a	1367	C	4.5
38	1g	71	PRO	4.5
43	2l	100	ILE	4.5
32	2a	1034	G	4.5
32	2a	1355	G	4.5
32	1a	1252	A	4.5
39	2h	134	ILE	4.5
14	1S	6	ALA	4.5
48	2q	32	TYR	4.5
1	2A	2116	G	4.5
32	1a	1265	G	4.5
45	1n	28	GLY	4.5
16	2U	41	ALA	4.5
6	2G	62	LEU	4.5
40	2i	102	LEU	4.5
41	2j	42	THR	4.5
39	1h	58	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
39	1h	91	ARG	4.5
9	2N	8	GLN	4.5
12	2Q	100	GLY	4.5
1	1A	2124	G	4.5
33	2b	162	ILE	4.5
36	1e	118	ILE	4.5
39	1h	21	LYS	4.5
30	28	46	ARG	4.5
32	2a	1205	U	4.5
52	1u	24	ARG	4.5
20	2Y	35	TYR	4.5
32	2a	112	G	4.5
32	2a	622	A	4.5
35	1d	138	TYR	4.5
26	24	66	SER	4.5
32	2a	1195	C	4.5
1	2A	2119	A	4.5
1	2A	2166	G	4.5
40	1i	65	VAL	4.5
16	2U	42	ALA	4.5
9	2N	37	LYS	4.5
34	1c	172	ARG	4.4
6	2G	97	ASP	4.4
38	1g	13	GLN	4.4
16	2U	46	ALA	4.4
32	2a	1067	A	4.4
38	1g	73	MET	4.4
41	1j	55	LYS	4.4
16	2U	49	HIS	4.4
32	1a	1033	G	4.4
1	2A	2128	C	4.4
32	2a	1103	C	4.4
41	2j	78	ASN	4.4
14	1S	5	THR	4.4
32	1a	1260	C	4.4
32	2a	1307	U	4.4
35	2d	74	GLN	4.4
41	2j	61	GLU	4.4
1	2A	2171	A	4.4
31	29	8	LYS	4.4
34	1c	162	GLN	4.4
45	2n	27	CYS	4.4

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Mol	Chain	Res	Type	RSRZ
32	2a	324	G	4.4
50	2s	39	THR	4.4
23	21	29	GLY	4.4
45	2n	8	GLU	4.4
32	1a	134	A	4.4
32	2a	1364	U	4.4
32	2a	877	C	4.4
28	26	11	LEU	4.4
26	24	64	GLY	4.4
32	2a	262	A	4.4
32	2a	1345	U	4.4
47	2p	5	ARG	4.4
41	1j	40	LEU	4.4
47	1p	23	ASP	4.4
33	2b	107	THR	4.4
1	1A	887	A	4.4
32	2a	1329	A	4.4
47	1p	1	MET	4.4
31	29	23	VAL	4.4
32	2a	1108	G	4.4
32	2a	1356	G	4.4
48	1q	10	VAL	4.4
51	1t	64	ASP	4.4
41	2j	68	HIS	4.4
47	1p	28	ARG	4.4
32	2a	878	G	4.4
34	1c	11	ARG	4.4
32	2a	1375	A	4.4
1	1A	2111	C	4.4
32	2a	1321	C	4.4
46	1o	15	PHE	4.4
1	1A	1062	G	4.3
12	2Q	34	LEU	4.3
32	1a	1276	G	4.3
42	2k	119	CYS	4.3
50	1s	61	TYR	4.3
38	1g	76	ARG	4.3
47	2p	18	ARG	4.3
1	1A	2163	C	4.3
19	2X	1	MET	4.3
32	1a	1328	C	4.3
46	1o	28	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
3	2D	221	VAL	4.3
36	1e	24	ARG	4.3
50	1s	38	SER	4.3
46	1o	59	MET	4.3
32	1a	217	C	4.3
32	2a	1097	C	4.3
47	2p	74	LEU	4.3
33	2b	57	PHE	4.3
9	2N	84	LYS	4.3
14	2S	35	ILE	4.3
32	2a	377	G	4.3
33	2b	196	LEU	4.3
34	1c	192	THR	4.3
43	2l	64	TYR	4.3
32	2a	1109	C	4.3
51	2t	63	ILE	4.3
32	2a	1357	A	4.3
35	1d	137	SER	4.3
45	2n	60	SER	4.3
32	1a	1315	U	4.3
32	2a	757	U	4.3
33	2b	100	GLY	4.3
51	1t	18	GLN	4.3
34	1c	177	THR	4.3
32	1a	1032	G	4.3
32	1a	1224	G	4.3
32	2a	1258	G	4.3
51	2t	14	LYS	4.3
6	1G	2	PRO	4.3
32	1a	1342	C	4.3
32	2a	1328	C	4.3
41	1j	73	ASP	4.3
51	2t	17	ARG	4.3
3	2D	40	THR	4.3
21	2Z	199	LYS	4.3
39	2h	133	LEU	4.3
1	2A	1085	A	4.3
32	1a	1151	A	4.3
40	1i	13	ALA	4.3
51	1t	62	LEU	4.3
14	2S	30	ARG	4.3
16	2U	40	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
45	1n	8	GLU	4.3
1	2A	34	C	4.3
43	1l	122	THR	4.3
32	2a	1358	U	4.3
33	2b	144	ARG	4.3
35	2d	66	ARG	4.3
6	2G	93	THR	4.3
32	1a	1363	C	4.3
32	2a	1233	G	4.3
41	1j	8	LEU	4.3
50	2s	68	GLY	4.3
40	1i	61	ALA	4.3
32	1a	1066	C	4.2
38	1g	101	LEU	4.2
47	2p	11	SER	4.2
40	1i	11	LYS	4.2
30	28	27	THR	4.2
38	1g	151	TYR	4.2
35	1d	157	LEU	4.2
47	2p	30	GLY	4.2
24	12	69	ARG	4.2
26	24	68	ARG	4.2
32	1a	1355	G	4.2
38	2g	10	ARG	4.2
33	1b	147	LYS	4.2
36	2e	17	ALA	4.2
38	1g	2	ALA	4.2
46	2o	51	HIS	4.2
45	2n	23	ARG	4.2
1	2A	2167	U	4.2
9	2N	42	TRP	4.2
46	2o	61	GLY	4.2
32	1a	1272	G	4.2
40	2i	93	ARG	4.2
46	1o	63	ARG	4.2
1	2A	2107	C	4.2
32	1a	1001	A	4.2
32	2a	1344	C	4.2
6	2G	58	GLN	4.2
1	1A	2296	U	4.2
21	2Z	197	ILE	4.2
34	2c	206	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
44	1m	30	ALA	4.2
1	1A	2115	G	4.2
32	1a	112	G	4.2
32	2a	1285	A	4.2
22	20	76	GLY	4.2
34	2c	158	GLY	4.2
40	1i	24	GLY	4.2
50	2s	82	GLY	4.2
48	1q	6	LEU	4.2
1	1A	2126	A	4.2
1	2A	2152	G	4.2
32	1a	1294	G	4.2
1	1A	2164	C	4.2
22	20	74	ARG	4.2
36	1e	22	GLY	4.2
50	1s	18	LYS	4.2
11	2P	58	THR	4.2
45	1n	44	LEU	4.2
1	1A	1101	U	4.2
41	2j	17	ASP	4.2
34	1c	175	LEU	4.2
39	2h	85	ARG	4.2
40	1i	102	LEU	4.2
40	2i	67	GLY	4.2
1	2A	1973	G	4.2
51	1t	70	SER	4.2
47	1p	15	PRO	4.2
32	2a	1043	C	4.1
32	2a	1044	A	4.1
32	2a	1360	A	4.1
40	2i	96	LEU	4.1
41	1j	20	ALA	4.1
51	2t	59	ALA	4.1
32	2a	1058	G	4.1
32	2a	1271	G	4.1
34	2c	157	ILE	4.1
43	1l	124	LYS	4.1
22	20	21	LEU	4.1
34	1c	200	ALA	4.1
32	2a	784	C	4.1
32	2a	800	G	4.1
33	2b	109	SER	4.1

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Mol	Chain	Res	Type	RSRZ
6	1G	72	ARG	4.1
1	1A	2320	A	4.1
1	2A	2170	A	4.1
32	1a	1147	C	4.1
32	2a	60	A	4.1
40	2i	27	THR	4.1
14	2S	9	ARG	4.1
48	2q	36	ILE	4.1
32	1a	959	A	4.1
40	1i	31	GLN	4.1
41	1j	70	ARG	4.1
45	1n	23	ARG	4.1
50	1s	12	ASP	4.1
1	1A	2141	G	4.1
32	1a	1026	G	4.1
32	2a	1331	G	4.1
26	24	7	PRO	4.1
16	2U	35	ALA	4.1
32	1a	1141	C	4.1
35	1d	76	ARG	4.1
32	2a	977	A	4.1
39	2h	88	LYS	4.1
46	2o	60	VAL	4.1
38	2g	95	ARG	4.1
32	1a	42	G	4.1
39	2h	31	PHE	4.1
32	1a	1209	C	4.1
50	2s	75	ALA	4.1
26	24	67	TYR	4.1
43	1l	98	TYR	4.1
32	2a	1369	C	4.1
39	1h	18	ARG	4.1
39	2h	15	ASN	4.1
41	2j	51	ARG	4.1
32	1a	1002	G	4.1
51	1t	82	SER	4.1
51	1t	76	ALA	4.1
50	1s	52	TYR	4.1
22	10	75	LEU	4.1
17	2V	75	PHE	4.1
40	2i	76	ALA	4.1
32	1a	1031	G	4.1

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Mol	Chain	Res	Type	RSRZ
32	2a	43	C	4.1
50	1s	54	GLY	4.1
32	2a	1031	G	4.1
39	1h	31	PHE	4.0
50	1s	48	THR	4.0
47	2p	2	VAL	4.0
14	2S	95	HIS	4.0
1	1A	2148	G	4.0
32	1a	957	U	4.0
32	2a	949	A	4.0
48	1q	4	LYS	4.0
43	2l	99	HIS	4.0
34	1c	156	ARG	4.0
1	1A	2108	C	4.0
38	1g	90	GLU	4.0
13	1R	69	ASP	4.0
24	12	70	GLN	4.0
32	2a	107	G	4.0
33	1b	198	ASP	4.0
47	1p	60	LEU	4.0
31	29	15	LYS	4.0
16	2U	37	GLU	4.0
47	2p	34	GLU	4.0
32	1a	1030(B)	C	4.0
41	1j	26	ALA	4.0
17	2V	84	LYS	4.0
41	2j	53	PRO	4.0
32	1a	1064	G	4.0
32	2a	947	G	4.0
16	2U	48	ALA	4.0
38	1g	133	GLY	4.0
1	2A	2140	C	4.0
50	1s	79	THR	4.0
32	2a	1289	A	4.0
51	2t	16	HIS	4.0
14	1S	17	ARG	4.0
14	1S	93	LYS	4.0
14	2S	87	PHE	4.0
6	2G	159	VAL	4.0
44	1m	65	LYS	4.0
32	2a	1180	A	4.0
40	2i	61	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	2A	1091	G	4.0
32	1a	1030(A)	G	4.0
11	2P	15	ARG	4.0
34	1c	14	ILE	4.0
41	2j	50	ILE	4.0
51	1t	55	ILE	4.0
30	18	33	ASN	4.0
7	2H	112	PRO	4.0
40	1i	51	ARG	4.0
51	1t	8	ARG	4.0
51	2t	64	ASP	4.0
48	1q	33	GLY	4.0
36	1e	21	ALA	4.0
51	2t	76	ALA	4.0
13	2R	5	LYS	4.0
23	21	33	LYS	4.0
31	19	8	LYS	4.0
32	1a	1045	C	4.0
32	1a	1303	C	4.0
32	1a	977	A	4.0
6	1G	39	ILE	4.0
51	2t	7	LYS	4.0
1	1A	2153	G	4.0
50	2s	41	VAL	4.0
38	1g	15	ASP	4.0
1	2A	1932	A	4.0
40	2i	77	ILE	4.0
44	2m	6	GLY	3.9
51	1t	10	LEU	3.9
32	1a	1028	C	3.9
32	2a	1218	C	3.9
45	2n	22	THR	3.9
8	1I	117	GLU	3.9
40	2i	53	VAL	3.9
23	11	23	LYS	3.9
41	1j	39	PRO	3.9
33	1b	188	ALA	3.9
32	2a	822	C	3.9
50	2s	80	TYR	3.9
46	2o	64	ARG	3.9
49	2r	71	LYS	3.9
32	2a	323	U	3.9

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Mol	Chain	Res	Type	RSRZ
32	2a	782	A	3.9
31	29	20	HIS	3.9
32	2a	221	C	3.9
32	2a	1234	C	3.9
32	2a	1139	G	3.9
32	2a	101	A	3.9
43	2l	7	ILE	3.9
51	1t	25	ARG	3.9
35	2d	135	LEU	3.9
33	2b	161	ALA	3.9
1	2A	2110	G	3.9
32	2a	1385	G	3.9
32	2a	1041	A	3.9
39	1h	20	TYR	3.9
43	1l	112	ASP	3.9
6	2G	67	LYS	3.9
28	16	54	ILE	3.9
38	1g	29	LYS	3.9
14	2S	13	ARG	3.9
32	2a	404	U	3.9
32	2a	956	U	3.9
35	1d	148	VAL	3.9
38	1g	37	ASN	3.9
20	2Y	68	HIS	3.9
41	1j	56	HIS	3.9
41	1j	23	ILE	3.9
41	1j	75	ILE	3.9
31	29	3	VAL	3.9
32	1a	379	C	3.9
32	2a	623	C	3.9
50	2s	60	VAL	3.9
43	2l	32	PHE	3.9
7	2H	159	GLU	3.9
1	1A	1067	A	3.9
1	2A	229	A	3.9
45	1n	32	SER	3.9
12	2Q	74	TYR	3.9
47	2p	6	LEU	3.9
20	2Y	43	ASN	3.9
22	10	74	ARG	3.9
32	1a	1039	C	3.9
32	2a	756	C	3.9

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Mol	Chain	Res	Type	RSRZ
32	2a	1037	C	3.9
32	2a	1515	C	3.9
46	2o	63	ARG	3.9
6	2G	152	LEU	3.9
30	28	47	LYS	3.9
40	1i	97	LYS	3.9
1	2A	2117	A	3.9
32	1a	1176	A	3.9
32	1a	1329	A	3.9
32	1a	201	C	3.9
32	2a	1113	C	3.9
11	2P	29	LYS	3.9
40	1i	27	THR	3.9
46	2o	66	LEU	3.9
41	2j	19	SER	3.9
50	1s	15	LEU	3.8
16	2U	47	TYR	3.8
32	1a	1038	C	3.8
32	1a	1223	C	3.8
32	2a	754	C	3.8
40	2i	72	GLY	3.8
47	2p	4	ILE	3.8
40	2i	46	ALA	3.8
45	2n	3	ARG	3.8
48	1q	63	ARG	3.8
3	1D	50	THR	3.8
32	1a	1125	U	3.8
32	2a	1002	G	3.8
33	1b	70	PHE	3.8
6	1G	88	ILE	3.8
22	20	77	ARG	3.8
32	2a	743	U	3.8
39	1h	5	PRO	3.8
1	1A	226	G	3.8
24	22	1	MET	3.8
32	1a	755	G	3.8
19	2X	79	ALA	3.8
38	2g	69	VAL	3.8
43	1l	99	HIS	3.8
39	1h	4	ASP	3.8
43	2l	28	LYS	3.8
20	1Y	2	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
34	2c	179	ARG	3.8
44	1m	108	ARG	3.8
32	2a	1219	U	3.8
34	1c	169	ALA	3.8
38	1g	39	ALA	3.8
1	2A	2136	C	3.8
32	1a	224	C	3.8
32	2a	783	C	3.8
14	2S	94	TYR	3.8
44	2m	84	ILE	3.8
33	2b	102	LEU	3.8
11	2P	64	LYS	3.8
45	1n	33	VAL	3.8
33	1b	57	PHE	3.8
41	2j	10	GLY	3.8
32	1a	756	C	3.8
1	1A	2151	G	3.8
33	2b	133	LYS	3.8
44	1m	96	LEU	3.8
1	1A	1083	U	3.8
11	2P	65	ARG	3.8
48	1q	59	ILE	3.8
32	2a	400	C	3.8
32	2a	1063	C	3.8
38	1g	7	ALA	3.8
1	1A	1094	U	3.8
34	1c	157	ILE	3.8
1	2A	866	A	3.8
38	2g	91	VAL	3.8
1	2A	2146	C	3.8
32	2a	1514	C	3.8
39	2h	131	GLY	3.8
40	2i	122	ALA	3.8
6	2G	161	THR	3.8
11	2P	36	LYS	3.8
22	20	78	TYR	3.8
40	1i	12	GLU	3.8
32	1a	1220	G	3.8
31	19	7	VAL	3.8
39	2h	93	VAL	3.8
46	2o	47	LYS	3.8
43	1l	7	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
44	1m	43	THR	3.8
32	2a	1070	U	3.8
40	1i	18	PHE	3.8
1	2A	2154	G	3.8
3	1D	253	GLN	3.8
44	1m	13	LYS	3.8
39	2h	136	GLU	3.8
1	1A	1070	A	3.8
30	28	16	ILE	3.8
48	1q	98	LEU	3.8
32	1a	784	C	3.8
3	2D	53	PHE	3.8
48	1q	34	LYS	3.7
49	2r	68	LYS	3.7
44	1m	19	LEU	3.7
30	28	14	VAL	3.7
32	2a	570	G	3.7
35	1d	6	GLY	3.7
47	1p	24	ALA	3.7
21	1Z	197	ILE	3.7
42	1k	124	LYS	3.7
51	2t	68	LYS	3.7
14	1S	9	ARG	3.7
38	2g	76	ARG	3.7
1	1A	2319	G	3.7
32	1a	113	G	3.7
32	1a	1048	G	3.7
47	1p	56	ALA	3.7
32	1a	985	C	3.7
39	1h	35	ILE	3.7
45	1n	21	TYR	3.7
48	1q	100	LYS	3.7
16	2U	8	VAL	3.7
41	2j	71	LEU	3.7
43	2l	13	LYS	3.7
1	1A	1068	G	3.7
39	2h	89	PRO	3.7
3	1D	227	ASN	3.7
30	28	11	LYS	3.7
50	2s	49	ILE	3.7
13	2R	47	PHE	3.7
38	1g	135	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
40	1i	59	PHE	3.7
32	2a	975	A	3.7
1	2A	1104	C	3.7
47	1p	20	VAL	3.7
44	2m	65	LYS	3.7
32	2a	1350	A	3.7
13	2R	68	ARG	3.7
34	2c	188	LEU	3.7
32	1a	820	U	3.7
32	2a	620	C	3.7
32	2a	1259	C	3.7
35	1d	74	GLN	3.7
44	2m	85	GLY	3.7
16	2U	28	ARG	3.7
32	2a	1304	G	3.7
6	1G	82	LEU	3.7
31	29	26	ILE	3.7
45	2n	42	ILE	3.7
1	2A	913	U	3.7
35	2d	8	VAL	3.7
32	2a	780	A	3.7
1	1A	2145	C	3.7
6	2G	85	GLY	3.7
33	2b	114	ARG	3.7
9	2N	116	LEU	3.7
35	2d	134	ASP	3.7
31	29	31	LYS	3.7
32	2a	998	G	3.7
32	2a	1057	G	3.7
38	2g	88	PRO	3.7
32	1a	501	C	3.7
47	1p	64	ALA	3.7
33	2b	137	ARG	3.7
47	2p	16	HIS	3.7
44	1m	95	GLY	3.6
32	1a	972	C	3.6
32	1a	1016	A	3.6
38	2g	5	ARG	3.6
39	2h	58	TYR	3.6
39	2h	94	TYR	3.6
41	2j	55	LYS	3.6
16	2U	20	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
32	1a	65	U	3.6
32	2a	1330	U	3.6
40	1i	64	THR	3.6
6	1G	160	VAL	3.6
44	2m	60	VAL	3.6
32	2a	1332	A	3.6
44	1m	26	GLY	3.6
15	2T	1	MET	3.6
3	1D	36	PRO	3.6
19	2X	34	ALA	3.6
43	1l	89	ARG	3.6
44	2m	107	ALA	3.6
33	2b	112	VAL	3.6
50	2s	77	THR	3.6
13	2R	69	ASP	3.6
1	2A	2121	G	3.6
13	1R	68	ARG	3.6
44	1m	80	ARG	3.6
1	2A	2143	C	3.6
32	1a	196	A	3.6
20	2Y	45	VAL	3.6
39	2h	86	ILE	3.6
47	1p	31	LYS	3.6
50	1s	70	LYS	3.6
48	2q	33	GLY	3.6
25	23	29	ARG	3.6
26	14	61	ARG	3.6
48	1q	74	LEU	3.6
16	2U	17	ILE	3.6
23	11	25	LYS	3.6
40	1i	37	PHE	3.6
31	19	25	VAL	3.6
32	2a	821	G	3.6
32	2a	1155	G	3.6
47	1p	7	ALA	3.6
48	1q	37	LYS	3.6
6	2G	100	TRP	3.6
16	2U	45	TYR	3.6
32	1a	389	A	3.6
32	1a	1027	C	3.6
32	2a	1236	A	3.6
46	1o	69	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
10	2O	34	THR	3.6
39	1h	112	LEU	3.6
40	1i	60	ASP	3.6
11	2P	60	MET	3.6
51	2t	29	LYS	3.6
33	1b	184	VAL	3.6
36	2e	86	ALA	3.6
39	2h	111	ILE	3.6
1	2A	2295	C	3.6
32	1a	1515	C	3.6
32	2a	787	A	3.6
38	2g	90	GLU	3.6
3	2D	36	PRO	3.6
38	2g	81	GLY	3.6
20	2Y	46	LYS	3.6
39	1h	36	LEU	3.6
1	1A	2129	C	3.6
1	1A	2142	C	3.6
32	1a	997	U	3.6
32	1a	1269	A	3.6
41	1j	16	LEU	3.6
44	1m	64	TRP	3.6
13	2R	14	SER	3.6
35	2d	115	ARG	3.6
37	2f	90	VAL	3.6
41	2j	6	ILE	3.6
32	1a	1346	A	3.6
47	1p	17	TYR	3.6
51	2t	88	VAL	3.6
32	1a	1063	C	3.6
51	1t	79	ARG	3.6
32	1a	1386	G	3.6
33	2b	95	GLN	3.6
41	1j	6	ILE	3.6
46	2o	72	ARG	3.5
32	2a	820	U	3.5
21	2Z	78	LYS	3.5
32	1a	744	C	3.5
1	2A	1969	A	3.5
28	26	20	ASN	3.5
32	2a	728	A	3.5
39	1h	19	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
16	2U	33	ARG	3.5
32	1a	1124	G	3.5
32	2a	104	G	3.5
33	2b	31	TYR	3.5
40	1i	128	ARG	3.5
46	2o	69	TYR	3.5
44	1m	111	LYS	3.5
32	1a	1211	U	3.5
20	2Y	71	LYS	3.5
51	1t	11	SER	3.5
33	1b	200	ILE	3.5
14	2S	3	ARG	3.5
43	1l	68	ALA	3.5
9	2N	109	LYS	3.5
32	2a	744	C	3.5
32	2a	1045	C	3.5
45	2n	21	TYR	3.5
6	2G	91	ARG	3.5
44	1m	4	ILE	3.5
35	1d	78	LEU	3.5
36	1e	86	ALA	3.5
48	1q	43	LEU	3.5
1	1A	2127	G	3.5
1	1A	2167	U	3.5
14	1S	92	TYR	3.5
45	1n	37	PHE	3.5
32	1a	1218	C	3.5
39	2h	91	ARG	3.5
51	2t	8	ARG	3.5
14	2S	11	LYS	3.5
35	2d	21	LEU	3.5
40	1i	43	ALA	3.5
19	2X	28	PHE	3.5
31	19	26	ILE	3.5
32	2a	951	G	3.5
34	1c	153	VAL	3.5
1	1A	34	C	3.5
32	2a	395	C	3.5
23	11	24	ALA	3.5
41	1j	18	ALA	3.5
14	2S	36	TYR	3.5
51	2t	19	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	2A	2124	G	3.5
32	2a	310	G	3.5
1	1A	2143	C	3.5
31	29	19	ARG	3.5
32	2a	63	C	3.5
3	2D	276	LYS	3.5
48	2q	34	LYS	3.5
22	20	45	PHE	3.5
33	2b	183	PRO	3.5
8	1I	41	GLU	3.5
35	1d	166	LYS	3.5
32	2a	1141	C	3.5
5	2F	41	LEU	3.5
51	1t	23	ARG	3.5
3	1D	228	PRO	3.5
38	2g	8	GLU	3.5
6	1G	34	LEU	3.5
40	2i	81	ILE	3.5
35	1d	59	ARG	3.5
47	1p	25	ARG	3.5
1	1A	2120	G	3.5
32	1a	1241	G	3.5
1	2A	614(A)	U	3.5
1	2A	1785	A	3.5
32	1a	1275	A	3.5
32	2a	1016	A	3.5
38	1g	21	VAL	3.5
16	2U	50	ARG	3.5
36	1e	88	LYS	3.5
40	2i	9	ARG	3.5
40	2i	99	LEU	3.5
48	1q	68	ARG	3.5
32	1a	783	C	3.4
41	2j	58	ASP	3.4
6	2G	142	PRO	3.4
35	1d	202	LEU	3.4
36	2e	31	LEU	3.4
51	2t	24	LEU	3.4
39	1h	22	GLU	3.4
40	1i	23	ASN	3.4
1	2A	1075	C	3.4
39	1h	72	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
39	1h	93	VAL	3.4
32	2a	1522	U	3.4
33	1b	149	LEU	3.4
36	2e	84	PHE	3.4
32	1a	610	G	3.4
13	2R	9	LYS	3.4
52	2u	18	TYR	3.4
32	1a	30	U	3.4
39	2h	130	GLY	3.4
22	20	46	LYS	3.4
45	1n	29	ARG	3.4
1	1A	2154	G	3.4
32	1a	1397	C	3.4
40	2i	82	ALA	3.4
36	2e	12	LEU	3.4
44	1m	101	GLN	3.4
51	1t	63	ILE	3.4
30	28	28	GLY	3.4
38	1g	88	PRO	3.4
6	2G	75	LYS	3.4
31	19	1	MET	3.4
31	29	2	LYS	3.4
32	2a	1521	G	3.4
34	1c	167	TRP	3.4
45	2n	26	ARG	3.4
50	2s	78	ARG	3.4
51	2t	30	LYS	3.4
13	1R	21	TYR	3.4
38	2g	99	LEU	3.4
48	1q	25	ARG	3.4
1	1A	2135	A	3.4
23	21	42	GLN	3.4
32	1a	324	G	3.4
32	2a	1211	U	3.4
14	2S	112	PHE	3.4
46	2o	87	ILE	3.4
1	2A	2108	C	3.4
39	2h	9	MET	3.4
48	2q	23	VAL	3.4
16	2U	12	ARG	3.4
32	1a	1267	C	3.4
32	2a	1254	C	3.4

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Mol	Chain	Res	Type	RSRZ
32	2a	1397	C	3.4
23	2l	48	LYS	3.4
40	1i	85	LEU	3.4
1	2A	1103	A	3.4
26	14	52	THR	3.4
33	2b	185	ILE	3.4
32	1a	1236	A	3.4
32	1a	1280	A	3.4
47	2p	65	GLN	3.4
11	2P	52	GLU	3.4
14	2S	89	ARG	3.4
40	1i	20	ARG	3.4
1	1A	2337	G	3.4
1	2A	2294	C	3.4
42	2k	125	PHE	3.4
48	1q	27	PHE	3.4
30	28	7	HIS	3.4
44	2m	67	GLU	3.4
34	1c	164	ARG	3.4
32	2a	102	G	3.4
36	2e	24	ARG	3.4
6	1G	90	LEU	3.3
41	2j	49	VAL	3.3
16	2U	25	TRP	3.3
40	2i	36	TYR	3.3
36	2e	27	ARG	3.3
30	28	61	LEU	3.3
32	1a	948	C	3.3
32	2a	401	C	3.3
39	1h	133	LEU	3.3
46	1o	32	LEU	3.3
1	1A	1099	G	3.3
32	2a	326	G	3.3
40	1i	33	PHE	3.3
35	2d	207	TYR	3.3
16	2U	36	ARG	3.3
32	2a	1093	A	3.3
1	1A	2138	C	3.3
40	1i	55	ALA	3.3
32	2a	727	G	3.3
32	2a	876	G	3.3
15	1T	114	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
34	1c	15	THR	3.3
41	1j	100	THR	3.3
44	2m	5	ALA	3.3
50	1s	33	THR	3.3
3	1D	219	PRO	3.3
7	2H	128	PRO	3.3
23	21	37	ILE	3.3
16	2U	56	ASP	3.3
31	19	12	ASP	3.3
6	2G	94	LEU	3.3
15	2T	99	LEU	3.3
34	2c	175	LEU	3.3
16	2U	9	VAL	3.3
32	2a	44	G	3.3
36	2e	18	ARG	3.3
32	1a	393	A	3.3
3	2D	250	TRP	3.3
32	1a	656	C	3.3
35	2d	101	LEU	3.3
48	1q	9	VAL	3.3
51	2t	86	ARG	3.3
43	1l	120	TYR	3.3
3	2D	219	PRO	3.3
32	1a	873	A	3.3
32	2a	1221	G	3.3
35	2d	139	ARG	3.3
51	1t	22	ARG	3.3
14	2S	40	ILE	3.3
30	28	58	ILE	3.3
32	1a	261	U	3.3
39	1h	15	ASN	3.3
52	2u	21	TYR	3.3
44	1m	63	THR	3.3
50	2s	76	PRO	3.3
14	1S	28	VAL	3.3
1	1A	2168	G	3.3
32	2a	994	A	3.3
33	1b	163	PHE	3.3
26	14	53	GLU	3.3
38	1g	22	LEU	3.3
8	2I	3	VAL	3.3
13	2R	43	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
25	23	17	LYS	3.3
26	24	65	ASP	3.3
31	19	28	GLU	3.3
32	1a	1030(D)	A	3.3
47	1p	3	LYS	3.3
3	2D	239	ARG	3.3
12	2Q	32	TYR	3.3
32	2a	1156	G	3.3
43	2l	15	ARG	3.3
48	2q	6	LEU	3.3
1	2A	560	C	3.3
1	2A	2139	C	3.3
14	1S	29	PHE	3.3
27	15	60	VAL	3.3
32	1a	311	C	3.3
45	1n	24	CYS	3.3
44	1m	36	LYS	3.3
3	2D	52	ARG	3.3
38	1g	32	ARG	3.3
44	1m	2	ALA	3.3
47	2p	26	ARG	3.3
6	2G	131	TYR	3.3
12	1Q	17	LEU	3.3
32	2a	974	A	3.3
32	2a	1170	A	3.3
48	1q	71	PHE	3.3
32	1a	104	G	3.3
32	1a	800	G	3.3
32	1a	1516	G	3.3
32	2a	328	C	3.3
32	2a	1098	C	3.3
39	1h	92	ARG	3.3
34	2c	178	LEU	3.3
45	2n	6	LEU	3.3
30	18	3	LYS	3.3
32	1a	1044	A	3.2
32	2a	959	A	3.2
32	2a	1333	A	3.2
33	1b	29	ALA	3.2
40	1i	103	THR	3.2
43	1l	6	THR	3.2
32	1a	984	C	3.2

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Mol	Chain	Res	Type	RSRZ
45	2n	24	CYS	3.2
48	1q	42	TYR	3.2
41	2j	22	LYS	3.2
48	1q	56	VAL	3.2
33	1b	96	ARG	3.2
6	2G	87	PRO	3.2
39	2h	99	GLU	3.2
44	1m	112	GLY	3.2
47	1p	10	GLY	3.2
30	28	12	LYS	3.2
38	1g	18	TYR	3.2
46	1o	70	LEU	3.2
32	2a	135	C	3.2
32	2a	1128	C	3.2
32	2a	1203	C	3.2
38	1g	87	VAL	3.2
46	2o	35	ARG	3.2
50	1s	41	VAL	3.2
32	1a	46	G	3.2
32	2a	42	G	3.2
39	2h	36	LEU	3.2
46	1o	34	LEU	3.2
1	2A	2130	U	3.2
30	28	48	PHE	3.2
32	2a	1020	U	3.2
10	1O	1	MET	3.2
32	1a	110	C	3.2
32	1a	549	C	3.2
32	2a	1140	C	3.2
44	2m	92	HIS	3.2
43	2l	9	GLN	3.2
28	16	10	LEU	3.2
32	2a	1030(A)	G	3.2
33	2b	149	LEU	3.2
51	1t	58	LYS	3.2
40	2i	86	VAL	3.2
51	2t	61	SER	3.2
33	2b	68	ILE	3.2
44	2m	26	GLY	3.2
51	1t	56	MET	3.2
1	2A	1974	C	3.2
17	2V	71	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
39	1h	63	LEU	3.2
32	2a	1182	G	3.2
32	1a	1219	U	3.2
35	2d	102	ASP	3.2
14	2S	34	HIS	3.2
43	2l	33	ARG	3.2
46	2o	54	ARG	3.2
22	20	70	GLN	3.2
32	2a	968	A	3.2
44	2m	76	ALA	3.2
6	2G	13	GLU	3.2
6	2G	137	GLU	3.2
17	1V	74	LYS	3.2
44	1m	20	THR	3.2
19	2X	9	LEU	3.2
33	1b	172	ILE	3.2
50	2s	62	ILE	3.2
32	2a	971	G	3.2
32	2a	1266	G	3.2
3	2D	62	TYR	3.2
22	20	69	PHE	3.2
32	1a	994	A	3.2
32	2a	781	A	3.2
48	1q	41	LYS	3.2
44	2m	8	GLU	3.2
3	2D	48	ARG	3.2
13	2R	17	ARG	3.2
32	2a	618	C	3.2
32	2a	1129	C	3.2
8	2l	38	LEU	3.2
34	1c	8	ILE	3.2
39	1h	59	LEU	3.2
30	18	36	LYS	3.2
9	2N	108	PRO	3.2
35	2d	68	TYR	3.2
48	1q	35	VAL	3.2
1	1A	2121	G	3.2
32	1a	1015	A	3.2
32	2a	1179	A	3.2
43	2l	10	LEU	3.2
32	2a	1069	C	3.2
44	1m	75	ALA	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	2G	176	LEU	3.2
32	2a	61	G	3.2
32	2a	1220	G	3.2
1	2A	1067	A	3.2
41	1j	33	GLN	3.2
31	19	24	TYR	3.2
40	1i	125	TYR	3.2
48	2q	42	TYR	3.2
50	1s	59	PRO	3.2
14	1S	11	LYS	3.2
35	2d	96	LEU	3.2
14	1S	3	ARG	3.2
43	2l	101	VAL	3.2
32	1a	66	G	3.2
32	2a	105	G	3.2
50	2s	47	HIS	3.2
32	1a	999	C	3.1
34	1c	199	LYS	3.1
45	2n	9	LYS	3.1
48	2q	4	LYS	3.1
12	2Q	92	GLY	3.1
32	2a	1049	U	3.1
30	28	22	VAL	3.1
47	2p	3	LYS	3.1
13	1R	44	LEU	3.1
22	20	47	PRO	3.1
1	2A	2144	U	3.1
32	1a	390	C	3.1
32	1a	973	G	3.1
32	2a	1030(C)	G	3.1
32	2a	1242	C	3.1
33	2b	70	PHE	3.1
16	2U	30	LYS	3.1
23	21	23	LYS	3.1
38	2g	6	ARG	3.1
32	1a	1245	A	3.1
32	2a	1157	A	3.1
38	2g	87	VAL	3.1
1	1A	2113	U	3.1
32	1a	230	G	3.1
32	1a	742	G	3.1
32	2a	308	C	3.1

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Mol	Chain	Res	Type	RSRZ
32	2a	934	C	3.1
14	2S	17	ARG	3.1
44	1m	91	ARG	3.1
3	1D	231	HIS	3.1
13	2R	13	HIS	3.1
38	1g	19	GLY	3.1
46	1o	58	MET	3.1
1	2A	2122	U	3.1
52	2u	24	ARG	3.1
41	2j	85	LEU	3.1
40	2i	80	GLY	3.1
47	2p	22	THR	3.1
33	2b	164	VAL	3.1
45	2n	30	ALA	3.1
36	1e	23	GLY	3.1
40	2i	100	GLY	3.1
41	2j	11	PHE	3.1
48	1q	36	ILE	3.1
1	2A	2175	C	3.1
11	2P	74	GLU	3.1
12	2Q	80	GLU	3.1
22	20	71	ASP	3.1
32	1a	403	C	3.1
1	1A	1058	G	3.1
1	1A	1973	G	3.1
4	2E	114	ALA	3.1
32	2a	402	G	3.1
32	2a	1386	G	3.1
6	1G	135	LEU	3.1
44	2m	96	LEU	3.1
14	1S	20	ARG	3.1
19	2X	32	PRO	3.1
47	2p	79	VAL	3.1
32	1a	754	C	3.1
32	1a	996	A	3.1
32	2a	932	C	3.1
32	2a	935	A	3.1
32	2a	1189	C	3.1
6	2G	74	LYS	3.1
38	2g	12	LEU	3.1
41	1j	27	ALA	3.1
17	1V	81	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
25	23	15	TYR	3.1
47	2p	39	TYR	3.1
3	1D	53	PHE	3.1
17	2V	86	GLY	3.1
26	14	54	GLY	3.1
32	1a	546	G	3.1
32	1a	785	G	3.1
32	2a	394	G	3.1
32	2a	546	G	3.1
6	2G	40	ASN	3.1
39	2h	87	SER	3.1
33	1b	171	ALA	3.1
35	1d	54	TYR	3.1
36	2e	16	THR	3.1
47	2p	48	TRP	3.1
32	1a	1261	A	3.1
46	1o	87	ILE	3.1
3	2D	39	LYS	3.1
26	24	69	LYS	3.1
32	1a	1356	G	3.1
42	2k	121	PRO	3.1
34	2c	192	THR	3.1
23	11	42	GLN	3.1
43	2l	12	ARG	3.1
52	2u	4	GLY	3.1
32	2a	106	C	3.1
45	2n	4	LYS	3.1
17	2V	87	HIS	3.1
47	1p	6	LEU	3.1
39	2h	54	ASP	3.1
43	2l	8	ASN	3.1
12	2Q	68	ILE	3.1
47	1p	22	THR	3.1
44	2m	27	LYS	3.1
46	2o	48	LYS	3.1
44	1m	82	MET	3.1
1	2A	2062	A	3.1
34	1c	39	ILE	3.0
51	2t	34	LYS	3.0
12	2Q	102	VAL	3.0
50	2s	67	VAL	3.0
5	2F	44	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
51	1t	20	LEU	3.0
20	2Y	65	ALA	3.0
40	2i	45	ALA	3.0
22	20	42	GLY	3.0
32	1a	312	C	3.0
32	1a	1357	A	3.0
32	2a	175	C	3.0
39	1h	131	GLY	3.0
40	1i	68	GLY	3.0
1	2A	2109	U	3.0
6	1G	71	THR	3.0
32	1a	982	U	3.0
38	2g	75	VAL	3.0
3	1D	38	LYS	3.0
16	2U	34	LYS	3.0
44	1m	27	LYS	3.0
51	2t	67	ALA	3.0
1	2A	232	G	3.0
1	2A	1559	G	3.0
3	2D	55	GLY	3.0
30	28	2	PRO	3.0
32	1a	993	G	3.0
32	1a	1193	G	3.0
32	1a	1338	G	3.0
41	2j	52	GLY	3.0
1	2A	912	C	3.0
1	2A	2333	A	3.0
2	1B	48	A	3.0
3	2D	51	VAL	3.0
32	1a	578	C	3.0
32	1a	1382	C	3.0
32	2a	134	A	3.0
32	2a	369	C	3.0
35	1d	115	ARG	3.0
38	1g	92	SER	3.0
44	1m	60	VAL	3.0
46	1o	81	LEU	3.0
51	2t	56	MET	3.0
3	2D	247	ALA	3.0
14	1S	12	PHE	3.0
3	2D	226	MET	3.0
9	2N	23	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
16	2U	18	LEU	3.0
46	2o	57	LEU	3.0
12	2Q	75	THR	3.0
32	1a	801	U	3.0
26	14	62	ARG	3.0
35	1d	207	TYR	3.0
40	1i	36	TYR	3.0
46	1o	78	TYR	3.0
6	1G	138	GLN	3.0
40	2i	29	ASN	3.0
16	2U	32	PHE	3.0
1	2A	859	G	3.0
1	2A	916	G	3.0
4	2E	124	GLY	3.0
32	1a	31	G	3.0
32	1a	143	A	3.0
32	2a	788	U	3.0
32	2a	1334	G	3.0
6	1G	94	LEU	3.0
13	1R	20	LEU	3.0
41	1j	21	GLN	3.0
13	2R	11	ASN	3.0
44	2m	102	ARG	3.0
3	2D	59	LYS	3.0
14	1S	8	GLU	3.0
40	2i	12	GLU	3.0
39	2h	95	VAL	3.0
1	1A	2152	G	3.0
11	1P	72	PRO	3.0
12	2Q	103	MET	3.0
11	2P	53	GLY	3.0
12	2Q	30	GLY	3.0
40	1i	80	GLY	3.0
45	2n	55	GLY	3.0
7	2H	157	TYR	3.0
39	2h	35	ILE	3.0
9	2N	103	VAL	3.0
12	2Q	132	VAL	3.0
46	2o	70	LEU	3.0
9	1N	115	ARG	3.0
14	2S	97	ARG	3.0
25	23	12	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
32	2a	366	C	3.0
32	2a	801	U	3.0
33	2b	105	PHE	3.0
32	2a	983	A	3.0
32	2a	1014	A	3.0
12	2Q	23	GLY	3.0
33	2b	93	VAL	3.0
48	1q	11	VAL	3.0
22	20	55	ARG	3.0
46	1o	56	LEU	3.0
6	2G	68	PRO	3.0
16	2U	13	LYS	3.0
30	28	21	LYS	3.0
38	2g	89	MET	3.0
6	1G	73	ALA	3.0
47	2p	24	ALA	3.0
9	2N	140	VAL	3.0
35	1d	118	ARG	3.0
50	1s	19	VAL	3.0
3	2D	147	LEU	3.0
22	20	75	LEU	3.0
32	2a	973	G	3.0
32	2a	1401	G	3.0
50	1s	63	THR	3.0
38	1g	93	PRO	3.0
31	29	28	GLU	3.0
38	1g	132	GLY	3.0
51	2t	79	ARG	3.0
32	1a	990	C	3.0
17	2V	85	LYS	3.0
32	1a	1268	A	3.0
11	2P	63	PRO	3.0
39	1h	82	HIS	3.0
40	1i	73	GLN	3.0
32	2a	1300	G	2.9
38	1g	23	VAL	2.9
38	1g	147	ALA	2.9
8	1I	38	LEU	2.9
32	1a	323	U	2.9
1	2A	564	C	2.9
32	2a	578	C	2.9
1	2A	1787	A	2.9

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Mol	Chain	Res	Type	RSRZ
3	2D	217	ARG	2.9
11	1P	70	GLN	2.9
32	2a	1261	A	2.9
38	1g	96	GLN	2.9
39	2h	27	PRO	2.9
39	2h	90	GLY	2.9
46	2o	38	ARG	2.9
16	2U	21	ALA	2.9
30	28	23	VAL	2.9
31	19	15	LYS	2.9
39	1h	94	TYR	2.9
41	2j	57	LYS	2.9
49	2r	76	LEU	2.9
38	2g	149	ARG	2.9
39	2h	12	ARG	2.9
32	1a	395	C	2.9
36	2e	121	LYS	2.9
38	1g	137	LYS	2.9
39	2h	120	THR	2.9
50	2s	63	THR	2.9
9	2N	107	LEU	2.9
47	2p	60	LEU	2.9
36	2e	15	ARG	2.9
3	2D	235	GLY	2.9
4	1E	155	LYS	2.9
39	1h	132	GLU	2.9
7	2H	169	VAL	2.9
23	11	37	ILE	2.9
36	2e	89	ILE	2.9
8	2I	35	LEU	2.9
11	2P	62	LEU	2.9
1	2A	1967	C	2.9
32	1a	824	C	2.9
32	2a	501	C	2.9
33	2b	92	TYR	2.9
44	1m	33	ALA	2.9
1	1A	529	A	2.9
32	1a	968	A	2.9
22	20	17	GLN	2.9
4	2E	151	TYR	2.9
40	2i	98	PRO	2.9
47	2p	15	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
14	1S	30	ARG	2.9
47	2p	25	ARG	2.9
1	1A	2107	C	2.9
1	2A	2137	C	2.9
32	2a	948	C	2.9
33	1b	179	LYS	2.9
32	1a	1213	A	2.9
46	2o	58	MET	2.9
34	1c	5	ILE	2.9
9	2N	111	PRO	2.9
38	2g	147	ALA	2.9
46	2o	46	HIS	2.9
1	2A	2159	G	2.9
32	1a	821	G	2.9
33	2b	58	ILE	2.9
35	2d	148	VAL	2.9
36	2e	82	VAL	2.9
48	2q	25	ARG	2.9
32	2a	873	A	2.9
32	2a	1398	A	2.9
43	1l	125	PRO	2.9
44	2m	113	PRO	2.9
9	2N	22	THR	2.9
9	2N	114	ARG	2.9
39	1h	95	VAL	2.9
1	2A	888	C	2.9
14	2S	6	ALA	2.9
32	2a	1018	C	2.9
1	2A	1816	G	2.9
1	2A	1930	G	2.9
32	1a	108	G	2.9
32	1a	380	G	2.9
32	1a	579	G	2.9
32	1a	1047	G	2.9
32	2a	551	U	2.9
41	1j	77	PRO	2.9
41	2j	40	LEU	2.9
44	2m	17	VAL	2.9
6	2G	66	GLN	2.9
8	2I	83	ALA	2.9
1	2A	558	G	2.9
26	24	19	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
32	1a	1221	G	2.9
32	2a	991	U	2.9
1	1A	257	A	2.9
10	2O	1	MET	2.9
32	1a	523	A	2.9
40	2i	74	ILE	2.9
6	1G	80	PHE	2.9
30	18	10	ALA	2.9
35	2d	138	TYR	2.9
3	2D	273	ARG	2.9
6	1G	36	LYS	2.9
6	2G	10	LYS	2.9
19	2X	31	HIS	2.9
23	11	21	ARG	2.9
45	1n	41	ARG	2.9
29	27	14	LYS	2.9
34	1c	158	GLY	2.9
13	1R	10	LEU	2.9
14	1S	35	ILE	2.9
32	1a	221	C	2.9
35	1d	94	LEU	2.9
39	2h	119	LEU	2.9
43	2l	18	VAL	2.9
48	2q	59	ILE	2.9
11	2P	51	PHE	2.9
12	2Q	65	PHE	2.9
35	1d	185	PHE	2.9
1	2A	1627	G	2.9
32	2a	46	G	2.9
50	2s	64	GLU	2.9
16	2U	19	LYS	2.9
30	28	15	LYS	2.9
44	2m	79	LYS	2.9
9	2N	113	GLY	2.9
35	1d	67	ILE	2.8
1	2A	2712	U	2.8
32	2a	1051	C	2.8
32	2a	1301	U	2.8
32	2a	1303	C	2.8
32	2a	1363	C	2.8
1	2A	1835	G	2.8
32	1a	313	A	2.8

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Mol	Chain	Res	Type	RSRZ
32	1a	937	A	2.8
32	1a	1093	A	2.8
19	2X	58	HIS	2.8
32	1a	1215	G	2.8
32	2a	396	G	2.8
33	2b	131	PRO	2.8
35	2d	78	LEU	2.8
47	1p	13	HIS	2.8
47	1p	73	LEU	2.8
21	2Z	191	VAL	2.8
36	2e	19	MET	2.8
46	2o	27	VAL	2.8
41	1j	11	PHE	2.8
27	25	10	LYS	2.8
38	1g	138	LYS	2.8
43	1l	64	TYR	2.8
12	1Q	33	GLY	2.8
12	2Q	7	MET	2.8
35	1d	136	PRO	2.8
31	19	2	LYS	2.8
32	1a	1156	G	2.8
32	2a	230	G	2.8
50	2s	50	ALA	2.8
16	1U	39	LEU	2.8
22	10	72	ARG	2.8
32	2a	656	C	2.8
25	23	20	LYS	2.8
44	1m	16	ASP	2.8
46	1o	48	LYS	2.8
21	2Z	52	SER	2.8
1	1A	2318	G	2.8
3	2D	60	ARG	2.8
6	2G	65	GLY	2.8
12	2Q	59	ARG	2.8
13	2R	10	LEU	2.8
22	10	42	GLY	2.8
23	21	49	VAL	2.8
32	2a	1343	G	2.8
48	2q	70	ARG	2.8
1	1A	2295	C	2.8
32	1a	624	C	2.8
43	2l	5	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
4	1E	162	ALA	2.8
39	2h	110	ALA	2.8
20	2Y	42	VAL	2.8
32	2a	716	A	2.8
34	2c	199	LYS	2.8
36	2e	47	LYS	2.8
40	1i	6	GLY	2.8
44	1m	105	THR	2.8
46	2o	3	ILE	2.8
48	2q	27	PHE	2.8
32	1a	757	U	2.8
32	2a	229	U	2.8
32	2a	1003	G	2.8
51	2t	60	GLU	2.8
5	2F	97	TYR	2.8
23	21	64	ALA	2.8
21	2Z	76	LEU	2.8
32	2a	1377	A	2.8
11	2P	61	ARG	2.8
13	1R	45	ARG	2.8
32	1a	1000	U	2.8
45	1n	10	ALA	2.8
32	2a	307	C	2.8
32	2a	741	G	2.8
43	1l	121	GLY	2.8
50	2s	56	GLN	2.8
38	1g	30	ILE	2.8
38	2g	35	LYS	2.8
32	2a	1351	U	2.8
35	1d	55	ALA	2.8
12	2Q	96	VAL	2.8
17	2V	80	GLN	2.8
48	2q	35	VAL	2.8
1	1A	2722	G	2.8
1	2A	2129	C	2.8
13	1R	42	LYS	2.8
23	21	40	ARG	2.8
30	18	25	MET	2.8
38	1g	95	ARG	2.8
38	2g	155	ARG	2.8
3	2D	58	HIS	2.8
39	1h	89	PRO	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1A	1095	A	2.8
1	2A	1081	U	2.8
32	2a	729	A	2.8
23	11	20	ARG	2.8
36	1e	89	ILE	2.8
1	2A	2179	C	2.8
4	2E	182	LEU	2.8
32	1a	877	C	2.8
34	2c	196	LEU	2.8
46	2o	32	LEU	2.8
4	1E	124	GLY	2.8
6	2G	98	ARG	2.8
12	2Q	18	LYS	2.8
17	2V	76	LYS	2.8
17	2V	79	VAL	2.8
32	2a	66	G	2.8
32	2a	585	G	2.8
19	2X	77	LYS	2.8
33	2b	132	LYS	2.8
45	2n	57	ARG	2.8
47	1p	65	GLN	2.8
48	1q	5	VAL	2.8
1	2A	2522	U	2.8
32	2a	1040	U	2.8
33	2b	117	GLU	2.8
1	1A	1762	A	2.8
4	1E	116	VAL	2.8
21	2Z	79	ARG	2.8
43	2l	69	TYR	2.8
46	1o	38	ARG	2.8
1	1A	1026	U	2.7
32	1a	988	G	2.7
32	1a	1040	U	2.7
32	1a	1126	U	2.7
36	2e	10	MET	2.7
38	1g	89	MET	2.7
1	2A	2713	A	2.7
30	28	13	ARG	2.7
32	2a	1204	A	2.7
34	2c	171	GLY	2.7
35	2d	73	ARG	2.7
38	1g	65	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
46	2o	8	LYS	2.7
9	2N	71	ILE	2.7
44	1m	84	ILE	2.7
1	2A	2066	C	2.7
32	1a	488	C	2.7
16	2U	16	LYS	2.7
1	1A	2338	G	2.7
32	2a	825	G	2.7
33	1b	93	VAL	2.7
32	1a	729	A	2.7
39	2h	100	ILE	2.7
44	1m	62	ASN	2.7
23	1l	98	LEU	2.7
41	1j	7	LYS	2.7
1	1A	2140	C	2.7
32	2a	1263	C	2.7
1	2A	1083	U	2.7
1	1A	1056	G	2.7
1	2A	2190	G	2.7
3	1D	275	LYS	2.7
7	2H	111	HIS	2.7
1	1A	984	A	2.7
28	26	50	ARG	2.7
48	1q	69	LYS	2.7
35	2d	108	LEU	2.7
41	2j	54	PHE	2.7
3	1D	49	ILE	2.7
30	18	29	LYS	2.7
30	28	19	SER	2.7
33	1b	162	ILE	2.7
40	1i	48	GLU	2.7
39	2h	74	PRO	2.7
6	1G	155	MET	2.7
13	1R	51	LEU	2.7
35	2d	120	LEU	2.7
36	1e	123	LEU	2.7
48	1q	29	HIS	2.7
50	2s	65	ASN	2.7
1	1A	2587	A	2.7
7	2H	165	ALA	2.7
20	1Y	69	ALA	2.7
32	2a	41	G	2.7

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Mol	Chain	Res	Type	RSRZ
32	2a	1523	G	2.7
34	2c	148	GLY	2.7
38	1g	70	LYS	2.7
40	1i	95	LYS	2.7
1	1A	1065	U	2.7
23	2l	65	SER	2.7
32	2a	194	C	2.7
32	2a	322	C	2.7
40	1i	21	PRO	2.7
48	1q	22	LEU	2.7
48	2q	7	THR	2.7
12	2Q	106	VAL	2.7
3	2D	64	ILE	2.7
16	1U	89	GLU	2.7
33	2b	201	ILE	2.7
1	1A	2335	A	2.7
1	1A	2602	A	2.7
1	1A	240	G	2.7
1	1A	1667	G	2.7
32	2a	1265	G	2.7
38	1g	58	PRO	2.7
46	2o	24	SER	2.7
22	10	57	PHE	2.7
32	1a	1528	U	2.7
51	1t	85	MET	2.7
35	1d	79	PHE	2.7
16	2U	53	ARG	2.7
19	2X	59	VAL	2.7
20	1Y	3	VAL	2.7
44	1m	102	ARG	2.7
33	1b	182	ILE	2.7
34	2c	77	ILE	2.7
11	2P	17	LYS	2.7
20	2Y	34	LYS	2.7
32	2a	1175	G	2.7
40	1i	83	ARG	2.7
42	1k	122	LYS	2.7
1	1A	1933	G	2.7
1	2A	2132	U	2.7
6	2G	160	VAL	2.7
8	2I	92	VAL	2.7
32	1a	953	G	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	1a	1208	C	2.7
39	2h	80	ILE	2.7
44	1m	59	TYR	2.7
9	2N	104	LYS	2.7
23	1l	47	GLN	2.7
34	1c	9	GLY	2.7
35	1d	75	PHE	2.7
43	1l	32	PHE	2.7
47	1p	26	ARG	2.7
16	2U	14	HIS	2.7
50	2s	42	PRO	2.7
32	1a	1130	A	2.7
32	2a	1363(A)	A	2.7
37	2f	6	VAL	2.7
45	1n	27	CYS	2.7
46	2o	73	GLU	2.7
18	2W	6	ILE	2.7
1	1A	2146	C	2.7
1	2A	1297	C	2.7
1	2A	2521	C	2.7
32	1a	1270	C	2.7
32	2a	979	C	2.7
32	2a	1048	G	2.7
32	2a	1260	C	2.7
34	2c	43	LEU	2.7
3	2D	223	GLY	2.7
41	1j	25	GLU	2.7
1	1A	1066	U	2.7
10	2O	26	LYS	2.7
11	2P	39	LYS	2.7
16	2U	66	ASN	2.7
38	1g	33	ASP	2.7
35	1d	14	ARG	2.7
35	1d	65	ARG	2.7
1	1A	1176	G	2.7
1	2A	1903	G	2.7
32	1a	1511	G	2.7
50	1s	44	MET	2.7
34	1c	6	HIS	2.7
34	1c	193	TYR	2.6
39	2h	6	ILE	2.7
33	2b	118	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
44	2m	91	ARG	2.6
33	2b	193	ASP	2.6
32	2a	1046	A	2.6
1	1A	2175	C	2.6
32	2a	980	C	2.6
33	2b	139	LYS	2.6
6	1G	25	TYR	2.6
13	2R	2	ARG	2.6
20	2Y	73	ARG	2.6
1	2A	1377	G	2.6
32	1a	1050	G	2.6
32	2a	113	G	2.6
33	1b	180	LEU	2.6
35	2d	152	SER	2.6
39	1h	39	LEU	2.6
50	1s	20	LEU	2.6
3	2D	45	ASN	2.6
32	1a	1020	U	2.6
1	1A	2062	A	2.6
1	2A	1046	A	2.6
32	1a	781	A	2.6
32	1a	938	A	2.6
32	1a	1004	A	2.6
50	1s	36	ARG	2.6
14	2S	26	LEU	2.6
34	1c	168	ALA	2.6
50	2s	16	LEU	2.6
32	2a	385	C	2.6
32	2a	796	C	2.6
3	1D	243	GLY	2.6
6	2G	155	MET	2.6
22	20	73	GLY	2.6
37	2f	92	LYS	2.6
38	1g	53	LYS	2.6
51	1t	29	LYS	2.6
13	2R	71	GLN	2.6
35	1d	122	ARG	2.6
13	1R	18	LEU	2.6
33	1b	58	ILE	2.6
1	2A	1786	A	2.6
32	2a	393	A	2.6
3	2D	275	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
30	18	43	GLN	2.6
47	2p	68	ASP	2.6
48	1q	13	ASP	2.6
1	1A	2334	G	2.6
32	1a	587	G	2.6
51	2t	52	ALA	2.6
46	2o	2	PRO	2.6
4	1E	113	PHE	2.6
23	11	48	LYS	2.6
3	1D	244	ARG	2.6
31	19	4	ARG	2.6
32	1a	621	A	2.6
33	2b	141	GLU	2.6
13	1R	65	LEU	2.6
40	2i	52	ALA	2.6
50	2s	32	LYS	2.6
51	1t	59	ALA	2.6
6	1G	87	PRO	2.6
32	1a	1292	U	2.6
1	1A	1666	G	2.6
1	1A	1828	G	2.6
1	2A	563	G	2.6
1	2A	1252	G	2.6
1	2A	2337	G	2.6
32	1a	111	G	2.6
32	2a	1050	G	2.6
33	2b	165	VAL	2.6
51	1t	37	SER	2.6
11	2P	45	LEU	2.6
46	2o	67	LEU	2.6
16	2U	24	TYR	2.6
30	28	64	TYR	2.6
50	1s	28	LYS	2.6
50	1s	80	TYR	2.6
51	2t	28	ALA	2.6
19	1X	60	ARG	2.6
1	1A	2122	U	2.6
6	1G	37	VAL	2.6
32	1a	222	U	2.6
34	1c	207	VAL	2.6
47	2p	13	HIS	2.6
12	2Q	72	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
41	2j	88	LEU	2.6
1	1A	389	G	2.6
1	1A	410	G	2.6
1	2A	2149	G	2.6
7	2H	59	ARG	2.6
32	1a	1274	G	2.6
43	1l	26	ALA	2.6
51	2t	77	ALA	2.6
32	2a	996	A	2.6
1	1A	2128	C	2.6
32	1a	934	C	2.6
20	1Y	71	LYS	2.6
50	2s	70	LYS	2.6
6	2G	135	LEU	2.6
51	2t	41	ILE	2.6
36	2e	132	ALA	2.6
43	1l	30	ALA	2.6
1	2A	2709	G	2.6
14	2S	91	PRO	2.6
32	1a	231	G	2.6
1	1A	1069	A	2.6
32	1a	728	A	2.6
32	1a	314	C	2.6
32	2a	136	C	2.6
35	2d	65	ARG	2.6
14	2S	12	PHE	2.6
40	2i	3	GLN	2.6
51	1t	77	ALA	2.6
30	18	44	LYS	2.6
35	1d	15	GLU	2.6
38	2g	146	GLU	2.6
45	1n	4	LYS	2.6
47	1p	68	ASP	2.6
31	29	30	PRO	2.6
44	1m	48	LEU	2.6
46	1o	39	LEU	2.6
16	1U	17	ILE	2.6
1	1A	952	G	2.6
1	2A	975(A)	G	2.6
32	1a	1013	G	2.6
32	1a	1513	A	2.6
32	2a	232	G	2.6

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Mol	Chain	Res	Type	RSRZ
32	2a	313	A	2.6
32	2a	786	G	2.6
1	1A	1097	U	2.6
2	1B	47	C	2.6
32	1a	290	C	2.6
34	2c	189	ALA	2.6
43	2l	30	ALA	2.6
3	1D	230	ASP	2.6
9	2N	81	GLY	2.6
31	29	11	CYS	2.6
47	2p	55	ARG	2.6
4	1E	159	HIS	2.6
48	2q	29	HIS	2.6
6	2G	8	LYS	2.5
1	2A	2765	A	2.5
1	1A	614(B)	G	2.5
1	2A	976	C	2.5
1	2A	1745(A)	C	2.5
23	1l	22	GLY	2.5
32	2a	263	A	2.5
32	1a	107	G	2.5
32	2a	731	G	2.5
45	1n	38	GLY	2.5
46	1o	35	ARG	2.5
9	2N	87	LEU	2.5
4	2E	123	ALA	2.5
5	2F	172	TRP	2.5
38	1g	56	GLN	2.5
5	2F	47	GLY	2.5
21	2Z	114	GLY	2.5
14	2S	110	LEU	2.5
1	2A	865	C	2.5
32	1a	327	A	2.5
32	2a	958	A	2.5
15	1T	65	LYS	2.5
1	2A	1772	G	2.5
3	1D	271	ILE	2.5
19	1X	8	ILE	2.5
20	2Y	19	LYS	2.5
3	2D	218	ARG	2.5
16	2U	59	ARG	2.5
41	2j	79	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
38	1g	103	TRP	2.5
39	2h	10	LEU	2.5
51	2t	55	ILE	2.5
1	2A	267	C	2.5
1	2A	2712(A)	A	2.5
15	1T	104	ASN	2.5
32	1a	175	C	2.5
32	2a	185	A	2.5
38	2g	71	PRO	2.5
51	1t	15	ARG	2.5
32	2a	589	C	2.5
7	2H	129	THR	2.5
36	1e	17	ALA	2.5
43	2l	26	ALA	2.5
32	2a	1295	G	2.5
33	1b	99	GLY	2.5
46	1o	25	THR	2.5
1	1A	2159	G	2.5
1	2A	1935	G	2.5
32	1a	758	G	2.5
32	1a	878	G	2.5
11	2P	54	GLY	2.5
21	1Z	99	TYR	2.5
22	20	52	GLY	2.5
33	1b	164	VAL	2.5
33	2b	188	ALA	2.5
35	1d	167	GLY	2.5
44	1m	6	GLY	2.5
46	2o	16	ALA	2.5
23	21	32	LYS	2.5
30	18	15	LYS	2.5
8	2l	30	LEU	2.5
25	23	26	LEU	2.5
32	1a	366	C	2.5
45	2n	53	LEU	2.5
30	28	30	ARG	2.5
43	2l	53	ARG	2.5
1	2A	1382	G	2.5
32	2a	388	G	2.5
32	2a	588	G	2.5
3	1D	248	SER	2.5
3	2D	212	SER	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1A	2265	U	2.5
6	2G	138	GLN	2.5
9	2N	110	GLY	2.5
11	1P	68	GLN	2.5
11	2P	71	VAL	2.5
45	2n	28	GLY	2.5
9	2N	45	ASN	2.5
51	2t	13	LEU	2.5
30	18	46	ARG	2.5
21	2Z	193	GLU	2.5
1	2A	1968	G	2.5
19	2X	7	VAL	2.5
3	2D	231	HIS	2.5
28	16	11	LEU	2.5
30	28	50	LEU	2.5
32	1a	585	G	2.5
32	1a	1521	G	2.5
32	2a	1013	G	2.5
34	2c	173	VAL	2.5
49	2r	34	TYR	2.5
32	2a	619	U	2.5
36	2e	130	ASN	2.5
33	1b	201	ILE	2.5
12	2Q	76	LYS	2.5
23	21	10	LYS	2.5
1	2A	535	C	2.5
1	2A	2274	A	2.5
32	1a	1210	C	2.5
32	1a	1514	C	2.5
32	2a	1297	C	2.5
3	2D	34	VAL	2.5
19	2X	76	ARG	2.5
31	29	7	VAL	2.5
35	1d	58	LEU	2.5
46	2o	31	LEU	2.5
33	2b	113	HIS	2.5
1	1A	906	G	2.5
5	2F	64	ILE	2.5
39	2h	83	ILE	2.5
47	1p	27	LYS	2.5
30	28	38	GLY	2.5
35	1d	203	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
40	2i	28	VAL	2.5
46	2o	77	ARG	2.5
3	1D	249	PRO	2.5
5	2F	42	ALA	2.5
3	2D	230	ASP	2.5
32	2a	795	C	2.5
11	2P	40	SER	2.5
19	1X	77	LYS	2.5
19	2X	60	ARG	2.5
32	1a	1135	U	2.5
32	1a	1232	U	2.5
1	2A	1125	G	2.5
31	19	3	VAL	2.5
32	1a	402	G	2.5
32	1a	1488	G	2.5
32	2a	1530	G	2.5
36	2e	85	GLY	2.5
10	1O	5	GLN	2.5
19	2X	6	ASP	2.5
25	23	19	GLN	2.5
42	2k	122	LYS	2.5
46	2o	71	GLN	2.5
1	1A	821	A	2.5
1	2A	515	A	2.5
32	1a	325	A	2.5
32	2a	653	A	2.5
32	2a	1019	C	2.5
46	1o	51	HIS	2.5
50	1s	21	GLU	2.5
13	2R	18	LEU	2.5
40	2i	19	LEU	2.5
41	2j	81	THR	2.5
26	24	8	LYS	2.5
32	1a	309	G	2.5
32	1a	1529	G	2.5
43	1l	33	ARG	2.5
52	2u	22	ARG	2.5
7	2H	113	VAL	2.4
19	2X	78	LYS	2.4
32	1a	353	A	2.4
32	2a	695	A	2.4
39	2h	135	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
39	1h	110	ALA	2.4
42	1k	59	TYR	2.4
12	2Q	73	PRO	2.4
20	2Y	2	ARG	2.4
42	2k	116	HIS	2.4
47	1p	40	ASP	2.4
1	1A	864	G	2.4
1	2A	2155	G	2.4
2	2B	69	G	2.4
5	1F	192	LEU	2.4
32	2a	1154	G	2.4
33	1b	118	LEU	2.4
35	1d	8	VAL	2.4
18	2W	9	TYR	2.4
1	1A	1932	A	2.4
10	2O	29	ASN	2.4
31	19	29	ASN	2.4
44	2m	23	TYR	2.4
48	1q	88	TYR	2.4
32	1a	1014	A	2.4
32	2a	197	A	2.4
32	2a	1091	U	2.4
47	1p	8	ARG	2.4
33	1b	27	LYS	2.4
50	1s	35	SER	2.4
12	1Q	28	ALA	2.4
34	1c	163	ALA	2.4
1	1A	1826	G	2.4
1	2A	531	C	2.4
1	1A	2114	A	2.4
1	1A	2150	U	2.4
8	1I	118	LYS	2.4
11	2P	38	GLN	2.4
32	2a	1214	C	2.4
36	1e	122	GLU	2.4
48	1q	58	GLU	2.4
16	2U	2	PRO	2.4
32	1a	1062	U	2.4
32	2a	1341	U	2.4
51	1t	34	LYS	2.4
3	1D	226	MET	2.4
6	2G	19	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
14	1S	14	VAL	2.4
39	1h	85	ARG	2.4
38	1g	62	PHE	2.4
19	2X	8	ILE	2.4
43	2l	91	LYS	2.4
48	1q	60	ILE	2.4
51	1t	65	LYS	2.4
1	1A	1983	C	2.4
10	2O	21	CYS	2.4
24	22	35	LEU	2.4
32	1a	554	C	2.4
32	2a	957	U	2.4
32	2a	981	U	2.4
39	1h	101	PRO	2.4
45	1n	3	ARG	2.4
50	1s	22	LEU	2.4
1	2A	832	G	2.4
1	2A	864	G	2.4
1	2A	911	A	2.4
1	2A	944	G	2.4
1	2A	1642	G	2.4
32	2a	384	G	2.4
9	1N	83	LYS	2.4
19	2X	36	LYS	2.4
10	2O	5	GLN	2.4
36	1e	130	ASN	2.4
13	2R	1	MET	2.4
1	1A	390	A	2.4
12	2Q	93	TYR	2.4
14	2S	51	ALA	2.4
16	1U	24	TYR	2.4
32	2a	172	A	2.4
32	2a	1213	A	2.4
41	2j	18	ALA	2.4
32	1a	306	G	2.4
32	2a	80	G	2.4
38	2g	96	GLN	2.4
30	28	49	VAL	2.4
23	11	32	LYS	2.4
33	1b	168	THR	2.4
4	1E	163	GLU	2.4
19	1X	79	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
35	2d	54	TYR	2.4
3	2D	49	ILE	2.4
4	1E	119	ARG	2.4
11	1P	15	ARG	2.4
16	2U	62	ILE	2.4
31	19	17	ILE	2.4
32	1a	1214	C	2.4
32	2a	311	C	2.4
32	2a	1027	C	2.4
39	2h	132	GLU	2.4
33	2b	214	ILE	2.4
35	2d	132	ARG	2.4
46	1o	64	ARG	2.4
12	1Q	34	LEU	2.4
32	2a	389	A	2.4
1	1A	1630	G	2.4
1	2A	2338	G	2.4
4	1E	115	GLY	2.4
14	2S	98	VAL	2.4
14	1S	91	PRO	2.4
32	1a	1173	G	2.4
35	2d	166	LYS	2.4
38	1g	148	ASN	2.4
33	1b	130	ARG	2.4
34	1c	184	TYR	2.4
41	2j	70	ARG	2.4
51	2t	12	ALA	2.4
32	1a	223	U	2.4
32	1a	952	U	2.4
32	1a	1301	U	2.4
32	1a	1302	U	2.4
12	2Q	22	LYS	2.4
32	1a	866	C	2.4
34	2c	195	VAL	2.4
48	2q	22	LEU	2.4
29	27	1	MET	2.4
36	1e	19	MET	2.4
32	1a	780	A	2.4
3	1D	247	ALA	2.4
21	2Z	81	ARG	2.4
31	29	4	ARG	2.4
44	2m	93	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
32	2a	799	G	2.4
47	1p	16	HIS	2.4
9	2N	82	LEU	2.4
32	2a	62	U	2.4
51	1t	13	LEU	2.4
34	2c	170	GLN	2.4
44	1m	17	VAL	2.4
1	1A	2021	C	2.4
28	16	50	ARG	2.4
32	1a	1217	C	2.4
1	1A	227	A	2.4
11	1P	30	THR	2.4
32	1a	814	A	2.4
34	1c	182	ILE	2.4
1	2A	1931	U	2.4
7	2H	166	GLY	2.4
32	1a	387	U	2.4
32	2a	1106	G	2.4
33	1b	152	PHE	2.4
34	1c	154	SER	2.4
3	2D	225	ALA	2.4
13	2R	40	LYS	2.4
33	1b	167	PRO	2.4
4	2E	134	ILE	2.4
32	2a	586	C	2.4
34	1c	180	ALA	2.4
47	2p	36	ILE	2.4
11	2P	6	LEU	2.4
28	26	9	LEU	2.4
30	28	60	LEU	2.4
33	1b	140	HIS	2.4
46	1o	67	LEU	2.4
51	1t	84	LEU	2.4
3	2D	43	ARG	2.3
30	28	9	GLY	2.3
32	1a	1123	A	2.3
33	2b	198	ASP	2.3
38	2g	140	ASP	2.3
39	1h	75	ARG	2.3
41	1j	54	PHE	2.3
1	1A	966	G	2.3
1	1A	1769	G	2.3

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Mol	Chain	Res	Type	RSRZ
12	1Q	68	ILE	2.3
12	2Q	107	ALA	2.3
15	1T	131	ALA	2.3
32	2a	31	G	2.3
32	2a	791	G	2.3
1	1A	2477	C	2.3
5	2F	169	ASN	2.3
20	1Y	72	VAL	2.3
32	2a	779	C	2.3
3	2D	166	GLN	2.3
32	1a	1055	A	2.3
32	2a	1105	A	2.3
25	23	51	ALA	2.3
32	1a	956	U	2.3
32	1a	991	U	2.3
38	1g	46	ALA	2.3
39	1h	100	ILE	2.3
40	1i	82	ALA	2.3
3	1D	239	ARG	2.3
43	1l	93	LEU	2.3
1	1A	1813	G	2.3
6	2G	29	TRP	2.3
16	2U	38	THR	2.3
32	1a	378	G	2.3
32	1a	1231	G	2.3
32	2a	548	G	2.3
36	2e	45	PHE	2.3
50	1s	65	ASN	2.3
1	1A	2606	C	2.3
1	2A	1124	C	2.3
12	2Q	113	GLN	2.3
32	1a	1335	C	2.3
1	1A	225	A	2.3
1	1A	1669	A	2.3
14	1S	10	ARG	2.3
23	1l	46	LEU	2.3
32	1a	609	A	2.3
32	1a	1339	A	2.3
35	2d	100	ARG	2.3
44	1m	11	ARG	2.3
48	1q	31	LEU	2.3
3	1D	221	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
32	2a	223	U	2.3
10	2O	79	PHE	2.3
35	1d	206	PHE	2.3
48	1q	21	VAL	2.3
50	2s	55	LYS	2.3
1	1A	1252	G	2.3
1	1A	1770	G	2.3
1	1A	1904	G	2.3
1	2A	867	C	2.3
1	2A	1296	G	2.3
31	19	22	ARG	2.3
5	1F	181	LEU	2.3
19	2X	69	TYR	2.3
32	1a	727	G	2.3
39	2h	104	ARG	2.3
3	2D	241	PRO	2.3
3	2D	246	PRO	2.3
6	1G	75	LYS	2.3
33	2b	123	ALA	2.3
45	2n	20	ALA	2.3
36	2e	128	PRO	2.3
1	1A	532	A	2.3
32	2a	961	U	2.3
32	2a	1090	U	2.3
9	2N	1	MET	2.3
46	2o	59	MET	2.3
3	2D	54	ARG	2.3
16	1U	38	THR	2.3
47	1p	57	ARG	2.3
3	1D	59	LYS	2.3
4	2E	187	ALA	2.3
13	1R	4	LEU	2.3
40	1i	32	ASP	2.3
13	1R	19	ALA	2.3
1	2A	2699	C	2.3
32	2a	386	C	2.3
32	2a	805	C	2.3
41	2j	77	PRO	2.3
44	1m	7	VAL	2.3
1	2A	272	G	2.3
1	2A	2112	G	2.3
32	2a	1520	G	2.3

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Mol	Chain	Res	Type	RSRZ
4	2E	163	GLU	2.3
5	2F	72	ARG	2.3
38	2g	31	MET	2.3
50	2s	14	HIS	2.3
6	1G	19	LEU	2.3
15	1T	105	LEU	2.3
34	2c	147	LYS	2.3
23	2l	18	ILE	2.3
35	1d	11	LEU	2.3
42	1k	98	LEU	2.3
9	2N	80	GLY	2.3
23	2l	31	GLY	2.3
7	1H	6	ARG	2.3
23	2l	41	ARG	2.3
42	1k	54	ARG	2.3
43	2l	71	PRO	2.3
50	2s	37	ARG	2.3
32	1a	1158	C	2.3
1	1A	271(Y)	U	2.3
31	19	32	HIS	2.3
32	1a	548	G	2.3
32	1a	1085	U	2.3
32	1a	1196	U	2.3
32	1a	1216	G	2.3
32	2a	1387	G	2.3
38	2g	13	GLN	2.3
37	2f	8	ILE	2.3
41	2j	69	ASN	2.3
49	1r	31	LEU	2.3
1	1A	1970	A	2.3
28	26	21	TYR	2.3
29	27	18	PHE	2.3
32	1a	262	A	2.3
32	1a	655	A	2.3
47	1p	2	VAL	2.3
3	2D	244	ARG	2.3
6	1G	136	ARG	2.3
8	2l	27	ARG	2.3
30	18	47	LYS	2.3
48	1q	86	GLU	2.3
1	1A	967	C	2.3
13	1R	52	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
32	1a	620	C	2.3
32	1a	995	C	2.3
32	1a	1322	C	2.3
11	1P	32	THR	2.3
22	20	72	ARG	2.3
31	19	23	VAL	2.3
1	1A	820	A	2.3
1	1A	946	G	2.3
1	1A	1674	G	2.3
1	1A	1825	A	2.3
1	1A	2123	G	2.3
12	2Q	38	GLU	2.3
28	16	38	LYS	2.3
32	1a	1127	G	2.3
32	2a	1033	G	2.3
20	2Y	106	LEU	2.3
24	22	60	LEU	2.3
48	1q	97	SER	2.3
3	1D	220	HIS	2.3
42	1k	126	ARG	2.3
48	1q	45	HIS	2.3
44	2m	28	ALA	2.3
1	1A	2130	U	2.3
1	2A	1082	U	2.3
1	2A	1640	C	2.3
6	1G	40	ASN	2.3
32	1a	555	C	2.3
22	10	43	THR	2.3
42	1k	57	THR	2.3
41	2j	86	MET	2.3
1	1A	411	G	2.3
1	2A	561	G	2.3
1	2A	782	A	2.3
32	1a	865	A	2.3
3	1D	225	ALA	2.3
3	1D	229	VAL	2.3
31	19	5	ALA	2.3
36	1e	47	LYS	2.3
12	2Q	105	GLU	2.3
34	1c	166	GLU	2.3
26	14	51	ASP	2.3
32	1a	114	U	2.3

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Mol	Chain	Res	Type	RSRZ
32	1a	405	U	2.3
32	2a	962	C	2.3
34	1c	181	ASN	2.3
13	2R	51	LEU	2.3
37	2f	89	MET	2.3
44	1m	57	ARG	2.3
48	1q	84	LEU	2.3
34	2c	5	ILE	2.3
35	2d	61	LYS	2.3
22	20	8	GLY	2.2
32	1a	499	A	2.3
39	2h	137	VAL	2.3
32	1a	44	G	2.2
32	1a	396	G	2.2
35	2d	23	GLY	2.2
3	2D	44	ASN	2.2
5	2F	32	LEU	2.2
12	2Q	37	LEU	2.2
19	1X	57	LEU	2.2
32	1a	1341	U	2.2
1	2A	1600	C	2.2
17	2V	70	ILE	2.2
32	2a	121	C	2.2
51	1t	30	LYS	2.2
44	1m	15	VAL	2.2
41	2j	26	ALA	2.2
43	2l	118	SER	2.2
44	2m	95	GLY	2.2
3	1D	218	ARG	2.2
9	2N	35	ARG	2.2
44	2m	108	ARG	2.2
19	2X	57	LEU	2.2
1	1A	388	G	2.2
10	1O	21	CYS	2.2
13	2R	4	LEU	2.2
21	2Z	201	LYS	2.2
26	14	2	LYS	2.2
32	1a	394	G	2.2
32	2a	331	G	2.2
32	2a	354	G	2.2
32	2a	579	G	2.2
39	1h	24	THR	2.2

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Mol	Chain	Res	Type	RSRZ
47	1p	19	ILE	2.2
20	2Y	72	VAL	2.2
32	2a	174	C	2.2
10	2O	2	ILE	2.2
41	2j	87	THR	2.2
51	1t	33	ILE	2.2
34	2c	174	PRO	2.2
1	2A	1347	G	2.2
10	2O	64	ARG	2.2
32	1a	505	G	2.2
32	2a	380	G	2.2
32	2a	776	G	2.2
32	2a	778	G	2.2
32	2a	976	G	2.2
45	1n	26	ARG	2.2
13	1R	5	LYS	2.2
13	2R	42	LYS	2.2
1	1A	385	C	2.2
1	2A	1080	C	2.2
11	1P	62	LEU	2.2
39	2h	39	LEU	2.2
3	2D	87	ASN	2.2
38	2g	141	VAL	2.2
1	1A	477	A	2.2
1	1A	1783	A	2.2
11	2P	16	ARG	2.2
16	2U	10	ARG	2.2
6	2G	26	GLN	2.2
11	2P	31	ALA	2.2
25	23	34	GLU	2.2
32	1a	441	A	2.2
33	2b	143	GLU	2.2
43	1l	117	ARG	2.2
47	1p	18	ARG	2.2
23	21	98	LEU	2.2
44	2m	48	LEU	2.2
51	2t	53	LEU	2.2
51	2t	84	LEU	2.2
1	2A	1904	G	2.2
1	2A	2545	G	2.2
11	2P	56	SER	2.2
1	2A	385	C	2.2

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Mol	Chain	Res	Type	RSRZ
22	10	53	MET	2.2
32	2a	785	G	2.2
51	2t	31	SER	2.2
32	1a	1018	C	2.2
32	2a	150	C	2.2
32	2a	1096	C	2.2
32	2a	1395	C	2.2
32	2a	1509	C	2.2
36	1e	26	PHE	2.2
47	1p	80	PHE	2.2
38	1g	140	ASP	2.2
31	19	34	GLN	2.2
33	2b	67	THR	2.2
39	1h	16	ALA	2.2
47	2p	64	ALA	2.2
17	1V	38	LEU	2.2
1	2A	2189	U	2.2
32	1a	487	A	2.2
3	1D	252	TRP	2.2
32	1a	743	U	2.2
32	2a	109	A	2.2
32	2a	1531	A	2.2
34	2c	33	LEU	2.2
11	2P	67	MET	2.2
13	1R	8	ARG	2.2
36	1e	45	PHE	2.2
1	1A	224	G	2.2
1	1A	2294	C	2.2
3	2D	42	GLY	2.2
15	2T	25	GLY	2.2
23	11	29	GLY	2.2
32	1a	41	G	2.2
32	1a	526	C	2.2
33	2b	134	GLU	2.2
33	1b	193	ASP	2.2
42	1k	25	TYR	2.2
44	1m	10	PRO	2.2
33	2b	215	LEU	2.2
1	2A	2150	U	2.2
9	1N	42	TRP	2.2
12	1Q	41	TRP	2.2
17	2V	78	LYS	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
26	14	1	MET	2.2
31	19	13	LYS	2.2
31	19	35	ARG	2.2
33	2b	153	ARG	2.2
49	1r	84	LYS	2.2
50	2s	38	SER	2.2
47	2p	37	GLY	2.2
8	2I	25	TYR	2.2
19	1X	34	ALA	2.2
33	2b	173	ALA	2.2
1	2A	1934	C	2.2
45	2n	54	PRO	2.2
1	1A	1377	G	2.2
1	2A	1299	G	2.2
1	2A	2592	G	2.2
5	2F	46	ARG	2.2
21	2Z	82	ARG	2.2
22	20	41	ARG	2.2
32	1a	115	G	2.2
23	21	14	VAL	2.2
26	24	10	VAL	2.2
32	1a	793	U	2.2
46	2o	6	GLU	2.2
43	2l	14	GLY	2.2
1	1A	548	A	2.2
1	2A	1901	A	2.2
19	1X	69	TYR	2.2
7	2H	175	LYS	2.2
10	1O	4	PRO	2.2
10	1O	26	LYS	2.2
16	2U	51	LYS	2.2
24	22	52	ASP	2.2
38	2g	4	ARG	2.2
48	2q	72	ARG	2.2
1	1A	1672	C	2.2
32	1a	545	C	2.2
32	2a	549	C	2.2
33	1b	97	TRP	2.2
37	1f	88	VAL	2.2
1	2A	1980	G	2.2
4	2E	125	GLY	2.2
32	2a	544	G	2.2

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Mol	Chain	Res	Type	RSRZ
4	1E	108	SER	2.2
6	1G	74	LYS	2.2
11	2P	50	ARG	2.2
12	1Q	18	LYS	2.2
16	1U	35	ALA	2.2
32	2a	114	U	2.2
32	2a	1212	U	2.2
33	1b	132	LYS	2.2
36	1e	91	LEU	2.2
44	2m	42	ALA	2.2
1	1A	945	A	2.2
33	2b	78	GLN	2.2
43	1l	31	PRO	2.2
47	1p	9	PHE	2.2
13	1R	66	VAL	2.2
19	2X	39	ILE	2.2
20	1Y	5	MET	2.2
28	16	20	ASN	2.2
1	2A	886	C	2.2
1	2A	1832	C	2.2
1	2A	2690	C	2.2
32	2a	1210	C	2.2
45	1n	55	GLY	2.2
12	1Q	20	ALA	2.2
13	2R	21	TYR	2.2
1	1A	944	G	2.2
1	1A	947	G	2.2
1	1A	1975	G	2.2
1	2A	1089	G	2.2
16	1U	32	PHE	2.2
19	2X	38	GLU	2.2
39	1h	111	ILE	2.2
48	1q	73	VAL	2.2
6	1G	84	LYS	2.2
23	21	21	ARG	2.2
30	18	28	GLY	2.2
30	18	39	LYS	2.2
38	1g	10	ARG	2.2
44	2m	94	ARG	2.2
4	2E	160	TYR	2.1
13	1R	67	LEU	2.1
38	2g	101	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	2A	915	C	2.1
32	2a	1342	C	2.1
13	1R	14	SER	2.1
12	1Q	99	PRO	2.1
5	2F	45	ARG	2.1
22	20	79	VAL	2.1
33	1b	144	ARG	2.1
37	1f	90	VAL	2.1
39	2h	101	PRO	2.1
1	1A	2581	G	2.1
1	2A	226	G	2.1
1	2A	1699	G	2.1
1	2A	2446	G	2.1
3	1D	223	GLY	2.1
32	1a	305	G	2.1
32	2a	111	G	2.1
7	2H	163	TYR	2.1
9	2N	73	THR	2.1
10	2O	32	TYR	2.1
17	1V	71	LEU	2.1
30	18	61	LEU	2.1
32	2a	1299	A	2.1
40	1i	56	LEU	2.1
1	1A	271(Z)	C	2.1
1	1A	2297	C	2.1
11	2P	49	ARG	2.1
14	2S	28	VAL	2.1
15	1T	109	GLU	2.1
17	1V	73	SER	2.1
32	2a	398	C	2.1
33	1b	53	ARG	2.1
33	2b	71	VAL	2.1
37	1f	92	LYS	2.1
42	1k	91	ARG	2.1
48	2q	38	ARG	2.1
1	1A	2132	U	2.1
38	1g	144	MET	2.1
13	1R	111	LEU	2.1
19	2X	5	TYR	2.1
1	1A	1969	A	2.1
1	2A	389	G	2.1
1	2A	508	G	2.1

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Mol	Chain	Res	Type	RSRZ
10	2O	67	LYS	2.1
22	10	39	ARG	2.1
32	1a	316	G	2.1
32	1a	916	G	2.1
32	1a	1191	A	2.1
32	1a	1295	G	2.1
32	2a	353	A	2.1
6	1G	63	ILE	2.1
6	1G	144	ILE	2.1
9	2N	46	VAL	2.1
11	1P	74	GLU	2.1
12	1Q	39	PRO	2.1
15	1T	1	MET	2.1
1	1A	2073	C	2.1
1	2A	2313	C	2.1
32	1a	817	C	2.1
32	1a	992	U	2.1
32	2a	110	C	2.1
32	2a	526	C	2.1
40	2i	91	ASP	2.1
6	2G	25	TYR	2.1
36	2e	133	TYR	2.1
24	22	49	LYS	2.1
39	2h	44	PHE	2.1
41	1j	32	ALA	2.1
13	1R	24	GLN	2.1
33	1b	185	ILE	2.1
39	1h	86	ILE	2.1
40	1i	124	GLN	2.1
43	1l	85	ILE	2.1
45	2n	56	VAL	2.1
1	1A	2446	G	2.1
1	2A	536	A	2.1
1	2A	1972	A	2.1
12	1Q	37	LEU	2.1
21	2Z	83	PRO	2.1
32	1a	1021	G	2.1
35	1d	101	LEU	2.1
38	2g	14	PRO	2.1
1	1A	1629	U	2.1
1	2A	504	U	2.1
1	2A	1064	C	2.1

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Mol	Chain	Res	Type	RSRZ
16	2U	22	LYS	2.1
30	28	5	LYS	2.1
31	19	18	ARG	2.1
40	2i	60	ASP	2.1
32	2a	132	C	2.1
39	2h	7	ALA	2.1
43	1l	119	LYS	2.1
19	2X	29	TRP	2.1
10	2O	65	THR	2.1
36	2e	51	VAL	2.1
46	2o	11	VAL	2.1
4	2E	112	GLY	2.1
18	2W	82	LEU	2.1
4	1E	8	LYS	2.1
22	10	46	LYS	2.1
25	23	10	LYS	2.1
42	2k	115	PRO	2.1
1	1A	1986	A	2.1
1	2A	1783	A	2.1
13	1R	47	PHE	2.1
14	1S	36	TYR	2.1
32	1a	1398	A	2.1
32	2a	923	A	2.1
32	2a	1252	A	2.1
38	2g	26	PHE	2.1
49	2r	81	PHE	2.1
1	1A	2155	G	2.1
1	2A	383	U	2.1
2	2B	41	U	2.1
32	1a	544	G	2.1
32	2a	550	G	2.1
33	2b	177	ALA	2.1
32	2a	580	U	2.1
1	2A	2700	C	2.1
11	1P	52	GLU	2.1
13	1R	76	VAL	2.1
32	2a	1359	C	2.1
39	2h	138	TRP	2.1
51	1t	60	GLU	2.1
23	11	13	ILE	2.1
38	2g	148	ASN	2.1
39	1h	83	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
51	1t	75	ASN	2.1
3	1D	215	LEU	2.1
9	2N	112	LEU	2.1
13	2R	22	ARG	2.1
22	20	44	ARG	2.1
33	2b	69	LEU	2.1
50	1s	78	ARG	2.1
23	11	65	SER	2.1
12	2Q	114	ALA	2.1
46	2o	78	TYR	2.1
22	20	68	GLU	2.1
1	2A	1301	A	2.1
32	2a	1102	A	2.1
38	2g	153	HIS	2.1
1	1A	1987	G	2.1
1	1A	1994	C	2.1
1	1A	2321	G	2.1
1	2A	581	C	2.1
1	2A	1975	G	2.1
6	1G	93	THR	2.1
32	2a	963	G	2.1
32	2a	1147	C	2.1
35	1d	168	ARG	2.1
43	2l	27	LEU	2.1
46	2o	5	LYS	2.1
5	1F	102	PRO	2.1
13	2R	80	PHE	2.1
48	1q	79	SER	2.1
52	1u	21	TYR	2.1
44	1m	8	GLU	2.1
3	2D	184	LYS	2.1
7	2H	172	LYS	2.1
12	1Q	97	VAL	2.1
16	2U	15	LYS	2.1
43	1l	110	VAL	2.1
44	1m	53	VAL	2.1
17	1V	83	ARG	2.1
36	1e	85	GLY	2.1
39	2h	75	ARG	2.1
48	2q	60	ILE	2.1
1	2A	1629	U	2.1
51	2t	36	LEU	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2541	A	2.1
32	1a	872	A	2.1
32	2a	59	A	2.1
32	2a	327	A	2.1
1	1A	1934	C	2.1
1	1A	1958	C	2.1
1	2A	530	G	2.1
1	2A	964	C	2.1
1	2A	1905	C	2.1
32	1a	292	G	2.1
32	1a	332	G	2.1
32	1a	1068	G	2.1
32	2a	803	G	2.1
32	2a	1526	G	2.1
36	1e	48	ALA	2.1
4	1E	165	VAL	2.1
16	1U	33	ARG	2.1
23	21	13	ILE	2.1
25	23	54	VAL	2.1
26	24	62	ARG	2.1
29	17	41	ARG	2.1
31	19	10	ILE	2.1
39	1h	87	SER	2.1
13	1R	13	HIS	2.1
9	2N	69	GLN	2.1
30	18	48	PHE	2.1
30	18	27	THR	2.1
44	2m	77	ASN	2.1
1	2A	1572	A	2.1
17	1V	44	LYS	2.1
3	2D	229	VAL	2.1
5	2F	49	ALA	2.1
12	1Q	98	LYS	2.1
13	2R	8	ARG	2.1
16	1U	28	ARG	2.1
20	1Y	16	ALA	2.1
30	28	63	PRO	2.1
32	2a	777	A	2.1
31	29	5	ALA	2.1
43	1l	23	LYS	2.1
47	1p	38	TYR	2.1
32	1a	618	C	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	36	C	2.1
1	1A	530	G	2.1
32	1a	799	G	2.1
32	1a	1520	G	2.1
32	2a	1283	G	2.1
32	2a	1529	G	2.1
50	2s	12	ASP	2.1
21	1Z	118	GLN	2.1
35	1d	62	GLN	2.1
17	1V	84	LYS	2.1
43	2l	16	GLU	2.1
52	1u	20	LYS	2.1
23	1l	34	THR	2.1
32	1a	571	U	2.1
6	1G	159	VAL	2.1
38	1g	150	ALA	2.1
1	2A	1156	A	2.1
21	2Z	125	LEU	2.1
32	1a	819	A	2.1
32	2a	1251	A	2.1
46	1o	82	ILE	2.1
33	2b	150	SER	2.1
43	2l	72	GLY	2.1
32	2a	379	C	2.1
49	2r	61	LYS	2.0
50	2s	66	MET	2.1
16	2U	52	ARG	2.0
1	2A	2120	G	2.0
38	1g	52	GLU	2.0
1	2A	384	U	2.0
4	2E	141	ILE	2.0
15	2T	110	ILE	2.0
33	1b	68	ILE	2.0
34	2c	202	ILE	2.0
6	2G	134	GLY	2.0
11	2P	34	GLY	2.0
39	1h	10	LEU	2.0
1	2A	1569	A	2.0
14	2S	19	LYS	2.0
10	2O	3	GLN	2.0
11	1P	56	SER	2.0
32	1a	864	A	2.0

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Mol	Chain	Res	Type	RSRZ
32	2a	1015	A	2.0
45	2n	36	PHE	2.0
49	1r	29	PHE	2.0
32	2a	224	C	2.0
32	2a	1112	C	2.0
26	14	63	TYR	2.0
4	2E	77	ILE	2.0
6	2G	88	ILE	2.0
20	2Y	75	ILE	2.0
23	11	18	ILE	2.0
1	2A	958	U	2.0
1	2A	1718	G	2.0
1	2A	2067	G	2.0
1	2A	2523	G	2.0
11	2P	22	GLY	2.0
26	14	69	LYS	2.0
32	1a	941	G	2.0
32	1a	1131	G	2.0
32	2a	500	G	2.0
32	2a	1178	G	2.0
33	2b	179	LYS	2.0
38	1g	143	ARG	2.0
3	2D	220	HIS	2.0
30	18	65	GLU	2.0
40	1i	87	GLN	2.0
45	2n	32	SER	2.0
1	1A	1354	A	2.0
1	1A	2590	A	2.0
7	2H	164	TYR	2.0
16	2U	63	VAL	2.0
1	1A	2828	C	2.0
1	2A	914	C	2.0
3	2D	61	LEU	2.0
6	1G	43	LEU	2.0
6	1G	133	LEU	2.0
8	1I	4	ILE	2.0
10	2O	30	ALA	2.0
17	1V	78	LYS	2.0
19	2X	53	LYS	2.0
44	1m	70	LEU	2.0
11	2P	21	ARG	2.0
14	1S	15	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
15	1T	71	GLY	2.0
25	23	27	GLY	2.0
33	2b	130	ARG	2.0
40	2i	24	GLY	2.0
48	1q	91	ARG	2.0
32	2a	1012	U	2.0
1	1A	308	G	2.0
7	2H	58	GLU	2.0
22	20	40	GLN	2.0
13	2R	27	SER	2.0
32	1a	1175	G	2.0
10	2O	24	VAL	2.0
33	2b	44	LEU	2.0
34	1c	146	ALA	2.0
1	1A	1786	A	2.0
11	1P	69	GLY	2.0
16	2U	64	ARG	2.0
36	2e	131	ILE	2.0
38	2g	38	LEU	2.0
32	2a	965	A	2.0
1	1A	1827	C	2.0
1	1A	2699	C	2.0
1	2A	2359	C	2.0
1	2A	2703	C	2.0
11	2P	23	PRO	2.0
32	1a	307	C	2.0
32	1a	868	C	2.0
32	2a	34	C	2.0
33	1b	59	GLU	2.0
1	1A	2449	U	2.0
4	1E	152	LYS	2.0
4	2E	7	VAL	2.0
6	2G	37	VAL	2.0
8	2I	21	VAL	2.0
16	1U	5	LYS	2.0
16	1U	8	VAL	2.0
19	1X	78	LYS	2.0
32	2a	1125	U	2.0
28	26	10	LEU	2.0
1	1A	972	G	2.0
1	1A	1989	G	2.0
1	2A	559	G	2.0

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Mol	Chain	Res	Type	RSRZ
1	2A	830	G	2.0
1	2A	1303	G	2.0
1	2A	1678	G	2.0
6	1G	89	GLY	2.0
12	1Q	24	GLY	2.0
15	1T	50	ILE	2.0
16	1U	36	ARG	2.0
16	2U	11	ARG	2.0
16	2U	29	SER	2.0
42	2k	51	LYS	2.0
45	1n	49	HIS	2.0
15	1T	102	ILE	2.0
47	2p	42	ARG	2.0
32	2a	1120	G	2.0
32	2a	1291	G	2.0
40	2i	30	GLY	2.0
1	1A	347	A	2.0
1	2A	945	A	2.0
1	2A	1247	A	2.0
1	2A	692	C	2.0
1	2A	2297	C	2.0
5	1F	48	THR	2.0
26	24	27	THR	2.0
32	1a	983	A	2.0
32	2a	1201	A	2.0
32	1a	48	C	2.0
32	1a	879	C	2.0
32	2a	1059	C	2.0
32	2a	1403	C	2.0
33	1b	73	THR	2.0
4	1E	151	TYR	2.0
5	1F	114	VAL	2.0
7	1H	105	LEU	2.0
9	2N	74	ARG	2.0
12	2Q	82	ARG	2.0
43	1l	102	ARG	2.0
43	2l	120	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
32	5MC	1a	967	21/22	0.72	0.37	101,111,125,127	0
32	2MG	1a	1207	24/25	0.84	0.36	97,115,130,140	0
32	5MC	2a	967	21/22	0.84	0.33	100,110,124,141	0
32	M2G	1a	966	25/26	0.85	0.32	96,110,117,129	0
43	0TD	2l	92	10/11	0.88	0.24	79,94,103,117	0
32	PSU	1a	516	20/21	0.89	0.17	92,103,110,110	0
32	PSU	2a	516	20/21	0.90	0.13	88,104,112,114	0
32	4OC	1a	1402	22/23	0.91	0.31	77,90,106,109	0
32	2MG	2a	1207	24/25	0.91	0.33	101,114,128,130	0
43	0TD	1l	92	10/11	0.91	0.38	76,97,100,136	0
1	5MU	2A	1915	21/22	0.91	0.17	89,104,108,127	0
1	PSU	1A	1917	20/21	0.92	0.14	83,98,110,113	0
1	5MU	1A	1915	21/22	0.92	0.17	91,100,109,124	0
32	5MC	2a	1404	21/22	0.92	0.28	70,87,106,107	0
32	4OC	2a	1402	22/23	0.92	0.46	94,102,113,115	0
1	PSU	2A	1917	20/21	0.92	0.14	83,98,115,116	0
1	PSU	1A	1911	20/21	0.92	0.16	82,93,98,102	0
32	5MC	2a	1400	21/22	0.93	0.46	87,100,110,117	0
32	5MC	1a	1404	21/22	0.93	0.26	72,90,104,107	0
32	5MC	1a	1407	21/22	0.93	0.37	71,88,94,103	0
32	M2G	2a	966	25/26	0.93	0.38	95,107,118,128	0
1	PSU	2A	1911	20/21	0.93	0.16	80,92,102,104	0
1	2MA	2A	2503	23/24	0.94	0.29	35,40,53,57	0
1	5MC	2A	1962	21/22	0.94	0.28	51,71,84,90	0
32	UR3	2a	1498	21/22	0.94	0.24	81,91,99,114	0
1	4OC	2A	1920	21/23	0.94	0.19	86,93,100,101	0
32	7MG	2a	527	24/25	0.94	0.22	83,97,107,118	0
1	4OC	1A	1920	21/23	0.94	0.21	82,92,98,101	0
1	OMG	2A	2251	24/25	0.94	0.37	43,54,59,62	0
32	5MC	1a	1400	21/22	0.94	0.29	72,98,109,116	0
32	MA6	1a	1519	24/25	0.94	0.41	61,84,94,101	0
32	7MG	1a	527	24/25	0.94	0.37	85,94,100,105	0
1	5MC	1A	1962	21/22	0.95	0.32	49,70,83,86	0
1	5MC	2A	1942	21/22	0.95	0.21	57,73,79,89	0
32	MA6	2a	1518	24/25	0.95	0.40	56,95,102,108	0
1	PSU	2A	2605	20/21	0.95	0.28	36,51,56,56	0
32	MA6	2a	1519	24/25	0.95	0.38	78,91,99,106	0
1	PSU	1A	2605	20/21	0.95	0.29	33,49,55,60	0
32	5MC	2a	1407	21/22	0.96	0.23	83,89,96,99	0
1	2MA	1A	2503	23/24	0.96	0.33	31,36,45,65	0
1	5MC	1A	1942	21/22	0.96	0.25	50,71,80,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MA6	1a	1518	24/25	0.96	0.33	58,81,89,95	0
1	5MU	2A	1939	21/22	0.96	0.37	45,59,65,67	0
32	UR3	1a	1498	21/22	0.96	0.22	80,88,95,99	0
1	OMG	1A	2251	24/25	0.97	0.29	34,50,55,60	0
1	2MU	2A	2552	21/23	0.97	0.21	38,47,60,60	0
1	2MU	1A	2552	21/23	0.97	0.30	37,44,57,60	0
1	5MU	1A	1939	21/22	0.97	0.28	42,55,63,65	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	2a	1640	1/1	0.34	0.18	84,84,84,84	0
53	MG	1a	3008	1/1	0.46	0.33	95,95,95,95	0
53	MG	2t	201	1/1	0.46	1.75	80,80,80,80	0
53	MG	1r	3001	1/1	0.46	0.25	87,87,87,87	0
53	MG	1a	3056	1/1	0.49	0.26	74,74,74,74	0
53	MG	2a	1632	1/1	0.53	0.25	89,89,89,89	0
53	MG	1g	3002	1/1	0.53	0.18	83,83,83,83	0
53	MG	1A	3739	1/1	0.56	0.15	36,36,36,36	0
53	MG	1a	3059	1/1	0.56	0.86	92,92,92,92	0
53	MG	2a	1709	1/1	0.56	0.10	105,105,105,105	0
53	MG	2a	1705	1/1	0.56	1.25	91,91,91,91	0
53	MG	2A	3433	1/1	0.56	0.29	65,65,65,65	0
53	MG	1a	3142	1/1	0.56	2.02	106,106,106,106	0
53	MG	2a	1607	1/1	0.57	0.18	85,85,85,85	0
53	MG	2A	3403	1/1	0.58	0.15	69,69,69,69	0
53	MG	1a	3076	1/1	0.58	0.18	87,87,87,87	0
53	MG	2F	301	1/1	0.58	0.24	62,62,62,62	0
53	MG	2a	1643	1/1	0.59	0.33	102,102,102,102	0
53	MG	1A	3250	1/1	0.59	0.51	80,80,80,80	0
53	MG	2a	1646	1/1	0.62	0.29	74,74,74,74	0
53	MG	2a	1633	1/1	0.62	0.21	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2a	1650	1/1	0.62	0.25	80,80,80,80	0
53	MG	2B	214	1/1	0.62	0.15	53,53,53,53	0
53	MG	1B	3008	1/1	0.63	0.45	69,69,69,69	0
53	MG	1a	3066	1/1	0.64	0.25	74,74,74,74	0
53	MG	1A	3747	1/1	0.64	0.28	58,58,58,58	0
53	MG	2A	3071	1/1	0.65	0.25	68,68,68,68	0
53	MG	1A	3255	1/1	0.65	0.79	57,57,57,57	0
53	MG	2A	3138	1/1	0.66	0.30	55,55,55,55	0
53	MG	2A	3103	1/1	0.66	0.12	76,76,76,76	0
53	MG	1A	3364	1/1	0.66	0.28	82,82,82,82	0
53	MG	1A	3360	1/1	0.66	0.47	77,77,77,77	0
53	MG	1h	8001	1/1	0.66	0.14	88,88,88,88	0
53	MG	1A	3239	1/1	0.67	0.27	56,56,56,56	0
53	MG	2A	3145	1/1	0.68	0.24	55,55,55,55	0
53	MG	2A	3312	1/1	0.68	0.16	70,70,70,70	0
53	MG	2A	3478	1/1	0.68	0.22	81,81,81,81	0
53	MG	2A	3276	1/1	0.69	0.19	57,57,57,57	0
53	MG	2a	1723	1/1	0.69	0.16	77,77,77,77	0
53	MG	2A	3378	1/1	0.69	0.18	69,69,69,69	0
53	MG	1W	3001	1/1	0.69	0.37	52,52,52,52	0
53	MG	2A	3321	1/1	0.69	0.32	47,47,47,47	0
53	MG	2A	3248	1/1	0.69	0.20	63,63,63,63	0
53	MG	2a	1671	1/1	0.69	0.32	70,70,70,70	0
53	MG	1a	3086	1/1	0.69	0.16	77,77,77,77	0
53	MG	1A	3236	1/1	0.69	0.23	64,64,64,64	0
53	MG	1q	201	1/1	0.69	0.14	79,79,79,79	0
53	MG	2A	3425	1/1	0.70	0.12	68,68,68,68	0
53	MG	1A	3264	1/1	0.70	0.36	68,68,68,68	0
53	MG	2A	3088	1/1	0.70	0.31	67,67,67,67	0
53	MG	1A	3496	1/1	0.70	0.31	73,73,73,73	0
53	MG	19	103	1/1	0.70	0.55	47,47,47,47	0
53	MG	1A	3601	1/1	0.70	0.17	43,43,43,43	0
53	MG	1A	3229	1/1	0.70	0.23	57,57,57,57	0
53	MG	1a	3109	1/1	0.70	0.16	100,100,100,100	0
53	MG	1a	3006	1/1	0.70	0.15	85,85,85,85	0
53	MG	2A	3229	1/1	0.71	0.54	72,72,72,72	0
53	MG	1N	3001	1/1	0.71	0.28	77,77,77,77	0
53	MG	1E	305	1/1	0.71	0.51	79,79,79,79	0
53	MG	1A	3283	1/1	0.71	0.41	71,71,71,71	0
53	MG	1B	3002	1/1	0.71	0.29	76,76,76,76	0
55	ZN	2n	501	1/1	0.71	0.06	160,160,160,160	0
53	MG	1H	202	1/1	0.71	0.33	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1a	3079	1/1	0.71	0.19	73,73,73,73	0
53	MG	2a	1682	1/1	0.71	0.22	76,76,76,76	0
53	MG	2A	3182	1/1	0.71	0.21	58,58,58,58	0
53	MG	2A	3149	1/1	0.72	0.40	52,52,52,52	0
53	MG	2a	1694	1/1	0.72	0.14	74,74,74,74	0
53	MG	2A	3221	1/1	0.72	0.17	59,59,59,59	0
53	MG	1A	3117	1/1	0.72	0.34	63,63,63,63	0
53	MG	2a	1716	1/1	0.73	0.13	85,85,85,85	0
53	MG	1A	3128	1/1	0.73	0.51	60,60,60,60	0
53	MG	1A	3094	1/1	0.73	0.14	73,73,73,73	0
53	MG	2A	3331	1/1	0.73	0.21	65,65,65,65	0
53	MG	1o	102	1/1	0.73	0.35	67,67,67,67	0
53	MG	1B	3005	1/1	0.73	0.21	52,52,52,52	0
53	MG	1A	3200	1/1	0.73	0.17	55,55,55,55	0
53	MG	2A	3315	1/1	0.73	0.15	59,59,59,59	0
53	MG	1A	3074	1/1	0.73	0.26	64,64,64,64	0
53	MG	1A	3732	1/1	0.73	0.55	76,76,76,76	0
53	MG	2A	3504	1/1	0.73	0.14	74,74,74,74	0
53	MG	2A	3025	1/1	0.73	0.47	58,58,58,58	0
53	MG	2A	3029	1/1	0.73	0.12	59,59,59,59	0
53	MG	2a	1620	1/1	0.73	0.20	89,89,89,89	0
53	MG	1A	3112	1/1	0.74	0.25	70,70,70,70	0
53	MG	2A	3502	1/1	0.74	0.15	94,94,94,94	0
53	MG	2A	3064	1/1	0.74	0.14	69,69,69,69	0
53	MG	2a	1617	1/1	0.74	0.20	71,71,71,71	0
53	MG	1A	3384	1/1	0.74	0.26	30,30,30,30	0
53	MG	2A	3444	1/1	0.74	0.25	59,59,59,59	0
53	MG	2A	3050	1/1	0.74	0.21	45,45,45,45	0
53	MG	1A	3306	1/1	0.74	0.32	56,56,56,56	0
53	MG	1a	3083	1/1	0.74	0.26	59,59,59,59	0
53	MG	1a	3053	1/1	0.74	0.15	60,60,60,60	0
53	MG	1A	3516	1/1	0.74	0.57	53,53,53,53	0
53	MG	1a	3131	1/1	0.75	0.23	91,91,91,91	0
53	MG	2A	3096	1/1	0.75	0.27	67,67,67,67	0
53	MG	1A	3035	1/1	0.75	0.46	52,52,52,52	0
53	MG	2A	3277	1/1	0.75	0.23	61,61,61,61	0
53	MG	1a	3092	1/1	0.75	0.09	104,104,104,104	0
53	MG	1e	201	1/1	0.75	0.44	73,73,73,73	0
53	MG	1a	3011	1/1	0.75	0.15	64,64,64,64	0
53	MG	1A	3464	1/1	0.75	0.25	36,36,36,36	0
53	MG	2a	1715	1/1	0.75	0.17	84,84,84,84	0
53	MG	2A	3364	1/1	0.75	0.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3109	1/1	0.75	0.29	69,69,69,69	0
53	MG	1B	3010	1/1	0.76	0.28	51,51,51,51	0
53	MG	1A	3556	1/1	0.76	0.48	77,77,77,77	0
53	MG	2A	3078	1/1	0.76	0.20	62,62,62,62	0
53	MG	1A	3014	1/1	0.76	0.56	52,52,52,52	0
53	MG	1A	3445	1/1	0.76	0.21	90,90,90,90	0
53	MG	2a	1672	1/1	0.76	0.20	61,61,61,61	0
53	MG	2A	3423	1/1	0.76	0.59	67,67,67,67	0
53	MG	2a	1699	1/1	0.76	0.34	85,85,85,85	0
53	MG	2A	3020	1/1	0.76	0.15	54,54,54,54	0
53	MG	1A	3130	1/1	0.76	0.38	63,63,63,63	0
53	MG	2a	1622	1/1	0.76	0.16	83,83,83,83	0
53	MG	1A	3718	1/1	0.77	0.21	76,76,76,76	0
53	MG	2A	3430	1/1	0.77	0.14	63,63,63,63	0
53	MG	2B	204	1/1	0.77	0.21	63,63,63,63	0
53	MG	2A	3269	1/1	0.77	0.21	75,75,75,75	0
53	MG	2A	3365	1/1	0.77	0.11	75,75,75,75	0
53	MG	1A	3417	1/1	0.77	0.28	59,59,59,59	0
53	MG	2a	1614	1/1	0.77	0.20	84,84,84,84	0
53	MG	1A	3543	1/1	0.77	0.16	60,60,60,60	0
53	MG	1a	3037	1/1	0.78	0.10	84,84,84,84	0
53	MG	2A	3323	1/1	0.78	0.42	74,74,74,74	0
53	MG	1A	3465	1/1	0.78	0.19	62,62,62,62	0
53	MG	1N	3002	1/1	0.78	0.11	92,92,92,92	0
53	MG	2O	201	1/1	0.78	0.21	48,48,48,48	0
53	MG	2A	3342	1/1	0.78	0.12	61,61,61,61	0
53	MG	2B	213	1/1	0.78	0.20	70,70,70,70	0
53	MG	1a	3117	1/1	0.78	0.25	78,78,78,78	0
53	MG	1l	202	1/1	0.78	0.17	81,81,81,81	0
53	MG	1A	3027	1/1	0.78	0.13	66,66,66,66	0
53	MG	1a	3040	1/1	0.78	0.21	76,76,76,76	0
53	MG	2a	1657	1/1	0.78	0.20	68,68,68,68	0
53	MG	2A	3049	1/1	0.78	0.15	57,57,57,57	0
53	MG	1A	3164	1/1	0.78	0.32	53,53,53,53	0
53	MG	2A	3151	1/1	0.79	0.27	64,64,64,64	0
53	MG	2a	1616	1/1	0.79	0.16	92,92,92,92	0
53	MG	2A	3257	1/1	0.79	0.34	60,60,60,60	0
53	MG	2Q	3003	1/1	0.79	0.25	45,45,45,45	0
53	MG	2A	3147	1/1	0.79	0.77	53,53,53,53	0
53	MG	1A	3712	1/1	0.79	0.20	53,53,53,53	0
53	MG	1A	3058	1/1	0.79	0.32	49,49,49,49	0
53	MG	1A	3744	1/1	0.79	0.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1a	3026	1/1	0.79	0.44	65,65,65,65	0
53	MG	1A	3659	1/1	0.79	0.25	85,85,85,85	0
53	MG	1a	3072	1/1	0.79	0.37	83,83,83,83	0
53	MG	2A	3270	1/1	0.79	0.26	65,65,65,65	0
53	MG	1A	3727	1/1	0.79	0.27	80,80,80,80	0
53	MG	2I	3001	1/1	0.79	0.20	81,81,81,81	0
53	MG	1A	3512	1/1	0.79	0.28	64,64,64,64	0
53	MG	1A	3079	1/1	0.79	0.20	74,74,74,74	0
53	MG	2A	3382	1/1	0.79	0.15	51,51,51,51	0
53	MG	1A	3163	1/1	0.79	0.26	54,54,54,54	0
53	MG	1A	3060	1/1	0.79	0.48	53,53,53,53	0
53	MG	1A	3136	1/1	0.79	0.51	63,63,63,63	0
53	MG	2A	3081	1/1	0.79	0.30	82,82,82,82	0
53	MG	2a	1727	1/1	0.79	0.18	76,76,76,76	0
53	MG	1B	3006	1/1	0.79	0.17	47,47,47,47	0
53	MG	1I	3001	1/1	0.80	0.57	73,73,73,73	0
53	MG	1A	3158	1/1	0.80	0.25	55,55,55,55	0
53	MG	1A	3013	1/1	0.80	0.44	69,69,69,69	0
53	MG	1A	3551	1/1	0.80	0.19	58,58,58,58	0
53	MG	2A	3133	1/1	0.80	0.29	63,63,63,63	0
53	MG	2A	3067	1/1	0.80	0.20	56,56,56,56	0
53	MG	2A	3448	1/1	0.80	0.22	80,80,80,80	0
53	MG	2A	3189	1/1	0.80	0.22	55,55,55,55	0
53	MG	1A	3397	1/1	0.80	0.14	35,35,35,35	0
53	MG	1a	3021	1/1	0.80	0.15	86,86,86,86	0
53	MG	1A	3303	1/1	0.80	0.26	52,52,52,52	0
53	MG	2A	3152	1/1	0.80	0.31	48,48,48,48	0
53	MG	2A	3123	1/1	0.80	0.42	68,68,68,68	0
53	MG	2A	3164	1/1	0.80	0.27	57,57,57,57	0
53	MG	1a	3143	1/1	0.80	0.17	57,57,57,57	0
53	MG	2a	1728	1/1	0.80	0.23	85,85,85,85	0
53	MG	1A	3051	1/1	0.80	0.22	60,60,60,60	0
53	MG	1A	3088	1/1	0.80	0.20	71,71,71,71	0
53	MG	1D	307	1/1	0.80	0.21	63,63,63,63	0
53	MG	2A	3016	1/1	0.80	0.36	70,70,70,70	0
53	MG	2B	209	1/1	0.80	0.35	64,64,64,64	0
53	MG	1A	3070	1/1	0.80	0.36	74,74,74,74	0
53	MG	2A	3010	1/1	0.80	0.35	67,67,67,67	0
53	MG	2A	3439	1/1	0.81	0.19	49,49,49,49	0
53	MG	1A	3007	1/1	0.81	0.23	56,56,56,56	0
53	MG	1B	3015	1/1	0.81	0.36	64,64,64,64	0
53	MG	1A	3132	1/1	0.81	0.23	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	1A	3256	1/1	0.81	0.22	52,52,52,52	0
53	MG	2a	1713	1/1	0.81	0.11	100,100,100,100	0
53	MG	2A	3289	1/1	0.81	0.28	50,50,50,50	0
53	MG	2A	3072	1/1	0.81	0.28	71,71,71,71	0
53	MG	1A	3598	1/1	0.81	0.15	109,109,109,109	0
53	MG	2a	1604	1/1	0.81	0.48	59,59,59,59	0
53	MG	2a	1670	1/1	0.81	0.16	67,67,67,67	0
53	MG	1A	3331	1/1	0.81	0.15	56,56,56,56	0
53	MG	2a	1652	1/1	0.81	0.24	80,80,80,80	0
53	MG	1A	3674	1/1	0.81	0.17	82,82,82,82	0
53	MG	1a	3068	1/1	0.81	0.62	90,90,90,90	0
53	MG	1A	3528	1/1	0.81	0.15	72,72,72,72	0
53	MG	1A	3281	1/1	0.81	0.34	56,56,56,56	0
53	MG	1A	3378	1/1	0.81	0.30	72,72,72,72	0
53	MG	1a	3078	1/1	0.81	0.22	65,65,65,65	0
55	ZN	24	501	1/1	0.81	0.07	173,173,173,173	0
53	MG	2A	3003	1/1	0.81	0.49	68,68,68,68	0
53	MG	2A	3381	1/1	0.81	0.20	69,69,69,69	0
53	MG	1A	3392	1/1	0.81	0.16	34,34,34,34	0
53	MG	1A	3305	1/1	0.81	0.32	60,60,60,60	0
53	MG	1A	3290	1/1	0.81	0.18	51,51,51,51	0
53	MG	1A	3353	1/1	0.81	0.18	60,60,60,60	0
53	MG	1a	3074	1/1	0.81	0.11	67,67,67,67	0
53	MG	1a	3051	1/1	0.81	0.24	54,54,54,54	0
53	MG	2B	211	1/1	0.81	0.17	62,62,62,62	0
53	MG	2A	3027	1/1	0.81	0.23	63,63,63,63	0
53	MG	1A	3396	1/1	0.81	0.26	59,59,59,59	0
53	MG	2a	1725	1/1	0.81	0.23	97,97,97,97	0
53	MG	2A	3157	1/1	0.82	0.21	55,55,55,55	0
53	MG	1A	3104	1/1	0.82	0.25	58,58,58,58	0
53	MG	2A	3253	1/1	0.82	0.20	54,54,54,54	0
53	MG	1A	3194	1/1	0.82	0.26	51,51,51,51	0
53	MG	1A	3106	1/1	0.82	0.22	55,55,55,55	0
53	MG	1A	3251	1/1	0.82	0.29	59,59,59,59	0
53	MG	1A	3057	1/1	0.82	1.00	47,47,47,47	0
53	MG	1A	3084	1/1	0.82	0.26	73,73,73,73	0
53	MG	2Q	3002	1/1	0.82	0.24	51,51,51,51	0
53	MG	2A	3013	1/1	0.82	0.39	80,80,80,80	0
53	MG	2A	3045	1/1	0.82	0.19	61,61,61,61	0
53	MG	1a	3025	1/1	0.82	0.28	84,84,84,84	0
53	MG	2A	3398	1/1	0.82	0.14	61,61,61,61	0
53	MG	1A	3525	1/1	0.82	0.54	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3245	1/1	0.82	0.24	46,46,46,46	0
53	MG	1A	3676	1/1	0.82	0.12	89,89,89,89	0
53	MG	2A	3009	1/1	0.82	0.77	57,57,57,57	0
53	MG	1A	3691	1/1	0.82	0.13	84,84,84,84	0
53	MG	1a	3100	1/1	0.82	0.16	92,92,92,92	0
53	MG	2A	3092	1/1	0.82	0.58	68,68,68,68	0
53	MG	2A	3191	1/1	0.82	0.21	54,54,54,54	0
53	MG	1A	3630	1/1	0.82	0.20	70,70,70,70	0
53	MG	1a	3055	1/1	0.82	0.43	74,74,74,74	0
53	MG	2A	3420	1/1	0.82	0.60	54,54,54,54	0
53	MG	1A	3228	1/1	0.82	0.20	65,65,65,65	0
53	MG	2A	3307	1/1	0.82	0.20	69,69,69,69	0
53	MG	1A	3538	1/1	0.82	0.18	65,65,65,65	0
53	MG	15	106	1/1	0.82	0.17	86,86,86,86	0
53	MG	1A	3008	1/1	0.82	0.41	57,57,57,57	0
53	MG	2A	3030	1/1	0.83	0.13	73,73,73,73	0
53	MG	1B	3011	1/1	0.83	0.14	58,58,58,58	0
53	MG	1A	3102	1/1	0.83	0.10	85,85,85,85	0
53	MG	2A	3216	1/1	0.83	0.41	65,65,65,65	0
53	MG	1A	3453	1/1	0.83	0.47	87,87,87,87	0
53	MG	2a	1667	1/1	0.83	0.26	74,74,74,74	0
53	MG	2A	3408	1/1	0.83	0.23	43,43,43,43	0
53	MG	2A	3161	1/1	0.83	0.17	54,54,54,54	0
53	MG	1A	3657	1/1	0.83	0.18	44,44,44,44	0
53	MG	2F	302	1/1	0.83	0.12	64,64,64,64	0
53	MG	1A	3227	1/1	0.83	0.47	61,61,61,61	0
53	MG	1a	3045	1/1	0.83	0.17	76,76,76,76	0
53	MG	1a	3036	1/1	0.83	0.21	88,88,88,88	0
53	MG	1A	3491	1/1	0.83	0.14	65,65,65,65	0
53	MG	1a	3018	1/1	0.83	0.19	86,86,86,86	0
53	MG	1A	3446	1/1	0.83	0.41	76,76,76,76	0
53	MG	2A	3217	1/1	0.83	0.30	64,64,64,64	0
53	MG	1Z	8001	1/1	0.83	0.20	58,58,58,58	0
53	MG	1a	3061	1/1	0.83	0.14	78,78,78,78	0
53	MG	2A	3240	1/1	0.83	0.19	60,60,60,60	0
53	MG	1A	3359	1/1	0.83	0.39	66,66,66,66	0
53	MG	2a	1704	1/1	0.83	0.06	110,110,110,110	0
53	MG	2a	1627	1/1	0.83	0.71	78,78,78,78	0
53	MG	2A	3267	1/1	0.83	0.51	70,70,70,70	0
53	MG	1A	3766	1/1	0.83	1.03	47,47,47,47	0
53	MG	2a	1707	1/1	0.83	0.13	82,82,82,82	0
53	MG	2A	3202	1/1	0.83	0.25	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	3263	1/1	0.83	0.18	61,61,61,61	0
53	MG	1A	3560	1/1	0.83	0.52	66,66,66,66	0
53	MG	1A	3062	1/1	0.83	0.20	71,71,71,71	0
53	MG	2A	3121	1/1	0.83	0.15	62,62,62,62	0
53	MG	1A	3383	1/1	0.83	0.45	71,71,71,71	0
53	MG	1Q	202	1/1	0.83	0.24	35,35,35,35	0
53	MG	1A	3118	1/1	0.84	0.26	53,53,53,53	0
53	MG	1A	3361	1/1	0.84	0.19	69,69,69,69	0
53	MG	2A	3192	1/1	0.84	0.22	62,62,62,62	0
53	MG	1A	3139	1/1	0.84	0.18	57,57,57,57	0
53	MG	1a	3052	1/1	0.84	0.58	75,75,75,75	0
53	MG	1A	3763	1/1	0.84	0.54	51,51,51,51	0
53	MG	1A	3133	1/1	0.84	0.29	69,69,69,69	0
53	MG	1A	3184	1/1	0.84	0.20	55,55,55,55	0
53	MG	2A	3435	1/1	0.84	0.22	88,88,88,88	0
53	MG	2A	3468	1/1	0.84	0.10	58,58,58,58	0
53	MG	2k	3001	1/1	0.84	0.12	86,86,86,86	0
53	MG	2A	3110	1/1	0.84	0.23	45,45,45,45	0
53	MG	2a	1718	1/1	0.84	0.27	93,93,93,93	0
53	MG	2A	3427	1/1	0.84	0.09	84,84,84,84	0
53	MG	2a	1687	1/1	0.84	0.38	76,76,76,76	0
53	MG	1a	3007	1/1	0.84	0.29	64,64,64,64	0
53	MG	1V	3002	1/1	0.84	0.43	62,62,62,62	0
53	MG	1A	3182	1/1	0.84	0.29	39,39,39,39	0
53	MG	1A	3053	1/1	0.84	0.81	49,49,49,49	0
53	MG	1l	201	1/1	0.84	0.23	73,73,73,73	0
53	MG	1a	3116	1/1	0.84	0.31	137,137,137,137	0
53	MG	2A	3322	1/1	0.84	0.30	53,53,53,53	0
53	MG	2A	3087	1/1	0.84	0.34	64,64,64,64	0
53	MG	2B	205	1/1	0.84	0.28	73,73,73,73	0
53	MG	1A	3237	1/1	0.84	0.31	41,41,41,41	0
53	MG	1a	3042	1/1	0.84	0.15	64,64,64,64	0
53	MG	2A	3368	1/1	0.84	0.85	77,77,77,77	0
53	MG	1A	3159	1/1	0.84	0.23	49,49,49,49	0
53	MG	2A	3132	1/1	0.84	0.22	56,56,56,56	0
53	MG	1a	3077	1/1	0.84	0.19	69,69,69,69	0
53	MG	1A	3608	1/1	0.84	0.13	55,55,55,55	0
53	MG	2A	3101	1/1	0.84	0.24	50,50,50,50	0
53	MG	1A	3607	1/1	0.84	0.16	86,86,86,86	0
53	MG	1a	3136	1/1	0.84	0.18	83,83,83,83	0
53	MG	1G	8002	1/1	0.84	0.17	88,88,88,88	0
53	MG	2A	3001	1/1	0.84	0.14	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	2l	3001	1/1	0.84	0.14	53,53,53,53	0
53	MG	2A	3332	1/1	0.84	0.29	66,66,66,66	0
53	MG	1a	3041	1/1	0.84	0.37	96,96,96,96	0
53	MG	1A	3068	1/1	0.84	0.16	67,67,67,67	0
53	MG	1A	3096	1/1	0.85	0.24	62,62,62,62	0
53	MG	1A	3052	1/1	0.85	0.29	61,61,61,61	0
53	MG	2a	1605	1/1	0.85	0.30	82,82,82,82	0
53	MG	2a	1706	1/1	0.85	0.10	98,98,98,98	0
53	MG	2A	3026	1/1	0.85	1.33	57,57,57,57	0
53	MG	1a	3112	1/1	0.85	0.12	91,91,91,91	0
53	MG	1A	3638	1/1	0.85	0.18	56,56,56,56	0
53	MG	1A	3481	1/1	0.85	0.26	55,55,55,55	0
53	MG	1A	3621	1/1	0.85	0.23	67,67,67,67	0
53	MG	2A	3105	1/1	0.85	0.41	74,74,74,74	0
53	MG	1A	3086	1/1	0.85	0.32	58,58,58,58	0
53	MG	1A	3717	1/1	0.85	0.24	79,79,79,79	0
53	MG	2A	3316	1/1	0.85	0.18	46,46,46,46	0
53	MG	2E	306	1/1	0.85	0.34	68,68,68,68	0
53	MG	2A	3313	1/1	0.85	0.18	63,63,63,63	0
53	MG	1A	3720	1/1	0.85	0.14	53,53,53,53	0
53	MG	1a	3060	1/1	0.85	0.14	81,81,81,81	0
53	MG	2A	3369	1/1	0.85	0.14	56,56,56,56	0
53	MG	2a	1692	1/1	0.85	0.22	82,82,82,82	0
53	MG	1A	3374	1/1	0.85	0.14	68,68,68,68	0
53	MG	1A	3030	1/1	0.85	0.21	61,61,61,61	0
53	MG	2a	1661	1/1	0.85	0.85	87,87,87,87	0
53	MG	1A	3619	1/1	0.85	0.14	55,55,55,55	0
53	MG	1A	3435	1/1	0.85	0.19	46,46,46,46	0
53	MG	1A	3114	1/1	0.85	0.17	66,66,66,66	0
53	MG	2A	3109	1/1	0.85	0.35	67,67,67,67	0
53	MG	2A	3153	1/1	0.85	0.16	59,59,59,59	0
53	MG	1A	3175	1/1	0.85	0.43	54,54,54,54	0
53	MG	1A	3073	1/1	0.85	0.17	62,62,62,62	0
53	MG	1A	3667	1/1	0.85	0.24	36,36,36,36	0
53	MG	2a	1712	1/1	0.85	0.17	103,103,103,103	0
53	MG	1A	3332	1/1	0.85	0.33	61,61,61,61	0
53	MG	1d	502	1/1	0.85	0.23	58,58,58,58	0
53	MG	2A	3127	1/1	0.85	0.28	66,66,66,66	0
53	MG	2A	3089	1/1	0.85	0.14	71,71,71,71	0
53	MG	1A	3017	1/1	0.85	0.19	56,56,56,56	0
53	MG	1A	3731	1/1	0.86	0.25	71,71,71,71	0
53	MG	1A	3594	1/1	0.86	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	2a	1691	1/1	0.86	0.33	76,76,76,76	0
53	MG	2A	3513	1/1	0.86	0.81	60,60,60,60	0
53	MG	1A	3313	1/1	0.86	0.71	52,52,52,52	0
53	MG	1A	3664	1/1	0.86	0.19	49,49,49,49	0
53	MG	1A	3495	1/1	0.86	0.20	49,49,49,49	0
53	MG	1A	3466	1/1	0.86	0.17	87,87,87,87	0
53	MG	1a	3067	1/1	0.86	0.13	80,80,80,80	0
53	MG	1A	3338	1/1	0.86	0.38	62,62,62,62	0
53	MG	1a	3114	1/1	0.86	0.21	100,100,100,100	0
53	MG	2a	1603	1/1	0.86	0.33	79,79,79,79	0
53	MG	2A	3084	1/1	0.86	0.19	49,49,49,49	0
53	MG	1A	3411	1/1	0.86	0.24	32,32,32,32	0
53	MG	2A	3500	1/1	0.86	0.09	64,64,64,64	0
53	MG	1A	3099	1/1	0.86	0.14	64,64,64,64	0
53	MG	2A	3338	1/1	0.86	0.19	49,49,49,49	0
53	MG	1a	3015	1/1	0.86	0.15	73,73,73,73	0
53	MG	2A	3015	1/1	0.86	0.59	45,45,45,45	0
53	MG	1A	3437	1/1	0.86	0.19	36,36,36,36	0
53	MG	1A	3347	1/1	0.86	0.19	52,52,52,52	0
53	MG	2A	3351	1/1	0.86	0.16	59,59,59,59	0
53	MG	1A	3436	1/1	0.86	0.24	49,49,49,49	0
53	MG	1A	3592	1/1	0.86	0.18	49,49,49,49	0
53	MG	2A	3385	1/1	0.86	0.39	71,71,71,71	0
53	MG	1a	3043	1/1	0.86	0.20	90,90,90,90	0
53	MG	2A	3057	1/1	0.86	0.44	65,65,65,65	0
53	MG	2A	3080	1/1	0.86	0.32	66,66,66,66	0
53	MG	1A	3715	1/1	0.86	0.10	84,84,84,84	0
53	MG	2A	3069	1/1	0.86	0.25	60,60,60,60	0
53	MG	1A	3322	1/1	0.86	0.30	47,47,47,47	0
53	MG	2a	1612	1/1	0.86	0.15	93,93,93,93	0
53	MG	2a	1637	1/1	0.86	0.71	65,65,65,65	0
53	MG	2A	3366	1/1	0.86	0.19	37,37,37,37	0
53	MG	2A	3426	1/1	0.86	0.16	56,56,56,56	0
53	MG	2A	3387	1/1	0.86	0.24	69,69,69,69	0
53	MG	1A	3257	1/1	0.86	0.22	53,53,53,53	0
53	MG	2A	3048	1/1	0.86	0.16	64,64,64,64	0
53	MG	2A	3311	1/1	0.86	0.15	50,50,50,50	0
53	MG	1A	3016	1/1	0.86	0.27	66,66,66,66	0
53	MG	2A	3255	1/1	0.86	0.17	71,71,71,71	0
53	MG	1A	3736	1/1	0.86	0.21	68,68,68,68	0
53	MG	2A	3073	1/1	0.86	0.09	61,61,61,61	0
53	MG	2a	1635	1/1	0.86	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3400	1/1	0.86	0.13	65,65,65,65	0
53	MG	2a	1631	1/1	0.86	0.22	59,59,59,59	0
53	MG	10	101	1/1	0.86	0.33	67,67,67,67	0
53	MG	1a	3049	1/1	0.86	0.20	80,80,80,80	0
53	MG	2A	3421	1/1	0.86	0.16	56,56,56,56	0
53	MG	2A	3473	1/1	0.86	0.18	57,57,57,57	0
53	MG	2A	3295	1/1	0.87	0.13	54,54,54,54	0
53	MG	2a	1711	1/1	0.87	0.13	105,105,105,105	0
53	MG	2A	3163	1/1	0.87	0.17	55,55,55,55	0
53	MG	1a	3082	1/1	0.87	0.32	70,70,70,70	0
53	MG	1A	3555	1/1	0.87	0.26	35,35,35,35	0
53	MG	2A	3344	1/1	0.87	0.23	54,54,54,54	0
53	MG	2a	1675	1/1	0.87	0.09	83,83,83,83	0
53	MG	1A	3129	1/1	0.87	0.34	54,54,54,54	0
53	MG	2A	3134	1/1	0.87	0.68	67,67,67,67	0
53	MG	1A	3286	1/1	0.87	0.31	44,44,44,44	0
53	MG	2A	3491	1/1	0.87	0.18	71,71,71,71	0
53	MG	1R	202	1/1	0.87	0.19	49,49,49,49	0
53	MG	1A	3368	1/1	0.87	0.27	62,62,62,62	0
53	MG	1G	8001	1/1	0.87	0.16	77,77,77,77	0
53	MG	1o	101	1/1	0.87	0.08	82,82,82,82	0
53	MG	2A	3278	1/1	0.87	0.32	56,56,56,56	0
53	MG	1A	3510	1/1	0.87	0.52	41,41,41,41	0
53	MG	1R	205	1/1	0.87	0.35	52,52,52,52	0
53	MG	2A	3413	1/1	0.87	1.14	71,71,71,71	0
53	MG	2A	3464	1/1	0.87	0.12	47,47,47,47	0
53	MG	2A	3509	1/1	0.87	0.23	61,61,61,61	0
53	MG	1a	3113	1/1	0.87	0.12	97,97,97,97	0
53	MG	2a	1676	1/1	0.87	0.27	58,58,58,58	0
53	MG	1A	3376	1/1	0.87	0.18	38,38,38,38	0
53	MG	1A	3388	1/1	0.87	0.37	53,53,53,53	0
53	MG	1A	3728	1/1	0.87	0.14	77,77,77,77	0
53	MG	1A	3350	1/1	0.87	0.25	59,59,59,59	0
53	MG	2a	1641	1/1	0.87	1.01	67,67,67,67	0
53	MG	1A	3215	1/1	0.87	0.44	59,59,59,59	0
53	MG	1A	3103	1/1	0.87	0.08	81,81,81,81	0
53	MG	1A	3154	1/1	0.87	0.13	50,50,50,50	0
53	MG	2A	3242	1/1	0.87	0.19	62,62,62,62	0
53	MG	2A	3345	1/1	0.87	0.20	55,55,55,55	0
53	MG	2A	3150	1/1	0.87	0.19	46,46,46,46	0
53	MG	1A	3210	1/1	0.87	0.16	60,60,60,60	0
53	MG	2A	3422	1/1	0.87	0.12	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1B	3018	1/1	0.87	0.40	69,69,69,69	0
53	MG	2a	1623	1/1	0.87	0.15	66,66,66,66	0
53	MG	2X	101	1/1	0.87	0.18	70,70,70,70	0
53	MG	2A	3263	1/1	0.87	0.16	50,50,50,50	0
53	MG	1A	3413	1/1	0.87	0.25	57,57,57,57	0
53	MG	1A	3221	1/1	0.87	0.25	70,70,70,70	0
53	MG	1A	3684	1/1	0.87	0.14	76,76,76,76	0
53	MG	2A	3371	1/1	0.87	0.10	36,36,36,36	0
53	MG	1A	3323	1/1	0.87	0.86	52,52,52,52	0
53	MG	2A	3406	1/1	0.87	0.17	49,49,49,49	0
53	MG	2B	202	1/1	0.87	0.33	85,85,85,85	0
53	MG	1A	3626	1/1	0.87	0.15	26,26,26,26	0
53	MG	2A	3040	1/1	0.88	0.15	66,66,66,66	0
53	MG	2A	3349	1/1	0.88	0.19	62,62,62,62	0
53	MG	1a	3030	1/1	0.88	0.11	59,59,59,59	0
53	MG	2D	301	1/1	0.88	0.48	76,76,76,76	0
53	MG	1V	3001	1/1	0.88	0.44	40,40,40,40	0
53	MG	2A	3449	1/1	0.88	0.25	59,59,59,59	0
53	MG	1A	3486	1/1	0.88	0.23	52,52,52,52	0
53	MG	1A	3180	1/1	0.88	0.87	57,57,57,57	0
53	MG	2A	3090	1/1	0.88	1.14	77,77,77,77	0
53	MG	2A	3475	1/1	0.88	0.10	57,57,57,57	0
53	MG	1B	3014	1/1	0.88	0.37	43,43,43,43	0
53	MG	2A	3370	1/1	0.88	0.12	59,59,59,59	0
53	MG	1a	3125	1/1	0.88	0.34	95,95,95,95	0
53	MG	1A	3447	1/1	0.88	0.23	59,59,59,59	0
53	MG	1a	3138	1/1	0.88	0.72	115,115,115,115	0
53	MG	1A	3289	1/1	0.88	0.19	39,39,39,39	0
53	MG	1A	3479	1/1	0.88	0.25	58,58,58,58	0
53	MG	1a	3134	1/1	0.88	0.12	94,94,94,94	0
53	MG	2A	3354	1/1	0.88	0.31	68,68,68,68	0
53	MG	2A	3046	1/1	0.88	0.23	45,45,45,45	0
53	MG	1A	3553	1/1	0.88	0.15	36,36,36,36	0
53	MG	2A	3051	1/1	0.88	0.33	69,69,69,69	0
53	MG	2A	3204	1/1	0.88	0.30	64,64,64,64	0
53	MG	2A	3372	1/1	0.88	0.16	34,34,34,34	0
53	MG	1A	3473	1/1	0.88	0.17	48,48,48,48	0
53	MG	1a	3093	1/1	0.88	0.13	71,71,71,71	0
53	MG	1A	3098	1/1	0.88	0.17	64,64,64,64	0
53	MG	1A	3469	1/1	0.88	0.28	77,77,77,77	0
53	MG	1D	302	1/1	0.88	0.11	58,58,58,58	0
53	MG	1A	3583	1/1	0.88	0.20	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	2A	3328	1/1	0.88	0.13	45,45,45,45	0
53	MG	2a	1606	1/1	0.88	0.15	55,55,55,55	0
53	MG	2A	3061	1/1	0.88	0.36	65,65,65,65	0
53	MG	2A	3122	1/1	0.88	0.42	47,47,47,47	0
53	MG	2A	3141	1/1	0.88	0.37	68,68,68,68	0
53	MG	1B	3012	1/1	0.88	0.18	64,64,64,64	0
53	MG	2a	1688	1/1	0.88	0.18	82,82,82,82	0
53	MG	2A	3200	1/1	0.88	0.41	54,54,54,54	0
53	MG	1A	3010	1/1	0.88	0.17	67,67,67,67	0
53	MG	1A	3666	1/1	0.88	0.61	41,41,41,41	0
53	MG	2A	3117	1/1	0.88	0.49	73,73,73,73	0
53	MG	1A	3586	1/1	0.88	0.30	41,41,41,41	0
53	MG	2A	3437	1/1	0.88	0.18	83,83,83,83	0
53	MG	1A	3346	1/1	0.88	0.26	71,71,71,71	0
53	MG	1A	3738	1/1	0.88	0.24	43,43,43,43	0
53	MG	1A	3726	1/1	0.88	0.12	56,56,56,56	0
53	MG	1E	304	1/1	0.88	0.24	43,43,43,43	0
53	MG	1A	3212	1/1	0.88	0.22	48,48,48,48	0
53	MG	1A	3379	1/1	0.88	0.13	71,71,71,71	0
53	MG	2A	3293	1/1	0.88	0.17	37,37,37,37	0
53	MG	2A	3384	1/1	0.88	0.14	45,45,45,45	0
53	MG	1A	3095	1/1	0.88	0.15	67,67,67,67	0
53	MG	2B	212	1/1	0.88	0.24	71,71,71,71	0
53	MG	1A	3266	1/1	0.88	0.46	65,65,65,65	0
53	MG	1B	3016	1/1	0.88	0.23	38,38,38,38	0
53	MG	2A	3488	1/1	0.88	0.15	66,66,66,66	0
53	MG	1a	3065	1/1	0.88	0.20	82,82,82,82	0
53	MG	2B	207	1/1	0.88	0.36	62,62,62,62	0
53	MG	1A	3546	1/1	0.88	0.11	77,77,77,77	0
53	MG	19	104	1/1	0.88	1.67	49,49,49,49	0
53	MG	2E	302	1/1	0.88	0.29	49,49,49,49	0
53	MG	2a	1615	1/1	0.88	0.12	79,79,79,79	0
53	MG	1A	3341	1/1	0.88	0.24	61,61,61,61	0
53	MG	2A	3497	1/1	0.88	0.07	86,86,86,86	0
53	MG	1D	306	1/1	0.88	0.46	87,87,87,87	0
53	MG	1A	3078	1/1	0.88	0.38	67,67,67,67	0
53	MG	1A	3701	1/1	0.88	0.17	58,58,58,58	0
53	MG	1a	3139	1/1	0.88	0.09	70,70,70,70	0
53	MG	1A	3345	1/1	0.88	0.32	56,56,56,56	0
53	MG	1A	3390	1/1	0.89	0.16	27,27,27,27	0
53	MG	1A	3452	1/1	0.89	0.12	63,63,63,63	0
53	MG	2A	3115	1/1	0.89	0.41	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3239	1/1	0.89	0.16	73,73,73,73	0
55	ZN	14	501	1/1	0.89	0.16	168,168,168,168	0
53	MG	2A	3184	1/1	0.89	0.24	52,52,52,52	0
53	MG	1A	3004	1/1	0.89	0.23	42,42,42,42	0
53	MG	1A	3213	1/1	0.89	0.28	64,64,64,64	0
53	MG	2A	3019	1/1	0.89	0.09	60,60,60,60	0
53	MG	1A	3722	1/1	0.89	0.57	62,62,62,62	0
53	MG	1a	3004	1/1	0.89	0.10	65,65,65,65	0
53	MG	2A	3093	1/1	0.89	0.66	64,64,64,64	0
53	MG	1A	3054	1/1	0.89	0.14	64,64,64,64	0
53	MG	1A	3764	1/1	0.89	0.73	41,41,41,41	0
53	MG	2a	1608	1/1	0.89	0.11	94,94,94,94	0
53	MG	2a	1683	1/1	0.89	0.16	89,89,89,89	0
53	MG	2B	206	1/1	0.89	0.12	74,74,74,74	0
53	MG	1A	3467	1/1	0.89	0.18	57,57,57,57	0
53	MG	1A	3262	1/1	0.89	0.57	55,55,55,55	0
53	MG	1a	3107	1/1	0.89	0.25	92,92,92,92	0
53	MG	1D	301	1/1	0.89	0.67	49,49,49,49	0
53	MG	1A	3265	1/1	0.89	0.58	66,66,66,66	0
53	MG	2A	3112	1/1	0.89	0.23	37,37,37,37	0
53	MG	1B	3013	1/1	0.89	0.23	41,41,41,41	0
53	MG	2A	3224	1/1	0.89	0.56	64,64,64,64	0
53	MG	1b	3001	1/1	0.89	0.08	90,90,90,90	0
53	MG	2A	3271	1/1	0.89	0.30	49,49,49,49	0
53	MG	1A	3026	1/1	0.89	0.15	48,48,48,48	0
53	MG	1A	3273	1/1	0.89	0.40	50,50,50,50	0
53	MG	1a	3022	1/1	0.89	0.22	77,77,77,77	0
53	MG	2A	3358	1/1	0.89	0.10	49,49,49,49	0
53	MG	1A	3277	1/1	0.89	0.28	39,39,39,39	0
53	MG	2A	3113	1/1	0.89	0.69	62,62,62,62	0
53	MG	2a	1693	1/1	0.89	0.38	82,82,82,82	0
53	MG	2a	1664	1/1	0.89	0.17	68,68,68,68	0
53	MG	2A	3314	1/1	0.89	0.38	55,55,55,55	0
53	MG	1A	3282	1/1	0.89	1.06	61,61,61,61	0
53	MG	1a	3097	1/1	0.89	0.39	82,82,82,82	0
53	MG	2B	203	1/1	0.89	0.25	76,76,76,76	0
53	MG	1A	3317	1/1	0.89	0.27	52,52,52,52	0
53	MG	2V	3001	1/1	0.89	0.20	46,46,46,46	0
53	MG	1A	3490	1/1	0.89	0.22	48,48,48,48	0
53	MG	1a	3108	1/1	0.89	0.19	61,61,61,61	0
53	MG	2A	3228	1/1	0.89	0.28	49,49,49,49	0
53	MG	1a	3141	1/1	0.89	0.16	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	3105	1/1	0.89	0.18	66,66,66,66	0
53	MG	1A	3011	1/1	0.89	0.27	49,49,49,49	0
53	MG	1A	3644	1/1	0.89	0.24	78,78,78,78	0
53	MG	2a	1629	1/1	0.89	0.18	61,61,61,61	0
53	MG	1A	3107	1/1	0.89	0.32	63,63,63,63	0
53	MG	1A	3100	1/1	0.89	1.08	36,36,36,36	0
53	MG	1a	3115	1/1	0.89	0.23	82,82,82,82	0
53	MG	1A	3768	1/1	0.89	1.00	45,45,45,45	0
53	MG	1A	3542	1/1	0.89	0.17	78,78,78,78	0
53	MG	1A	3661	1/1	0.89	0.17	21,21,21,21	0
53	MG	2A	3268	1/1	0.89	0.22	60,60,60,60	0
53	MG	1A	3050	1/1	0.89	0.23	78,78,78,78	0
53	MG	1A	3407	1/1	0.89	0.19	57,57,57,57	0
53	MG	1E	301	1/1	0.89	0.16	38,38,38,38	0
53	MG	2A	3457	1/1	0.89	0.07	78,78,78,78	0
53	MG	1A	3279	1/1	0.89	0.17	53,53,53,53	0
53	MG	1a	3127	1/1	0.89	0.12	73,73,73,73	0
53	MG	1a	3031	1/1	0.89	0.27	75,75,75,75	0
53	MG	2A	3041	1/1	0.89	0.12	65,65,65,65	0
53	MG	2a	1634	1/1	0.89	0.21	78,78,78,78	0
53	MG	1A	3617	1/1	0.89	0.11	93,93,93,93	0
53	MG	1a	3009	1/1	0.89	0.15	70,70,70,70	0
53	MG	2A	3274	1/1	0.89	0.28	71,71,71,71	0
53	MG	1a	3039	1/1	0.89	0.28	62,62,62,62	0
53	MG	1A	3591	1/1	0.89	0.28	61,61,61,61	0
53	MG	1A	3243	1/1	0.89	0.52	50,50,50,50	0
53	MG	1A	3595	1/1	0.89	0.24	68,68,68,68	0
53	MG	1A	3349	1/1	0.89	0.18	32,32,32,32	0
53	MG	2A	3494	1/1	0.89	0.13	66,66,66,66	0
53	MG	1A	3412	1/1	0.89	0.15	56,56,56,56	0
53	MG	2A	3452	1/1	0.89	0.27	67,67,67,67	0
53	MG	2A	3032	1/1	0.89	0.72	42,42,42,42	0
53	MG	1A	3707	1/1	0.89	1.00	38,38,38,38	0
53	MG	2N	8001	1/1	0.90	0.18	68,68,68,68	0
53	MG	1A	3552	1/1	0.90	0.21	72,72,72,72	0
53	MG	1A	3573	1/1	0.90	0.18	92,92,92,92	0
53	MG	1A	3723	1/1	0.90	0.17	62,62,62,62	0
53	MG	2A	3022	1/1	0.90	0.17	67,67,67,67	0
53	MG	2A	3008	1/1	0.90	0.59	60,60,60,60	0
53	MG	2P	201	1/1	0.90	0.15	49,49,49,49	0
53	MG	1A	3367	1/1	0.90	0.60	35,35,35,35	0
53	MG	1A	3713	1/1	0.90	0.59	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3074	1/1	0.90	0.31	64,64,64,64	0
53	MG	1A	3241	1/1	0.90	0.17	50,50,50,50	0
53	MG	2a	1662	1/1	0.90	0.17	74,74,74,74	0
53	MG	1A	3757	1/1	0.90	0.59	54,54,54,54	0
53	MG	1A	3287	1/1	0.90	0.23	49,49,49,49	0
53	MG	2A	3250	1/1	0.90	0.17	51,51,51,51	0
53	MG	2A	3075	1/1	0.90	0.15	73,73,73,73	0
53	MG	2A	3256	1/1	0.90	0.24	58,58,58,58	0
53	MG	1a	3110	1/1	0.90	0.12	82,82,82,82	0
53	MG	1A	3101	1/1	0.90	0.15	73,73,73,73	0
53	MG	1A	3081	1/1	0.90	1.07	46,46,46,46	0
53	MG	2a	1609	1/1	0.90	0.36	60,60,60,60	0
53	MG	1A	3137	1/1	0.90	0.21	40,40,40,40	0
53	MG	1A	3527	1/1	0.90	0.23	56,56,56,56	0
53	MG	2A	3023	1/1	0.90	0.23	63,63,63,63	0
53	MG	1A	3652	1/1	0.90	0.17	59,59,59,59	0
53	MG	1a	3035	1/1	0.90	0.14	84,84,84,84	0
53	MG	2A	3380	1/1	0.90	0.10	52,52,52,52	0
53	MG	1A	3125	1/1	0.90	0.18	49,49,49,49	0
53	MG	1A	3706	1/1	0.90	0.15	71,71,71,71	0
53	MG	1A	3541	1/1	0.90	0.17	72,72,72,72	0
53	MG	1A	3150	1/1	0.90	0.19	38,38,38,38	0
53	MG	2A	3060	1/1	0.90	0.22	52,52,52,52	0
53	MG	1A	3508	1/1	0.90	0.26	77,77,77,77	0
53	MG	2a	1644	1/1	0.90	0.33	91,91,91,91	0
53	MG	1a	3123	1/1	0.90	0.14	81,81,81,81	0
53	MG	2A	3291	1/1	0.90	0.28	45,45,45,45	0
53	MG	2A	3037	1/1	0.90	0.32	67,67,67,67	0
53	MG	2A	3405	1/1	0.90	0.21	49,49,49,49	0
53	MG	2A	3436	1/1	0.90	0.14	61,61,61,61	0
53	MG	1A	3724	1/1	0.90	0.16	38,38,38,38	0
53	MG	1X	101	1/1	0.90	0.33	42,42,42,42	0
53	MG	2a	1722	1/1	0.90	0.13	78,78,78,78	0
53	MG	2A	3094	1/1	0.90	0.16	76,76,76,76	0
53	MG	2A	3506	1/1	0.90	0.20	62,62,62,62	0
53	MG	2A	3187	1/1	0.90	0.16	45,45,45,45	0
53	MG	1A	3122	1/1	0.90	0.22	61,61,61,61	0
53	MG	2T	202	1/1	0.90	0.18	58,58,58,58	0
53	MG	2A	3485	1/1	0.90	0.21	58,58,58,58	0
53	MG	1a	3062	1/1	0.90	0.13	69,69,69,69	0
53	MG	2h	201	1/1	0.90	0.72	65,65,65,65	0
53	MG	2a	1642	1/1	0.90	0.14	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	2A	3173	1/1	0.90	0.18	32,32,32,32	0
53	MG	2a	1700	1/1	0.90	0.11	80,80,80,80	0
53	MG	2A	3171	1/1	0.90	0.21	62,62,62,62	0
53	MG	2A	3053	1/1	0.90	0.21	64,64,64,64	0
53	MG	2A	3499	1/1	0.90	0.12	54,54,54,54	0
53	MG	1F	305	1/1	0.90	0.14	41,41,41,41	0
53	MG	2A	3438	1/1	0.90	0.13	47,47,47,47	0
53	MG	2A	3007	1/1	0.90	0.13	56,56,56,56	0
53	MG	1A	3031	1/1	0.90	0.47	56,56,56,56	0
53	MG	1A	3647	1/1	0.90	0.18	66,66,66,66	0
53	MG	1A	3414	1/1	0.90	0.16	57,57,57,57	0
53	MG	1A	3208	1/1	0.90	0.33	47,47,47,47	0
53	MG	2a	1611	1/1	0.90	0.14	97,97,97,97	0
53	MG	1T	202	1/1	0.90	0.32	83,83,83,83	0
53	MG	1E	306	1/1	0.90	0.12	46,46,46,46	0
53	MG	1a	3088	1/1	0.90	0.20	107,107,107,107	0
53	MG	2A	3107	1/1	0.90	0.16	62,62,62,62	0
53	MG	1A	3069	1/1	0.90	0.26	63,63,63,63	0
53	MG	1A	3394	1/1	0.90	0.42	61,61,61,61	0
53	MG	2A	3226	1/1	0.90	0.13	49,49,49,49	0
53	MG	1A	3632	1/1	0.90	0.16	68,68,68,68	0
53	MG	2A	3388	1/1	0.90	0.55	61,61,61,61	0
53	MG	1a	3103	1/1	0.90	0.18	81,81,81,81	0
53	MG	2A	3395	1/1	0.90	0.29	72,72,72,72	0
53	MG	1A	3253	1/1	0.90	0.33	65,65,65,65	0
53	MG	2a	1685	1/1	0.90	0.12	55,55,55,55	0
53	MG	1A	3352	1/1	0.90	0.22	68,68,68,68	0
53	MG	1a	3121	1/1	0.90	0.12	94,94,94,94	0
53	MG	1A	3093	1/1	0.90	0.95	67,67,67,67	0
53	MG	2a	1625	1/1	0.90	0.10	69,69,69,69	0
53	MG	1A	3001	1/1	0.90	0.11	41,41,41,41	0
53	MG	1A	3517	1/1	0.90	0.25	69,69,69,69	0
53	MG	1a	3111	1/1	0.90	0.25	78,78,78,78	0
53	MG	2a	1602	1/1	0.91	0.30	88,88,88,88	0
53	MG	1A	3090	1/1	0.91	0.39	64,64,64,64	0
53	MG	2A	3166	1/1	0.91	0.36	53,53,53,53	0
53	MG	1A	3461	1/1	0.91	0.48	86,86,86,86	0
53	MG	2A	3348	1/1	0.91	0.48	58,58,58,58	0
53	MG	1A	3492	1/1	0.91	0.16	80,80,80,80	0
53	MG	2A	3363	1/1	0.91	0.12	52,52,52,52	0
53	MG	1A	3278	1/1	0.91	0.24	51,51,51,51	0
53	MG	1A	3193	1/1	0.91	0.29	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1a	3129	1/1	0.91	0.06	61,61,61,61	0
53	MG	1A	3402	1/1	0.91	0.21	50,50,50,50	0
53	MG	1a	3057	1/1	0.91	0.34	88,88,88,88	0
53	MG	1A	3047	1/1	0.91	0.20	59,59,59,59	0
53	MG	2a	1626	1/1	0.91	0.21	72,72,72,72	0
53	MG	2B	210	1/1	0.91	0.27	55,55,55,55	0
53	MG	1A	3308	1/1	0.91	0.28	68,68,68,68	0
53	MG	2A	3286	1/1	0.91	0.27	56,56,56,56	0
53	MG	1A	3609	1/1	0.91	0.26	56,56,56,56	0
53	MG	1A	3063	1/1	0.91	0.30	36,36,36,36	0
53	MG	1A	3274	1/1	0.91	0.22	61,61,61,61	0
53	MG	1A	3280	1/1	0.91	0.44	55,55,55,55	0
53	MG	1A	3544	1/1	0.91	0.82	64,64,64,64	0
53	MG	1a	3054	1/1	0.91	0.21	76,76,76,76	0
53	MG	1A	3245	1/1	0.91	0.20	48,48,48,48	0
53	MG	2A	3333	1/1	0.91	0.17	30,30,30,30	0
53	MG	1A	3330	1/1	0.91	0.27	66,66,66,66	0
53	MG	1T	204	1/1	0.91	0.24	83,83,83,83	0
53	MG	2B	217	1/1	0.91	0.09	98,98,98,98	0
53	MG	1A	3258	1/1	0.91	0.23	40,40,40,40	0
53	MG	17	101	1/1	0.91	0.13	38,38,38,38	0
53	MG	1A	3628	1/1	0.91	0.18	58,58,58,58	0
53	MG	1A	3651	1/1	0.91	0.22	78,78,78,78	0
53	MG	2A	3501	1/1	0.91	0.07	56,56,56,56	0
53	MG	2A	3493	1/1	0.91	0.23	52,52,52,52	0
53	MG	2A	3492	1/1	0.91	0.32	83,83,83,83	0
53	MG	1A	3658	1/1	0.91	0.16	35,35,35,35	0
53	MG	2A	3238	1/1	0.91	0.23	57,57,57,57	0
53	MG	1t	201	1/1	0.91	0.61	77,77,77,77	0
53	MG	1a	3135	1/1	0.91	0.57	105,105,105,105	0
53	MG	2A	3360	1/1	0.91	0.17	72,72,72,72	0
53	MG	2A	3097	1/1	0.91	0.61	67,67,67,67	0
53	MG	2A	3235	1/1	0.91	0.28	53,53,53,53	0
53	MG	1A	3304	1/1	0.91	0.15	38,38,38,38	0
53	MG	2A	3006	1/1	0.91	0.23	51,51,51,51	0
53	MG	2A	3160	1/1	0.91	0.28	53,53,53,53	0
53	MG	2a	1717	1/1	0.91	0.25	94,94,94,94	0
53	MG	2A	3496	1/1	0.91	0.13	68,68,68,68	0
53	MG	1A	3141	1/1	0.91	0.44	62,62,62,62	0
53	MG	1A	3614	1/1	0.91	0.45	64,64,64,64	0
53	MG	1A	3391	1/1	0.91	0.16	42,42,42,42	0
53	MG	2a	1658	1/1	0.91	0.29	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3021	1/1	0.91	0.22	46,46,46,46	0
53	MG	1A	3195	1/1	0.91	0.27	54,54,54,54	0
53	MG	1A	3310	1/1	0.91	1.11	49,49,49,49	0
53	MG	1a	3048	1/1	0.91	0.23	66,66,66,66	0
53	MG	1A	3429	1/1	0.91	0.27	63,63,63,63	0
53	MG	1A	3518	1/1	0.91	0.12	37,37,37,37	0
53	MG	1A	3484	1/1	0.91	0.09	54,54,54,54	0
53	MG	1a	3075	1/1	0.91	0.14	43,43,43,43	0
53	MG	1A	3038	1/1	0.91	0.20	35,35,35,35	0
53	MG	1A	3476	1/1	0.91	0.18	39,39,39,39	0
53	MG	1A	3124	1/1	0.91	0.19	40,40,40,40	0
53	MG	2B	219	1/1	0.91	0.06	79,79,79,79	0
53	MG	2A	3108	1/1	0.91	0.22	54,54,54,54	0
53	MG	1A	3366	1/1	0.91	0.25	37,37,37,37	0
53	MG	1A	3650	1/1	0.91	0.23	42,42,42,42	0
53	MG	1a	3098	1/1	0.91	0.12	75,75,75,75	0
53	MG	1a	3029	1/1	0.91	0.29	72,72,72,72	0
53	MG	2A	3063	1/1	0.91	0.41	41,41,41,41	0
53	MG	1A	3629	1/1	0.91	0.23	59,59,59,59	0
53	MG	1A	3171	1/1	0.91	0.38	46,46,46,46	0
53	MG	2A	3489	1/1	0.91	0.19	55,55,55,55	0
53	MG	1A	3319	1/1	0.91	0.54	70,70,70,70	0
53	MG	1A	3275	1/1	0.91	0.67	38,38,38,38	0
53	MG	2a	1720	1/1	0.91	0.31	75,75,75,75	0
53	MG	1A	3549	1/1	0.91	0.79	63,63,63,63	0
53	MG	1A	3216	1/1	0.91	0.25	55,55,55,55	0
53	MG	2a	1690	1/1	0.91	0.36	82,82,82,82	0
53	MG	2a	1660	1/1	0.91	0.13	64,64,64,64	0
53	MG	2a	1724	1/1	0.91	0.33	91,91,91,91	0
53	MG	1A	3342	1/1	0.91	0.21	72,72,72,72	0
53	MG	2A	3098	1/1	0.91	0.25	54,54,54,54	0
53	MG	2A	3476	1/1	0.91	0.39	75,75,75,75	0
53	MG	1A	3252	1/1	0.91	0.29	60,60,60,60	0
53	MG	2a	1636	1/1	0.91	0.59	60,60,60,60	0
53	MG	1a	3120	1/1	0.91	0.11	92,92,92,92	0
53	MG	2E	303	1/1	0.91	0.23	57,57,57,57	0
53	MG	2A	3410	1/1	0.91	0.21	44,44,44,44	0
53	MG	1A	3066	1/1	0.91	0.27	54,54,54,54	0
53	MG	1A	3421	1/1	0.91	0.28	40,40,40,40	0
53	MG	1A	3198	1/1	0.91	0.27	38,38,38,38	0
53	MG	1A	3131	1/1	0.91	0.33	68,68,68,68	0
53	MG	2A	3211	1/1	0.91	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3111	1/1	0.91	0.74	66,66,66,66	0
53	MG	1A	3048	1/1	0.91	0.24	48,48,48,48	0
53	MG	1A	3408	1/1	0.91	0.21	51,51,51,51	0
53	MG	2A	3377	1/1	0.91	0.22	50,50,50,50	0
53	MG	1A	3387	1/1	0.91	0.25	46,46,46,46	0
53	MG	1a	3085	1/1	0.91	0.38	45,45,45,45	0
53	MG	1A	3029	1/1	0.91	0.27	52,52,52,52	0
53	MG	1A	3623	1/1	0.91	0.22	94,94,94,94	0
53	MG	1A	3343	1/1	0.92	0.17	53,53,53,53	0
53	MG	1A	3631	1/1	0.92	0.21	53,53,53,53	0
53	MG	2A	3128	1/1	0.92	0.61	59,59,59,59	0
53	MG	1A	3217	1/1	0.92	0.29	57,57,57,57	0
53	MG	1A	3762	1/1	0.92	0.13	47,47,47,47	0
53	MG	1A	3123	1/1	0.92	0.47	56,56,56,56	0
53	MG	1a	3130	1/1	0.92	0.41	63,63,63,63	0
53	MG	1A	3348	1/1	0.92	0.14	51,51,51,51	0
53	MG	1a	3002	1/1	0.92	0.21	96,96,96,96	0
53	MG	2A	3326	1/1	0.92	0.21	55,55,55,55	0
53	MG	2A	3244	1/1	0.92	0.14	48,48,48,48	0
53	MG	2A	3077	1/1	0.92	0.16	53,53,53,53	0
53	MG	1A	3344	1/1	0.92	0.22	60,60,60,60	0
53	MG	1A	3515	1/1	0.92	0.17	75,75,75,75	0
53	MG	2A	3070	1/1	0.92	0.28	57,57,57,57	0
53	MG	1A	3155	1/1	0.92	0.23	53,53,53,53	0
53	MG	1l	3002	1/1	0.92	0.19	51,51,51,51	0
53	MG	1A	3223	1/1	0.92	0.17	71,71,71,71	0
53	MG	1A	3043	1/1	0.92	0.50	54,54,54,54	0
53	MG	1d	503	1/1	0.92	0.08	99,99,99,99	0
53	MG	1A	3205	1/1	0.92	0.14	40,40,40,40	0
53	MG	1A	3415	1/1	0.92	0.16	31,31,31,31	0
53	MG	1A	3480	1/1	0.92	0.22	61,61,61,61	0
53	MG	1A	3499	1/1	0.92	0.18	63,63,63,63	0
53	MG	2E	304	1/1	0.92	0.23	36,36,36,36	0
53	MG	1A	3428	1/1	0.92	0.41	39,39,39,39	0
53	MG	15	104	1/1	0.92	0.18	63,63,63,63	0
53	MG	1A	3576	1/1	0.92	0.25	19,19,19,19	0
53	MG	2A	3470	1/1	0.92	0.06	71,71,71,71	0
53	MG	1U	202	1/1	0.92	0.31	49,49,49,49	0
53	MG	2A	3461	1/1	0.92	0.08	65,65,65,65	0
53	MG	1A	3616	1/1	0.92	0.37	87,87,87,87	0
53	MG	1a	3140	1/1	0.92	0.27	101,101,101,101	0
53	MG	1A	3704	1/1	0.92	0.12	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	3028	1/1	0.92	0.14	59,59,59,59	0
53	MG	1a	3063	1/1	0.92	0.12	73,73,73,73	0
53	MG	1A	3425	1/1	0.92	0.17	39,39,39,39	0
53	MG	1a	3046	1/1	0.92	0.14	65,65,65,65	0
53	MG	1A	3316	1/1	0.92	0.43	68,68,68,68	0
54	HGR	2A	3515	36/36	0.92	0.41	36,61,70,76	0
53	MG	2A	3318	1/1	0.92	0.31	63,63,63,63	0
53	MG	1A	3363	1/1	0.92	0.56	60,60,60,60	0
53	MG	2a	1679	1/1	0.92	0.13	74,74,74,74	0
53	MG	19	105	1/1	0.92	0.33	74,74,74,74	0
53	MG	1A	3526	1/1	0.92	0.15	89,89,89,89	0
53	MG	1A	3199	1/1	0.92	0.21	45,45,45,45	0
53	MG	1A	3181	1/1	0.92	0.27	65,65,65,65	0
53	MG	2A	3386	1/1	0.92	0.22	55,55,55,55	0
53	MG	1A	3393	1/1	0.92	0.18	35,35,35,35	0
53	MG	1A	3569	1/1	0.92	0.62	67,67,67,67	0
53	MG	1A	3377	1/1	0.92	0.21	60,60,60,60	0
53	MG	2A	3391	1/1	0.92	0.22	51,51,51,51	0
53	MG	1g	3001	1/1	0.92	0.17	78,78,78,78	0
53	MG	2A	3341	1/1	0.92	0.28	45,45,45,45	0
53	MG	1A	3463	1/1	0.92	0.21	48,48,48,48	0
53	MG	2A	3201	1/1	0.92	0.25	62,62,62,62	0
53	MG	2a	1701	1/1	0.92	0.25	93,93,93,93	0
53	MG	15	105	1/1	0.92	0.29	47,47,47,47	0
53	MG	1A	3005	1/1	0.92	0.25	51,51,51,51	0
53	MG	2D	303	1/1	0.92	0.11	60,60,60,60	0
53	MG	2A	3319	1/1	0.92	0.26	50,50,50,50	0
53	MG	2A	3111	1/1	0.92	0.20	63,63,63,63	0
53	MG	2A	3129	1/1	0.92	0.20	55,55,55,55	0
53	MG	1A	3562	1/1	0.92	0.52	70,70,70,70	0
53	MG	2A	3517	1/1	0.92	0.20	45,45,45,45	0
53	MG	2A	3409	1/1	0.92	0.15	53,53,53,53	0
53	MG	2A	3330	1/1	0.92	0.27	47,47,47,47	0
53	MG	2A	3055	1/1	0.92	0.15	59,59,59,59	0
53	MG	28	8001	1/1	0.92	0.48	64,64,64,64	0
53	MG	1W	3002	1/1	0.92	0.29	51,51,51,51	0
53	MG	2A	3206	1/1	0.92	0.22	48,48,48,48	0
53	MG	1A	3080	1/1	0.92	0.21	67,67,67,67	0
53	MG	1A	3760	1/1	0.92	0.55	47,47,47,47	0
53	MG	1A	3730	1/1	0.92	0.16	52,52,52,52	0
53	MG	1A	3351	1/1	0.92	0.19	40,40,40,40	0
53	MG	2A	3514	1/1	0.92	0.27	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3508	1/1	0.92	0.43	65,65,65,65	0
53	MG	1A	3557	1/1	0.92	0.25	55,55,55,55	0
53	MG	2A	3454	1/1	0.92	0.12	61,61,61,61	0
53	MG	1D	303	1/1	0.92	0.21	25,25,25,25	0
53	MG	2a	1651	1/1	0.92	0.21	76,76,76,76	0
53	MG	1a	3003	1/1	0.92	0.15	77,77,77,77	0
53	MG	1A	3249	1/1	0.92	0.20	54,54,54,54	0
53	MG	1A	3312	1/1	0.92	1.20	44,44,44,44	0
53	MG	2A	3247	1/1	0.92	0.16	58,58,58,58	0
53	MG	2A	3036	1/1	0.92	0.40	55,55,55,55	0
53	MG	2A	3142	1/1	0.92	0.31	49,49,49,49	0
53	MG	1A	3083	1/1	0.92	0.67	61,61,61,61	0
53	MG	1A	3318	1/1	0.92	0.73	51,51,51,51	0
53	MG	2A	3392	1/1	0.92	0.31	51,51,51,51	0
53	MG	2A	3170	1/1	0.92	0.17	61,61,61,61	0
53	MG	1A	3410	1/1	0.92	0.20	43,43,43,43	0
53	MG	1A	3166	1/1	0.92	0.19	42,42,42,42	0
53	MG	2A	3034	1/1	0.92	0.13	60,60,60,60	0
53	MG	1A	3076	1/1	0.92	0.35	60,60,60,60	0
53	MG	1A	3087	1/1	0.92	0.79	61,61,61,61	0
53	MG	1A	3003	1/1	0.92	0.25	59,59,59,59	0
53	MG	2a	1697	1/1	0.92	0.11	48,48,48,48	0
53	MG	2A	3266	1/1	0.92	0.18	55,55,55,55	0
53	MG	1A	3126	1/1	0.92	0.29	55,55,55,55	0
53	MG	1A	3153	1/1	0.92	0.35	52,52,52,52	0
53	MG	1A	3188	1/1	0.92	0.33	39,39,39,39	0
53	MG	1A	3389	1/1	0.92	0.17	47,47,47,47	0
53	MG	1a	3044	1/1	0.93	0.17	61,61,61,61	0
53	MG	1A	3513	1/1	0.93	0.18	56,56,56,56	0
53	MG	1A	3110	1/1	0.93	0.80	51,51,51,51	0
53	MG	1A	3605	1/1	0.93	0.20	63,63,63,63	0
53	MG	1A	3514	1/1	0.93	0.40	83,83,83,83	0
53	MG	2A	3516	1/1	0.93	0.09	34,34,34,34	0
53	MG	2T	201	1/1	0.93	0.22	56,56,56,56	0
53	MG	1A	3382	1/1	0.93	0.18	56,56,56,56	0
53	MG	2A	3511	1/1	0.93	0.16	39,39,39,39	0
53	MG	1A	3295	1/1	0.93	0.30	57,57,57,57	0
53	MG	2A	3471	1/1	0.93	0.15	52,52,52,52	0
53	MG	1A	3635	1/1	0.93	0.12	56,56,56,56	0
53	MG	2A	3035	1/1	0.93	0.21	65,65,65,65	0
53	MG	1A	3404	1/1	0.93	0.16	63,63,63,63	0
53	MG	1A	3649	1/1	0.93	0.24	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1a	3087	1/1	0.93	0.11	87,87,87,87	0
53	MG	1A	3042	1/1	0.93	0.15	53,53,53,53	0
53	MG	1A	3403	1/1	0.93	0.11	68,68,68,68	0
53	MG	1A	3135	1/1	0.93	0.45	49,49,49,49	0
53	MG	2A	3044	1/1	0.93	0.09	57,57,57,57	0
53	MG	1a	3033	1/1	0.93	0.18	83,83,83,83	0
53	MG	2A	3039	1/1	0.93	0.21	51,51,51,51	0
53	MG	2A	3219	1/1	0.93	0.19	54,54,54,54	0
53	MG	1A	3085	1/1	0.93	0.21	58,58,58,58	0
53	MG	1A	3753	1/1	0.93	0.12	59,59,59,59	0
53	MG	2A	3058	1/1	0.93	0.19	52,52,52,52	0
53	MG	2A	3346	1/1	0.93	0.31	68,68,68,68	0
53	MG	2A	3357	1/1	0.93	0.49	73,73,73,73	0
53	MG	2A	3114	1/1	0.93	0.17	78,78,78,78	0
53	MG	2A	3353	1/1	0.93	0.18	64,64,64,64	0
53	MG	1A	3183	1/1	0.93	0.30	29,29,29,29	0
53	MG	1A	3233	1/1	0.93	0.16	58,58,58,58	0
53	MG	2A	3175	1/1	0.93	0.26	48,48,48,48	0
53	MG	2A	3443	1/1	0.93	0.08	88,88,88,88	0
53	MG	1A	3108	1/1	0.93	0.19	45,45,45,45	0
53	MG	1A	3254	1/1	0.93	0.27	48,48,48,48	0
53	MG	1E	303	1/1	0.93	0.35	45,45,45,45	0
53	MG	1a	3090	1/1	0.93	0.19	88,88,88,88	0
53	MG	1a	3023	1/1	0.93	0.36	51,51,51,51	0
53	MG	2A	3199	1/1	0.93	0.26	26,26,26,26	0
53	MG	1A	3533	1/1	0.93	0.22	90,90,90,90	0
53	MG	1A	3276	1/1	0.93	0.31	43,43,43,43	0
53	MG	1A	3590	1/1	0.93	0.32	54,54,54,54	0
53	MG	1A	3418	1/1	0.93	0.14	65,65,65,65	0
53	MG	2A	3136	1/1	0.93	0.26	62,62,62,62	0
53	MG	1A	3309	1/1	0.93	0.34	46,46,46,46	0
53	MG	2A	3082	1/1	0.93	0.78	69,69,69,69	0
53	MG	2A	3455	1/1	0.93	0.04	66,66,66,66	0
53	MG	1a	3020	1/1	0.93	0.08	86,86,86,86	0
53	MG	2A	3177	1/1	0.93	0.17	54,54,54,54	0
53	MG	2a	1677	1/1	0.93	0.08	82,82,82,82	0
53	MG	1A	3023	1/1	0.93	0.22	60,60,60,60	0
53	MG	1A	3399	1/1	0.93	0.15	64,64,64,64	0
53	MG	1A	3077	1/1	0.93	0.41	51,51,51,51	0
53	MG	1A	3075	1/1	0.93	1.22	57,57,57,57	0
53	MG	1A	3648	1/1	0.93	1.31	73,73,73,73	0
53	MG	1A	3019	1/1	0.93	0.14	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	2A	3140	1/1	0.93	0.23	68,68,68,68	0
53	MG	1a	3089	1/1	0.93	0.15	72,72,72,72	0
53	MG	2A	3144	1/1	0.93	0.81	49,49,49,49	0
53	MG	2A	3042	1/1	0.93	0.18	62,62,62,62	0
53	MG	2A	3383	1/1	0.93	0.18	79,79,79,79	0
53	MG	1A	3039	1/1	0.93	0.20	67,67,67,67	0
53	MG	1A	3680	1/1	0.93	0.20	41,41,41,41	0
53	MG	1A	3409	1/1	0.93	0.17	30,30,30,30	0
53	MG	1A	3385	1/1	0.93	0.16	58,58,58,58	0
53	MG	2a	1674	1/1	0.93	0.08	68,68,68,68	0
53	MG	2A	3137	1/1	0.93	0.20	56,56,56,56	0
53	MG	2A	3479	1/1	0.93	0.12	56,56,56,56	0
53	MG	2A	3447	1/1	0.93	0.09	72,72,72,72	0
53	MG	2a	1659	1/1	0.93	0.21	101,101,101,101	0
53	MG	10	103	1/1	0.93	0.20	39,39,39,39	0
53	MG	2A	3394	1/1	0.93	0.16	54,54,54,54	0
53	MG	1A	3091	1/1	0.93	0.16	76,76,76,76	0
53	MG	2A	3249	1/1	0.93	0.14	64,64,64,64	0
53	MG	1A	3152	1/1	0.93	0.17	30,30,30,30	0
53	MG	2A	3234	1/1	0.93	0.25	73,73,73,73	0
53	MG	1A	3401	1/1	0.93	0.70	71,71,71,71	0
53	MG	1f	8001	1/1	0.93	0.17	86,86,86,86	0
53	MG	2A	3262	1/1	0.93	0.28	30,30,30,30	0
53	MG	2A	3227	1/1	0.93	0.51	71,71,71,71	0
53	MG	2A	3417	1/1	0.93	0.19	60,60,60,60	0
53	MG	1F	302	1/1	0.93	0.48	43,43,43,43	0
53	MG	1A	3149	1/1	0.93	0.19	31,31,31,31	0
53	MG	1A	3028	1/1	0.93	0.27	61,61,61,61	0
53	MG	2A	3373	1/1	0.93	0.19	38,38,38,38	0
53	MG	1A	3655	1/1	0.93	0.32	77,77,77,77	0
53	MG	1A	3688	1/1	0.93	0.13	76,76,76,76	0
53	MG	1A	3625	1/1	0.93	0.69	49,49,49,49	0
53	MG	2a	1686	1/1	0.93	0.54	88,88,88,88	0
53	MG	2A	3462	1/1	0.93	0.11	73,73,73,73	0
53	MG	2A	3298	1/1	0.93	0.11	47,47,47,47	0
53	MG	1A	3362	1/1	0.93	0.21	63,63,63,63	0
53	MG	1A	3568	1/1	0.93	0.62	51,51,51,51	0
53	MG	2A	3162	1/1	0.93	0.20	52,52,52,52	0
53	MG	10	102	1/1	0.93	0.57	37,37,37,37	0
53	MG	1A	3302	1/1	0.93	0.21	63,63,63,63	0
53	MG	1A	3748	1/1	0.93	0.16	62,62,62,62	0
53	MG	1A	3321	1/1	0.93	0.19	54,54,54,54	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	0.93	0.25	50,50,50,50	0
53	MG	1A	3743	1/1	0.93	0.19	65,65,65,65	0
53	MG	2a	1645	1/1	0.93	0.32	64,64,64,64	0
53	MG	2A	3180	1/1	0.93	0.44	59,59,59,59	0
53	MG	2A	3337	1/1	0.93	0.67	53,53,53,53	0
53	MG	2a	1613	1/1	0.93	0.17	83,83,83,83	0
53	MG	2A	3282	1/1	0.93	0.25	59,59,59,59	0
53	MG	2a	1714	1/1	0.93	0.14	101,101,101,101	0
53	MG	2A	3482	1/1	0.93	0.41	72,72,72,72	0
53	MG	1k	3001	1/1	0.93	0.15	66,66,66,66	0
53	MG	2A	3460	1/1	0.93	0.12	69,69,69,69	0
53	MG	2A	3119	1/1	0.93	0.51	72,72,72,72	0
53	MG	1A	3197	1/1	0.93	0.23	74,74,74,74	0
53	MG	1A	3478	1/1	0.93	0.26	56,56,56,56	0
53	MG	1A	3574	1/1	0.93	0.23	82,82,82,82	0
53	MG	1A	3642	1/1	0.93	0.20	88,88,88,88	0
53	MG	1A	3138	1/1	0.93	0.36	56,56,56,56	0
53	MG	2a	1702	1/1	0.94	0.18	62,62,62,62	0
53	MG	1A	3375	1/1	0.94	0.23	69,69,69,69	0
53	MG	1a	3081	1/1	0.94	0.25	63,63,63,63	0
53	MG	1A	3624	1/1	0.94	0.18	19,19,19,19	0
53	MG	1A	3214	1/1	0.94	0.47	41,41,41,41	0
53	MG	2A	3017	1/1	0.94	0.17	58,58,58,58	0
53	MG	1A	3056	1/1	0.94	0.18	40,40,40,40	0
53	MG	1Q	201	1/1	0.94	0.24	50,50,50,50	0
53	MG	1a	3012	1/1	0.94	0.13	75,75,75,75	0
53	MG	1A	3721	1/1	0.94	0.14	69,69,69,69	0
53	MG	1a	3137	1/1	0.94	0.30	86,86,86,86	0
53	MG	1A	3176	1/1	0.94	0.14	24,24,24,24	0
53	MG	1A	3686	1/1	0.94	0.12	59,59,59,59	0
53	MG	1A	3769	1/1	0.94	0.16	35,35,35,35	0
53	MG	1A	3678	1/1	0.94	0.14	33,33,33,33	0
53	MG	1A	3327	1/1	0.94	0.96	62,62,62,62	0
53	MG	1B	3021	1/1	0.94	0.21	64,64,64,64	0
53	MG	2A	3352	1/1	0.94	0.20	49,49,49,49	0
53	MG	1A	3160	1/1	0.94	0.34	51,51,51,51	0
53	MG	2A	3375	1/1	0.94	0.10	51,51,51,51	0
55	ZN	2Y	501	1/1	0.94	0.22	92,92,92,92	0
53	MG	2A	3442	1/1	0.94	0.14	37,37,37,37	0
53	MG	2A	3450	1/1	0.94	0.36	84,84,84,84	0
53	MG	1B	3017	1/1	0.94	0.16	54,54,54,54	0
53	MG	2A	3167	1/1	0.94	0.31	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	1A	3524	1/1	0.94	0.11	91,91,91,91	0
53	MG	1A	3179	1/1	0.94	0.51	37,37,37,37	0
53	MG	1A	3733	1/1	0.94	0.18	42,42,42,42	0
53	MG	2B	201	1/1	0.94	0.16	75,75,75,75	0
53	MG	2A	3031	1/1	0.94	0.13	60,60,60,60	0
53	MG	2A	3220	1/1	0.94	0.31	37,37,37,37	0
53	MG	1A	3588	1/1	0.94	0.08	61,61,61,61	0
53	MG	2A	3396	1/1	0.94	0.31	68,68,68,68	0
53	MG	1A	3032	1/1	0.94	0.17	30,30,30,30	0
53	MG	2B	218	1/1	0.94	0.17	62,62,62,62	0
53	MG	1A	3587	1/1	0.94	0.38	51,51,51,51	0
53	MG	1A	3174	1/1	0.94	0.53	44,44,44,44	0
53	MG	10	104	1/1	0.94	0.29	57,57,57,57	0
53	MG	1A	3537	1/1	0.94	0.27	59,59,59,59	0
53	MG	2a	1689	1/1	0.94	1.23	88,88,88,88	0
53	MG	1A	3015	1/1	0.94	0.20	48,48,48,48	0
53	MG	1A	3424	1/1	0.94	0.18	48,48,48,48	0
53	MG	1A	3272	1/1	0.94	0.22	53,53,53,53	0
53	MG	2a	1655	1/1	0.94	0.23	78,78,78,78	0
53	MG	2A	3106	1/1	0.94	0.15	54,54,54,54	0
53	MG	2A	3165	1/1	0.94	0.21	54,54,54,54	0
53	MG	1A	3729	1/1	0.94	0.12	57,57,57,57	0
53	MG	28	8002	1/1	0.94	0.15	51,51,51,51	0
53	MG	2A	3340	1/1	0.94	0.43	53,53,53,53	0
53	MG	1A	3092	1/1	0.94	0.43	74,74,74,74	0
53	MG	2A	3004	1/1	0.94	0.16	53,53,53,53	0
53	MG	2A	3329	1/1	0.94	0.30	58,58,58,58	0
53	MG	1A	3285	1/1	0.94	0.28	46,46,46,46	0
53	MG	2A	3014	1/1	0.94	0.22	53,53,53,53	0
53	MG	2A	3510	1/1	0.94	0.17	38,38,38,38	0
53	MG	2A	3260	1/1	0.94	0.22	41,41,41,41	0
53	MG	2A	3264	1/1	0.94	0.29	30,30,30,30	0
53	MG	1A	3040	1/1	0.94	0.21	57,57,57,57	0
53	MG	1A	3395	1/1	0.94	0.20	54,54,54,54	0
53	MG	1A	3147	1/1	0.94	0.24	32,32,32,32	0
53	MG	2A	3415	1/1	0.94	0.08	61,61,61,61	0
53	MG	1A	3685	1/1	0.94	0.12	56,56,56,56	0
53	MG	1a	3128	1/1	0.94	0.39	93,93,93,93	0
53	MG	1A	3120	1/1	0.94	0.25	53,53,53,53	0
53	MG	1A	3025	1/1	0.94	0.16	57,57,57,57	0
53	MG	1A	3041	1/1	0.94	0.90	59,59,59,59	0
53	MG	1A	3767	1/1	0.94	1.71	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3285	1/1	0.94	0.13	46,46,46,46	0
53	MG	1A	3072	1/1	0.94	0.37	58,58,58,58	0
53	MG	2D	302	1/1	0.94	0.33	49,49,49,49	0
53	MG	2A	3459	1/1	0.94	0.14	53,53,53,53	0
53	MG	2Q	3001	1/1	0.94	0.11	66,66,66,66	0
53	MG	1Q	203	1/1	0.94	0.19	53,53,53,53	0
53	MG	2A	3011	1/1	0.94	0.23	52,52,52,52	0
54	HGR	1A	3749	36/36	0.94	0.33	24,38,52,65	0
53	MG	1a	3001	1/1	0.94	0.21	60,60,60,60	0
53	MG	1A	3071	1/1	0.94	1.09	37,37,37,37	0
53	MG	2A	3445	1/1	0.94	0.15	46,46,46,46	0
53	MG	1T	203	1/1	0.94	0.14	58,58,58,58	0
53	MG	2A	3507	1/1	0.94	0.53	93,93,93,93	0
53	MG	1A	3116	1/1	0.94	0.18	48,48,48,48	0
53	MG	2A	3225	1/1	0.94	0.21	57,57,57,57	0
53	MG	1A	3545	1/1	0.94	0.10	89,89,89,89	0
53	MG	2a	1663	1/1	0.94	0.18	62,62,62,62	0
53	MG	1A	3506	1/1	0.94	0.20	50,50,50,50	0
53	MG	1F	303	1/1	0.94	0.16	40,40,40,40	0
53	MG	2B	216	1/1	0.94	0.16	81,81,81,81	0
53	MG	2A	3043	1/1	0.94	0.14	43,43,43,43	0
53	MG	2A	3412	1/1	0.94	0.09	58,58,58,58	0
53	MG	2a	1628	1/1	0.94	0.24	55,55,55,55	0
53	MG	1A	3593	1/1	0.94	0.18	34,34,34,34	0
53	MG	2A	3402	1/1	0.94	0.12	53,53,53,53	0
53	MG	2a	1710	1/1	0.94	0.13	76,76,76,76	0
53	MG	2A	3214	1/1	0.94	0.34	35,35,35,35	0
53	MG	1A	3354	1/1	0.94	0.42	63,63,63,63	0
53	MG	2A	3172	1/1	0.94	0.61	52,52,52,52	0
53	MG	2A	3230	1/1	0.94	0.12	46,46,46,46	0
53	MG	2A	3290	1/1	0.94	0.29	49,49,49,49	0
53	MG	1A	3456	1/1	0.94	0.14	43,43,43,43	0
53	MG	1A	3589	1/1	0.94	0.10	91,91,91,91	0
53	MG	2a	1654	1/1	0.94	0.09	67,67,67,67	0
53	MG	2A	3156	1/1	0.94	0.15	50,50,50,50	0
53	MG	1a	3126	1/1	0.94	0.11	104,104,104,104	0
53	MG	2A	3258	1/1	0.94	0.17	53,53,53,53	0
53	MG	1A	3641	1/1	0.94	0.21	78,78,78,78	0
53	MG	1D	305	1/1	0.94	0.15	52,52,52,52	0
53	MG	2A	3304	1/1	0.94	0.16	57,57,57,57	0
53	MG	2A	3416	1/1	0.94	0.24	45,45,45,45	0
53	MG	2A	3207	1/1	0.94	0.22	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3119	1/1	0.94	0.30	31,31,31,31	0
53	MG	1A	3369	1/1	0.94	0.21	47,47,47,47	0
53	MG	1A	3320	1/1	0.94	0.12	46,46,46,46	0
53	MG	2A	3467	1/1	0.94	0.07	60,60,60,60	0
53	MG	1A	3270	1/1	0.94	0.54	62,62,62,62	0
53	MG	1A	3219	1/1	0.94	0.26	60,60,60,60	0
53	MG	1A	3340	1/1	0.94	0.24	50,50,50,50	0
53	MG	2A	3062	1/1	0.94	0.28	58,58,58,58	0
53	MG	1A	3218	1/1	0.94	0.33	57,57,57,57	0
53	MG	1A	3627	1/1	0.94	0.11	52,52,52,52	0
53	MG	1a	3091	1/1	0.94	0.21	62,62,62,62	0
53	MG	2A	3441	1/1	0.94	0.12	57,57,57,57	0
53	MG	1A	3529	1/1	0.94	0.52	55,55,55,55	0
53	MG	1A	3559	1/1	0.94	0.17	58,58,58,58	0
53	MG	2A	3411	1/1	0.94	0.09	44,44,44,44	0
53	MG	1A	3511	1/1	0.94	0.11	67,67,67,67	0
53	MG	2A	3066	1/1	0.94	0.15	51,51,51,51	0
53	MG	1a	3010	1/1	0.94	0.12	83,83,83,83	0
53	MG	1A	3144	1/1	0.94	0.37	48,48,48,48	0
53	MG	1A	3089	1/1	0.94	0.23	61,61,61,61	0
53	MG	2A	3047	1/1	0.94	0.11	59,59,59,59	0
53	MG	1A	3151	1/1	0.94	0.25	62,62,62,62	0
53	MG	1A	3692	1/1	0.94	0.20	36,36,36,36	0
53	MG	2A	3272	1/1	0.94	0.19	41,41,41,41	0
53	MG	1A	3558	1/1	0.94	0.18	53,53,53,53	0
53	MG	2A	3068	1/1	0.94	0.15	59,59,59,59	0
53	MG	2B	215	1/1	0.94	0.12	69,69,69,69	0
53	MG	1A	3406	1/1	0.94	0.12	50,50,50,50	0
53	MG	1A	3531	1/1	0.94	0.51	78,78,78,78	0
53	MG	1A	3021	1/1	0.94	0.26	27,27,27,27	0
53	MG	2A	3343	1/1	0.94	0.38	50,50,50,50	0
53	MG	1A	3504	1/1	0.94	0.32	53,53,53,53	0
53	MG	1A	3044	1/1	0.94	0.15	55,55,55,55	0
53	MG	2A	3091	1/1	0.94	0.51	68,68,68,68	0
53	MG	2A	3325	1/1	0.94	0.28	53,53,53,53	0
53	MG	1F	306	1/1	0.94	0.53	48,48,48,48	0
53	MG	2A	3288	1/1	0.94	0.11	32,32,32,32	0
53	MG	1A	3226	1/1	0.94	0.14	40,40,40,40	0
53	MG	1A	3207	1/1	0.94	0.29	49,49,49,49	0
53	MG	1A	3584	1/1	0.94	0.43	61,61,61,61	0
53	MG	1A	3577	1/1	0.94	0.13	42,42,42,42	0
53	MG	1a	3034	1/1	0.94	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	3176	1/1	0.94	0.20	32,32,32,32	0
53	MG	2A	3440	1/1	0.94	0.14	43,43,43,43	0
53	MG	1R	204	1/1	0.94	0.16	25,25,25,25	0
53	MG	1a	3064	1/1	0.94	0.15	75,75,75,75	0
53	MG	2A	3193	1/1	0.95	0.15	27,27,27,27	0
53	MG	1A	3293	1/1	0.95	0.30	43,43,43,43	0
53	MG	1A	3494	1/1	0.95	0.22	63,63,63,63	0
53	MG	2A	3085	1/1	0.95	0.98	70,70,70,70	0
53	MG	2a	1601	1/1	0.95	0.29	71,71,71,71	0
53	MG	2A	3306	1/1	0.95	0.24	68,68,68,68	0
53	MG	1a	3118	1/1	0.95	0.29	92,92,92,92	0
53	MG	2a	1698	1/1	0.95	0.15	79,79,79,79	0
53	MG	1A	3530	1/1	0.95	0.13	37,37,37,37	0
53	MG	1a	3038	1/1	0.95	0.29	52,52,52,52	0
53	MG	2A	3356	1/1	0.95	0.21	56,56,56,56	0
53	MG	2W	3001	1/1	0.95	0.21	58,58,58,58	0
53	MG	1A	3333	1/1	0.95	0.21	39,39,39,39	0
53	MG	1A	3248	1/1	0.95	0.27	55,55,55,55	0
53	MG	1a	3071	1/1	0.95	0.09	68,68,68,68	0
53	MG	1A	3561	1/1	0.95	0.88	70,70,70,70	0
53	MG	1A	3336	1/1	0.95	0.37	34,34,34,34	0
53	MG	2A	3469	1/1	0.95	0.13	56,56,56,56	0
53	MG	2a	1681	1/1	0.95	0.23	64,64,64,64	0
53	MG	2A	3024	1/1	0.95	0.33	57,57,57,57	0
53	MG	1A	3521	1/1	0.95	0.16	64,64,64,64	0
53	MG	2a	1630	1/1	0.95	0.37	66,66,66,66	0
53	MG	1A	3600	1/1	0.95	0.65	46,46,46,46	0
53	MG	18	101	1/1	0.95	0.24	51,51,51,51	0
53	MG	1A	3582	1/1	0.95	0.13	61,61,61,61	0
53	MG	2A	3076	1/1	0.95	0.32	59,59,59,59	0
53	MG	1A	3209	1/1	0.95	0.11	35,35,35,35	0
53	MG	15	101	1/1	0.95	0.28	64,64,64,64	0
53	MG	1a	3024	1/1	0.95	0.64	68,68,68,68	0
53	MG	2A	3477	1/1	0.95	0.39	64,64,64,64	0
53	MG	1A	3754	1/1	0.95	0.44	28,28,28,28	0
53	MG	1A	3311	1/1	0.95	0.26	53,53,53,53	0
53	MG	19	101	1/1	0.95	0.20	40,40,40,40	0
53	MG	1A	3370	1/1	0.95	0.45	57,57,57,57	0
53	MG	1A	3373	1/1	0.95	0.24	63,63,63,63	0
53	MG	1A	3371	1/1	0.95	0.14	43,43,43,43	0
53	MG	2A	3362	1/1	0.95	0.35	51,51,51,51	0
53	MG	1A	3339	1/1	0.95	0.28	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	2A	3495	1/1	0.95	0.07	64,64,64,64	0
53	MG	1A	3714	1/1	0.95	0.26	74,74,74,74	0
53	MG	2A	3181	1/1	0.95	0.13	58,58,58,58	0
53	MG	10	106	1/1	0.95	0.35	78,78,78,78	0
53	MG	2A	3336	1/1	0.95	0.26	66,66,66,66	0
53	MG	2A	3028	1/1	0.95	0.13	57,57,57,57	0
53	MG	1a	3073	1/1	0.95	0.10	72,72,72,72	0
53	MG	2a	1668	1/1	0.95	0.18	76,76,76,76	0
53	MG	1A	3196	1/1	0.95	0.18	31,31,31,31	0
53	MG	1A	3260	1/1	0.95	0.30	29,29,29,29	0
53	MG	2A	3518	1/1	0.95	0.32	47,47,47,47	0
53	MG	1D	304	1/1	0.95	0.19	66,66,66,66	0
53	MG	2A	3347	1/1	0.95	0.15	56,56,56,56	0
53	MG	1T	201	1/1	0.95	0.16	68,68,68,68	0
53	MG	1A	3380	1/1	0.95	0.18	47,47,47,47	0
53	MG	1A	3434	1/1	0.95	0.18	24,24,24,24	0
53	MG	1a	3124	1/1	0.95	0.18	100,100,100,100	0
53	MG	2A	3169	1/1	0.95	0.29	48,48,48,48	0
53	MG	1A	3612	1/1	0.95	0.24	51,51,51,51	0
53	MG	2A	3339	1/1	0.95	0.24	40,40,40,40	0
53	MG	1A	3471	1/1	0.95	0.14	54,54,54,54	0
53	MG	1A	3242	1/1	0.95	0.33	35,35,35,35	0
53	MG	2A	3265	1/1	0.95	0.12	60,60,60,60	0
53	MG	2A	3300	1/1	0.95	0.21	41,41,41,41	0
53	MG	2a	1680	1/1	0.95	0.34	56,56,56,56	0
53	MG	1A	3689	1/1	0.95	0.11	75,75,75,75	0
53	MG	2A	3095	1/1	0.95	0.99	71,71,71,71	0
53	MG	2e	3001	1/1	0.95	0.44	74,74,74,74	0
53	MG	2a	1656	1/1	0.95	0.30	52,52,52,52	0
53	MG	2A	3374	1/1	0.95	0.11	48,48,48,48	0
53	MG	1A	3067	1/1	0.95	0.29	66,66,66,66	0
53	MG	1a	3106	1/1	0.95	0.13	74,74,74,74	0
53	MG	1A	3020	1/1	0.95	0.17	35,35,35,35	0
53	MG	1A	3498	1/1	0.95	0.50	65,65,65,65	0
53	MG	2A	3135	1/1	0.95	1.16	65,65,65,65	0
53	MG	1A	3535	1/1	0.95	0.29	68,68,68,68	0
53	MG	2A	3299	1/1	0.95	0.28	56,56,56,56	0
53	MG	13	101	1/1	0.95	0.18	50,50,50,50	0
53	MG	2A	3294	1/1	0.95	0.11	53,53,53,53	0
53	MG	1a	3133	1/1	0.95	0.17	81,81,81,81	0
53	MG	1A	3700	1/1	0.95	0.16	39,39,39,39	0
53	MG	2A	3126	1/1	0.95	0.46	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	3190	1/1	0.95	0.23	31,31,31,31	0
53	MG	1B	3023	1/1	0.95	0.09	68,68,68,68	0
53	MG	1a	3017	1/1	0.95	0.14	71,71,71,71	0
53	MG	2A	3487	1/1	0.95	0.13	59,59,59,59	0
53	MG	2A	3431	1/1	0.95	0.20	63,63,63,63	0
53	MG	1A	3082	1/1	0.95	0.89	42,42,42,42	0
53	MG	2A	3118	1/1	0.95	0.12	78,78,78,78	0
53	MG	1A	3146	1/1	0.95	0.54	47,47,47,47	0
53	MG	2A	3429	1/1	0.95	0.12	71,71,71,71	0
53	MG	1A	3426	1/1	0.95	0.27	56,56,56,56	0
53	MG	1A	3477	1/1	0.95	0.19	49,49,49,49	0
53	MG	1A	3554	1/1	0.95	0.23	66,66,66,66	0
53	MG	1a	3005	1/1	0.95	0.19	53,53,53,53	0
53	MG	1A	3502	1/1	0.95	0.18	52,52,52,52	0
53	MG	1A	3602	1/1	0.95	0.27	50,50,50,50	0
53	MG	2A	3065	1/1	0.95	0.27	37,37,37,37	0
53	MG	1A	3687	1/1	0.95	0.27	74,74,74,74	0
53	MG	1A	3267	1/1	0.95	0.38	42,42,42,42	0
53	MG	1A	3483	1/1	0.95	0.16	32,32,32,32	0
53	MG	2A	3086	1/1	0.95	0.89	70,70,70,70	0
53	MG	1A	3419	1/1	0.95	0.21	40,40,40,40	0
53	MG	10	105	1/1	0.95	0.14	62,62,62,62	0
53	MG	1A	3326	1/1	0.95	0.22	44,44,44,44	0
53	MG	2A	3419	1/1	0.95	0.15	36,36,36,36	0
53	MG	2A	3154	1/1	0.95	0.19	36,36,36,36	0
53	MG	2A	3018	1/1	0.95	0.23	74,74,74,74	0
53	MG	2A	3418	1/1	0.95	0.10	63,63,63,63	0
53	MG	1A	3018	1/1	0.95	0.23	64,64,64,64	0
53	MG	2A	3424	1/1	0.95	0.18	63,63,63,63	0
53	MG	1A	3672	1/1	0.95	0.08	33,33,33,33	0
53	MG	2A	3124	1/1	0.95	0.15	44,44,44,44	0
53	MG	1A	3519	1/1	0.95	0.22	75,75,75,75	0
53	MG	2A	3186	1/1	0.95	0.24	31,31,31,31	0
53	MG	2a	1618	1/1	0.95	0.21	63,63,63,63	0
53	MG	2A	3195	1/1	0.95	0.16	57,57,57,57	0
53	MG	1B	3009	1/1	0.95	0.17	41,41,41,41	0
53	MG	1A	3487	1/1	0.95	0.24	45,45,45,45	0
53	MG	2A	3505	1/1	0.95	0.17	77,77,77,77	0
53	MG	1a	3013	1/1	0.95	0.10	54,54,54,54	0
53	MG	1A	3566	1/1	0.95	0.20	58,58,58,58	0
53	MG	1A	3247	1/1	0.95	0.15	32,32,32,32	0
53	MG	2A	3399	1/1	0.95	0.15	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	2A	3361	1/1	0.95	0.43	64,64,64,64	0
53	MG	1A	3134	1/1	0.95	0.15	63,63,63,63	0
55	ZN	1n	101	1/1	0.95	0.04	159,159,159,159	0
53	MG	2A	3503	1/1	0.95	0.16	67,67,67,67	0
53	MG	2A	3350	1/1	0.95	0.17	72,72,72,72	0
53	MG	1B	3020	1/1	0.95	0.23	42,42,42,42	0
53	MG	2O	202	1/1	0.95	0.31	47,47,47,47	0
53	MG	2A	3428	1/1	0.95	0.61	83,83,83,83	0
53	MG	2A	3320	1/1	0.95	0.16	73,73,73,73	0
53	MG	1A	3442	1/1	0.95	0.13	68,68,68,68	0
53	MG	1A	3636	1/1	0.95	0.16	31,31,31,31	0
53	MG	1B	3007	1/1	0.95	0.38	43,43,43,43	0
53	MG	1A	3489	1/1	0.95	0.07	69,69,69,69	0
53	MG	2A	3130	1/1	0.95	0.14	57,57,57,57	0
53	MG	2A	3376	1/1	0.95	0.26	77,77,77,77	0
53	MG	1a	3016	1/1	0.95	0.27	77,77,77,77	0
53	MG	2A	3309	1/1	0.95	0.26	50,50,50,50	0
53	MG	1A	3178	1/1	0.95	0.18	30,30,30,30	0
53	MG	1A	3606	1/1	0.95	0.26	58,58,58,58	0
53	MG	2A	3223	1/1	0.95	0.18	61,61,61,61	0
53	MG	1A	3694	1/1	0.95	0.22	76,76,76,76	0
53	MG	1A	3740	1/1	0.95	0.28	48,48,48,48	0
53	MG	1a	3084	1/1	0.95	0.13	60,60,60,60	0
53	MG	1A	3356	1/1	0.95	0.30	41,41,41,41	0
53	MG	2T	203	1/1	0.95	0.19	52,52,52,52	0
53	MG	1a	3132	1/1	0.95	0.11	65,65,65,65	0
53	MG	1A	3656	1/1	0.95	0.12	56,56,56,56	0
53	MG	1a	3069	1/1	0.95	0.21	75,75,75,75	0
53	MG	2A	3432	1/1	0.95	0.26	62,62,62,62	0
53	MG	1A	3033	1/1	0.95	0.40	37,37,37,37	0
53	MG	2a	1673	1/1	0.95	0.21	55,55,55,55	0
53	MG	1A	3220	1/1	0.95	0.30	38,38,38,38	0
53	MG	1A	3681	1/1	0.95	0.56	63,63,63,63	0
53	MG	1F	301	1/1	0.95	0.09	66,66,66,66	0
53	MG	2A	3275	1/1	0.95	0.22	37,37,37,37	0
53	MG	1A	3470	1/1	0.95	0.27	71,71,71,71	0
53	MG	2A	3292	1/1	0.95	0.20	49,49,49,49	0
53	MG	1A	3231	1/1	0.95	0.11	46,46,46,46	0
53	MG	2A	3241	1/1	0.95	0.34	53,53,53,53	0
53	MG	1A	3059	1/1	0.96	0.15	76,76,76,76	0
53	MG	2A	3079	1/1	0.96	0.13	54,54,54,54	0
53	MG	1A	3563	1/1	0.96	0.14	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	1A	3444	1/1	0.96	0.18	54,54,54,54	0
53	MG	1A	3682	1/1	0.96	0.25	63,63,63,63	0
53	MG	1A	3244	1/1	0.96	0.18	53,53,53,53	0
53	MG	1A	3055	1/1	0.96	0.45	58,58,58,58	0
53	MG	1a	3019	1/1	0.96	0.14	81,81,81,81	0
53	MG	1A	3441	1/1	0.96	0.15	52,52,52,52	0
53	MG	2A	3158	1/1	0.96	0.20	54,54,54,54	0
53	MG	1A	3540	1/1	0.96	0.34	48,48,48,48	0
53	MG	1A	3653	1/1	0.96	0.12	54,54,54,54	0
53	MG	1A	3299	1/1	0.96	0.23	37,37,37,37	0
53	MG	1A	3741	1/1	0.96	0.22	36,36,36,36	0
53	MG	1A	3064	1/1	0.96	0.22	57,57,57,57	0
53	MG	1a	3104	1/1	0.96	0.11	92,92,92,92	0
53	MG	1A	3372	1/1	0.96	0.19	59,59,59,59	0
53	MG	1A	3669	1/1	0.96	0.10	61,61,61,61	0
53	MG	2A	3231	1/1	0.96	0.28	49,49,49,49	0
53	MG	2a	1726	1/1	0.96	0.21	62,62,62,62	0
53	MG	1A	3416	1/1	0.96	0.21	41,41,41,41	0
53	MG	1A	3565	1/1	0.96	0.10	69,69,69,69	0
53	MG	1A	3675	1/1	0.96	0.15	63,63,63,63	0
55	ZN	29	501	1/1	0.96	0.09	89,89,89,89	0
53	MG	2A	3083	1/1	0.96	0.13	50,50,50,50	0
53	MG	1A	3157	1/1	0.96	0.19	38,38,38,38	0
53	MG	1B	3004	1/1	0.96	0.25	66,66,66,66	0
53	MG	1A	3232	1/1	0.96	0.19	60,60,60,60	0
53	MG	1A	3459	1/1	0.96	0.23	45,45,45,45	0
53	MG	20	8001	1/1	0.96	0.11	49,49,49,49	0
53	MG	1A	3170	1/1	0.96	0.14	56,56,56,56	0
53	MG	1A	3433	1/1	0.96	0.34	47,47,47,47	0
53	MG	1a	3080	1/1	0.96	0.30	66,66,66,66	0
53	MG	2Y	502	1/1	0.96	0.20	57,57,57,57	0
53	MG	2A	3466	1/1	0.96	0.10	63,63,63,63	0
53	MG	2A	3324	1/1	0.96	0.29	51,51,51,51	0
53	MG	1A	3719	1/1	0.96	0.29	71,71,71,71	0
53	MG	1A	3475	1/1	0.96	0.20	65,65,65,65	0
53	MG	1A	3488	1/1	0.96	0.26	69,69,69,69	0
53	MG	1A	3334	1/1	0.96	0.32	37,37,37,37	0
53	MG	1A	3567	1/1	0.96	0.19	97,97,97,97	0
53	MG	2a	1648	1/1	0.96	0.23	52,52,52,52	0
53	MG	1A	3705	1/1	0.96	0.18	42,42,42,42	0
53	MG	1R	203	1/1	0.96	0.89	47,47,47,47	0
53	MG	1A	3539	1/1	0.96	0.18	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	1A	3121	1/1	0.96	0.22	50,50,50,50	0
53	MG	1A	3211	1/1	0.96	0.16	50,50,50,50	0
53	MG	1A	3430	1/1	0.96	0.15	49,49,49,49	0
53	MG	2A	3002	1/1	0.96	0.07	55,55,55,55	0
53	MG	1a	3095	1/1	0.96	0.09	66,66,66,66	0
53	MG	1A	3271	1/1	0.96	0.16	44,44,44,44	0
53	MG	2A	3146	1/1	0.96	0.18	49,49,49,49	0
53	MG	1B	3022	1/1	0.96	0.20	32,32,32,32	0
53	MG	2A	3194	1/1	0.96	0.45	33,33,33,33	0
53	MG	1A	3451	1/1	0.96	0.23	51,51,51,51	0
53	MG	1A	3259	1/1	0.96	0.33	39,39,39,39	0
53	MG	2A	3059	1/1	0.96	0.22	42,42,42,42	0
53	MG	2A	3434	1/1	0.96	0.30	57,57,57,57	0
53	MG	1A	3432	1/1	0.96	0.30	58,58,58,58	0
53	MG	1A	3314	1/1	0.96	0.23	57,57,57,57	0
53	MG	1A	3703	1/1	0.96	0.23	62,62,62,62	0
53	MG	1A	3329	1/1	0.96	0.35	37,37,37,37	0
53	MG	1A	3500	1/1	0.96	0.19	68,68,68,68	0
53	MG	2A	3100	1/1	0.96	0.16	59,59,59,59	0
53	MG	1A	3357	1/1	0.96	0.23	41,41,41,41	0
53	MG	1A	3548	1/1	0.96	0.39	69,69,69,69	0
53	MG	1A	3482	1/1	0.96	0.17	55,55,55,55	0
53	MG	2A	3481	1/1	0.96	0.26	66,66,66,66	0
53	MG	1A	3458	1/1	0.96	0.11	27,27,27,27	0
53	MG	1A	3036	1/1	0.96	0.36	76,76,76,76	0
53	MG	1A	3660	1/1	0.96	0.13	50,50,50,50	0
53	MG	1A	3307	1/1	0.96	0.32	34,34,34,34	0
53	MG	1A	3751	1/1	0.96	0.13	37,37,37,37	0
53	MG	1A	3185	1/1	0.96	0.46	51,51,51,51	0
53	MG	1A	3677	1/1	0.96	0.34	46,46,46,46	0
53	MG	2A	3012	1/1	0.96	0.14	51,51,51,51	0
53	MG	1A	3750	1/1	0.96	0.13	73,73,73,73	0
53	MG	2a	1665	1/1	0.96	0.33	76,76,76,76	0
53	MG	2A	3335	1/1	0.96	0.19	48,48,48,48	0
53	MG	1A	3734	1/1	0.96	0.87	69,69,69,69	0
53	MG	1A	3640	1/1	0.96	0.15	43,43,43,43	0
53	MG	2A	3236	1/1	0.96	0.45	42,42,42,42	0
53	MG	1A	3646	1/1	0.96	0.08	64,64,64,64	0
53	MG	2A	3512	1/1	0.96	0.16	46,46,46,46	0
53	MG	1A	3570	1/1	0.96	0.20	62,62,62,62	0
53	MG	1A	3365	1/1	0.96	0.22	38,38,38,38	0
53	MG	1A	3585	1/1	0.96	0.12	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	2a	1703	1/1	0.96	0.16	91,91,91,91	0
53	MG	2A	3463	1/1	0.96	0.12	70,70,70,70	0
53	MG	1A	3246	1/1	0.96	0.13	40,40,40,40	0
53	MG	1A	3505	1/1	0.96	0.20	51,51,51,51	0
53	MG	1a	3122	1/1	0.96	0.18	60,60,60,60	0
53	MG	1A	3509	1/1	0.96	0.12	77,77,77,77	0
53	MG	1A	3696	1/1	0.96	0.18	57,57,57,57	0
53	MG	2A	3334	1/1	0.96	0.39	55,55,55,55	0
53	MG	1B	3003	1/1	0.96	0.48	60,60,60,60	0
53	MG	1a	3014	1/1	0.96	0.22	88,88,88,88	0
53	MG	1A	3455	1/1	0.96	0.23	65,65,65,65	0
53	MG	1A	3297	1/1	0.96	0.45	40,40,40,40	0
53	MG	1A	3745	1/1	0.96	0.29	81,81,81,81	0
53	MG	1A	3173	1/1	0.96	0.37	48,48,48,48	0
53	MG	1A	3613	1/1	0.96	0.32	48,48,48,48	0
53	MG	1a	3094	1/1	0.96	0.23	88,88,88,88	0
53	MG	2A	3246	1/1	0.96	0.19	38,38,38,38	0
53	MG	2A	3208	1/1	0.96	0.29	27,27,27,27	0
53	MG	2A	3397	1/1	0.96	0.10	54,54,54,54	0
53	MG	2A	3287	1/1	0.96	0.28	63,63,63,63	0
53	MG	1A	3448	1/1	0.96	0.20	64,64,64,64	0
53	MG	1A	3618	1/1	0.96	0.24	81,81,81,81	0
53	MG	1a	3050	1/1	0.96	0.11	67,67,67,67	0
53	MG	2A	3401	1/1	0.96	0.18	52,52,52,52	0
53	MG	1A	3572	1/1	0.96	0.13	74,74,74,74	0
53	MG	1F	304	1/1	0.96	0.15	39,39,39,39	0
53	MG	2a	1638	1/1	0.96	0.28	74,74,74,74	0
53	MG	2a	1684	1/1	0.96	0.14	75,75,75,75	0
53	MG	2A	3168	1/1	0.96	0.27	57,57,57,57	0
53	MG	1A	3328	1/1	0.96	0.46	61,61,61,61	0
53	MG	1A	3599	1/1	0.96	0.39	54,54,54,54	0
53	MG	2A	3056	1/1	0.96	0.10	60,60,60,60	0
53	MG	1A	3172	1/1	0.96	0.34	23,23,23,23	0
53	MG	1A	3012	1/1	0.96	0.67	47,47,47,47	0
53	MG	1A	3034	1/1	0.96	0.97	50,50,50,50	0
53	MG	1A	3710	1/1	0.96	0.26	52,52,52,52	0
53	MG	1A	3633	1/1	0.96	0.24	57,57,57,57	0
53	MG	2a	1696	1/1	0.96	0.60	67,67,67,67	0
53	MG	2A	3104	1/1	0.96	0.25	79,79,79,79	0
53	MG	1A	3358	1/1	0.96	0.35	58,58,58,58	0
53	MG	1A	3746	1/1	0.96	0.40	55,55,55,55	0
53	MG	1A	3620	1/1	0.96	0.32	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2E	301	1/1	0.96	0.12	47,47,47,47	0
53	MG	2A	3179	1/1	0.96	0.20	39,39,39,39	0
53	MG	1A	3615	1/1	0.96	0.32	73,73,73,73	0
53	MG	1U	201	1/1	0.96	0.11	23,23,23,23	0
53	MG	1A	3202	1/1	0.96	0.42	33,33,33,33	0
53	MG	2A	3474	1/1	0.96	0.12	65,65,65,65	0
53	MG	2A	3456	1/1	0.97	0.12	63,63,63,63	0
53	MG	2A	3052	1/1	0.97	0.85	66,66,66,66	0
53	MG	1A	3235	1/1	0.97	0.18	36,36,36,36	0
53	MG	2A	3296	1/1	0.97	0.23	39,39,39,39	0
53	MG	1A	3742	1/1	0.97	0.17	36,36,36,36	0
53	MG	1A	3634	1/1	0.97	0.22	58,58,58,58	0
53	MG	2A	3233	1/1	0.97	0.11	60,60,60,60	0
53	MG	1A	3520	1/1	0.97	0.25	74,74,74,74	0
53	MG	2A	3486	1/1	0.97	0.16	63,63,63,63	0
53	MG	1A	3673	1/1	0.97	0.14	32,32,32,32	0
53	MG	1A	3268	1/1	0.97	0.22	23,23,23,23	0
53	MG	1A	3162	1/1	0.97	0.21	51,51,51,51	0
53	MG	1A	3564	1/1	0.97	0.14	46,46,46,46	0
53	MG	2A	3453	1/1	0.97	0.09	66,66,66,66	0
53	MG	2a	1721	1/1	0.97	0.31	80,80,80,80	0
53	MG	1A	3002	1/1	0.97	0.26	51,51,51,51	0
53	MG	1A	3765	1/1	0.97	0.95	54,54,54,54	0
53	MG	1A	3485	1/1	0.97	0.17	72,72,72,72	0
53	MG	1A	3702	1/1	0.97	0.22	76,76,76,76	0
53	MG	2a	1639	1/1	0.97	0.74	69,69,69,69	0
53	MG	2A	3317	1/1	0.97	0.23	59,59,59,59	0
53	MG	1A	3581	1/1	0.97	0.60	64,64,64,64	0
53	MG	1A	3534	1/1	0.97	0.23	35,35,35,35	0
53	MG	1A	3697	1/1	0.97	0.17	37,37,37,37	0
53	MG	2A	3273	1/1	0.97	0.10	55,55,55,55	0
53	MG	1A	3168	1/1	0.97	0.22	26,26,26,26	0
53	MG	2A	3414	1/1	0.97	0.14	70,70,70,70	0
53	MG	1A	3547	1/1	0.97	0.13	62,62,62,62	0
53	MG	1A	3693	1/1	0.97	0.27	41,41,41,41	0
53	MG	1a	3047	1/1	0.97	0.30	80,80,80,80	0
53	MG	1a	3027	1/1	0.97	0.14	65,65,65,65	0
53	MG	1A	3315	1/1	0.97	0.22	53,53,53,53	0
53	MG	1A	3690	1/1	0.97	0.26	46,46,46,46	0
53	MG	1A	3755	1/1	0.97	0.22	63,63,63,63	0
53	MG	1A	3699	1/1	0.97	0.28	78,78,78,78	0
53	MG	1A	3161	1/1	0.97	0.61	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	2A	3120	1/1	0.97	0.16	64,64,64,64	0
53	MG	2A	3155	1/1	0.97	0.12	50,50,50,50	0
53	MG	2A	3483	1/1	0.97	0.09	50,50,50,50	0
53	MG	2A	3196	1/1	0.97	0.19	27,27,27,27	0
53	MG	2A	3297	1/1	0.97	0.17	48,48,48,48	0
53	MG	1A	3711	1/1	0.97	0.23	57,57,57,57	0
53	MG	1A	3420	1/1	0.97	0.26	28,28,28,28	0
53	MG	1a	3096	1/1	0.97	0.10	63,63,63,63	0
53	MG	1P	202	1/1	0.97	0.15	72,72,72,72	0
53	MG	1A	3532	1/1	0.97	0.16	73,73,73,73	0
56	SF4	2d	501	8/8	0.97	0.20	87,107,123,125	0
53	MG	1A	3422	1/1	0.97	0.30	22,22,22,22	0
53	MG	1A	3454	1/1	0.97	0.14	57,57,57,57	0
53	MG	1B	3001	1/1	0.97	0.25	70,70,70,70	0
53	MG	2a	1649	1/1	0.97	0.11	55,55,55,55	0
53	MG	1A	3761	1/1	0.97	0.21	75,75,75,75	0
53	MG	1A	3662	1/1	0.97	0.18	82,82,82,82	0
53	MG	2A	3215	1/1	0.97	0.22	32,32,32,32	0
53	MG	1A	3167	1/1	0.97	0.24	20,20,20,20	0
53	MG	1A	3224	1/1	0.97	0.29	30,30,30,30	0
53	MG	2A	3139	1/1	0.97	0.39	35,35,35,35	0
55	ZN	26	501	1/1	0.97	0.18	84,84,84,84	0
53	MG	2A	3308	1/1	0.97	0.17	36,36,36,36	0
53	MG	1A	3439	1/1	0.97	0.23	54,54,54,54	0
53	MG	1A	3230	1/1	0.97	0.29	23,23,23,23	0
53	MG	2A	3203	1/1	0.97	0.15	28,28,28,28	0
53	MG	1A	3663	1/1	0.97	0.38	47,47,47,47	0
53	MG	2A	3303	1/1	0.97	0.22	39,39,39,39	0
53	MG	2A	3185	1/1	0.97	0.18	35,35,35,35	0
53	MG	1U	203	1/1	0.97	0.75	73,73,73,73	0
53	MG	2A	3005	1/1	0.97	0.23	51,51,51,51	0
53	MG	1a	3032	1/1	0.97	0.23	56,56,56,56	0
53	MG	1A	3597	1/1	0.97	0.24	40,40,40,40	0
53	MG	1A	3443	1/1	0.97	0.17	69,69,69,69	0
53	MG	1a	3070	1/1	0.97	0.17	69,69,69,69	0
53	MG	2a	1708	1/1	0.97	0.16	73,73,73,73	0
53	MG	2A	3252	1/1	0.97	0.27	42,42,42,42	0
53	MG	2A	3283	1/1	0.97	0.26	46,46,46,46	0
53	MG	1A	3294	1/1	0.97	0.30	39,39,39,39	0
53	MG	1A	3639	1/1	0.97	0.14	26,26,26,26	0
53	MG	1A	3460	1/1	0.97	0.08	50,50,50,50	0
53	MG	2A	3498	1/1	0.97	0.12	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2B	208	1/1	0.97	0.12	79,79,79,79	0
53	MG	1A	3497	1/1	0.97	0.17	35,35,35,35	0
53	MG	1A	3335	1/1	0.97	0.35	42,42,42,42	0
53	MG	2a	1719	1/1	0.97	0.10	93,93,93,93	0
53	MG	1A	3679	1/1	0.97	0.22	38,38,38,38	0
53	MG	1A	3097	1/1	0.97	0.35	50,50,50,50	0
53	MG	2A	3188	1/1	0.97	0.42	66,66,66,66	0
53	MG	17	102	1/1	0.97	0.62	50,50,50,50	0
53	MG	1A	3536	1/1	0.97	0.18	52,52,52,52	0
53	MG	1A	3022	1/1	0.97	0.37	58,58,58,58	0
53	MG	1A	3752	1/1	0.97	0.31	47,47,47,47	0
53	MG	1A	3643	1/1	0.97	0.11	31,31,31,31	0
53	MG	2A	3446	1/1	0.97	0.11	59,59,59,59	0
53	MG	1a	3102	1/1	0.97	0.15	58,58,58,58	0
53	MG	2A	3038	1/1	0.97	0.09	56,56,56,56	0
53	MG	2A	3213	1/1	0.97	0.19	64,64,64,64	0
53	MG	1A	3291	1/1	0.97	0.23	49,49,49,49	0
53	MG	2A	3480	1/1	0.97	0.08	72,72,72,72	0
53	MG	2A	3404	1/1	0.97	0.09	44,44,44,44	0
53	MG	1A	3206	1/1	0.97	0.29	67,67,67,67	0
53	MG	2A	3125	1/1	0.97	0.16	33,33,33,33	0
53	MG	1A	3611	1/1	0.97	0.38	51,51,51,51	0
53	MG	1A	3695	1/1	0.97	0.47	57,57,57,57	0
53	MG	1A	3405	1/1	0.97	0.16	45,45,45,45	0
53	MG	1A	3579	1/1	0.97	0.15	68,68,68,68	0
53	MG	1A	3431	1/1	0.97	0.26	62,62,62,62	0
53	MG	1A	3523	1/1	0.97	0.14	73,73,73,73	0
53	MG	1A	3325	1/1	0.97	0.15	50,50,50,50	0
53	MG	2a	1695	1/1	0.97	0.16	88,88,88,88	0
53	MG	2A	3472	1/1	0.97	0.13	57,57,57,57	0
53	MG	2A	3143	1/1	0.97	0.28	47,47,47,47	0
53	MG	1a	3101	1/1	0.97	0.09	65,65,65,65	0
53	MG	1A	3474	1/1	0.97	0.20	57,57,57,57	0
53	MG	2A	3305	1/1	0.97	0.22	40,40,40,40	0
53	MG	1A	3337	1/1	0.97	0.49	26,26,26,26	0
53	MG	1A	3725	1/1	0.97	0.51	71,71,71,71	0
53	MG	1A	3049	1/1	0.97	0.25	51,51,51,51	0
53	MG	1A	3024	1/1	0.97	1.37	62,62,62,62	0
53	MG	2a	1647	1/1	0.97	0.49	64,64,64,64	0
53	MG	1A	3449	1/1	0.97	0.21	57,57,57,57	0
53	MG	1A	3578	1/1	0.97	0.13	30,30,30,30	0
53	MG	1A	3065	1/1	0.97	0.34	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	3218	1/1	0.97	0.27	44,44,44,44	0
53	MG	1A	3571	1/1	0.97	0.16	69,69,69,69	0
53	MG	1A	3115	1/1	0.97	0.18	53,53,53,53	0
53	MG	1a	3099	1/1	0.98	0.23	67,67,67,67	0
53	MG	1A	3261	1/1	0.98	0.17	59,59,59,59	0
55	ZN	15	103	1/1	0.98	0.24	43,43,43,43	0
55	ZN	19	102	1/1	0.98	0.22	51,51,51,51	0
53	MG	1A	3637	1/1	0.98	0.17	42,42,42,42	0
53	MG	1A	3234	1/1	0.98	0.33	44,44,44,44	0
53	MG	1A	3709	1/1	0.98	0.15	75,75,75,75	0
53	MG	1A	3398	1/1	0.98	0.15	55,55,55,55	0
53	MG	2A	3458	1/1	0.98	0.16	44,44,44,44	0
53	MG	1A	3009	1/1	0.98	0.23	45,45,45,45	0
53	MG	2A	3099	1/1	0.98	0.21	46,46,46,46	0
53	MG	1A	3288	1/1	0.98	0.40	47,47,47,47	0
53	MG	1A	3596	1/1	0.98	0.11	58,58,58,58	0
53	MG	1A	3292	1/1	0.98	0.17	42,42,42,42	0
53	MG	1A	3450	1/1	0.98	0.16	40,40,40,40	0
53	MG	1A	3522	1/1	0.98	0.21	70,70,70,70	0
53	MG	2A	3198	1/1	0.98	0.30	40,40,40,40	0
53	MG	1A	3604	1/1	0.98	0.23	64,64,64,64	0
53	MG	2A	3116	1/1	0.98	0.17	51,51,51,51	0
53	MG	2A	3389	1/1	0.98	0.17	64,64,64,64	0
53	MG	1A	3503	1/1	0.98	0.32	43,43,43,43	0
53	MG	2a	1653	1/1	0.98	0.24	67,67,67,67	0
53	MG	1A	3708	1/1	0.98	0.28	44,44,44,44	0
53	MG	2A	3355	1/1	0.98	0.09	62,62,62,62	0
53	MG	1A	3427	1/1	0.98	0.31	39,39,39,39	0
53	MG	1A	3142	1/1	0.98	0.32	45,45,45,45	0
53	MG	1B	3019	1/1	0.98	0.20	40,40,40,40	0
53	MG	1A	3468	1/1	0.98	0.21	73,73,73,73	0
53	MG	2A	3490	1/1	0.98	0.17	51,51,51,51	0
53	MG	2a	1624	1/1	0.98	0.13	55,55,55,55	0
53	MG	2A	3237	1/1	0.98	0.20	56,56,56,56	0
53	MG	1E	302	1/1	0.98	0.15	43,43,43,43	0
53	MG	1A	3737	1/1	0.98	0.49	23,23,23,23	0
53	MG	1A	3550	1/1	0.98	0.12	23,23,23,23	0
53	MG	2A	3209	1/1	0.98	0.14	50,50,50,50	0
53	MG	2A	3212	1/1	0.98	0.37	37,37,37,37	0
53	MG	2A	3379	1/1	0.98	0.18	47,47,47,47	0
53	MG	1A	3440	1/1	0.98	0.18	65,65,65,65	0
53	MG	1A	3201	1/1	0.98	0.37	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2a	1669	1/1	0.98	0.10	71,71,71,71	0
53	MG	2A	3210	1/1	0.98	0.16	37,37,37,37	0
53	MG	1A	3187	1/1	0.98	0.34	31,31,31,31	0
53	MG	1A	3140	1/1	0.98	0.13	53,53,53,53	0
56	SF4	1d	501	8/8	0.98	0.19	85,105,119,125	0
53	MG	1A	3225	1/1	0.98	0.30	52,52,52,52	0
53	MG	1A	3400	1/1	0.98	0.14	58,58,58,58	0
53	MG	2R	8001	1/1	0.98	0.19	30,30,30,30	0
53	MG	2a	1666	1/1	0.98	0.14	66,66,66,66	0
53	MG	1A	3381	1/1	0.98	0.28	48,48,48,48	0
53	MG	1A	3037	1/1	0.98	0.18	57,57,57,57	0
53	MG	2A	3451	1/1	0.98	0.21	71,71,71,71	0
53	MG	2A	3407	1/1	0.98	0.22	49,49,49,49	0
53	MG	2A	3251	1/1	0.98	0.25	41,41,41,41	0
53	MG	1A	3580	1/1	0.98	0.22	38,38,38,38	0
53	MG	1A	3177	1/1	0.98	0.27	35,35,35,35	0
53	MG	2A	3259	1/1	0.98	0.30	45,45,45,45	0
53	MG	1A	3759	1/1	0.98	0.16	32,32,32,32	0
53	MG	1A	3296	1/1	0.98	0.20	24,24,24,24	0
53	MG	1A	3240	1/1	0.98	0.38	28,28,28,28	0
53	MG	1A	3501	1/1	0.98	0.11	59,59,59,59	0
53	MG	2A	3301	1/1	0.98	0.14	45,45,45,45	0
53	MG	2A	3254	1/1	0.98	0.36	47,47,47,47	0
53	MG	1A	3127	1/1	0.98	0.21	60,60,60,60	0
53	MG	1A	3423	1/1	0.98	0.20	63,63,63,63	0
53	MG	1A	3113	1/1	0.98	0.29	63,63,63,63	0
53	MG	2A	3327	1/1	0.98	0.32	51,51,51,51	0
53	MG	1A	3046	1/1	0.98	0.27	51,51,51,51	0
53	MG	2a	1619	1/1	0.98	0.12	81,81,81,81	0
53	MG	1R	201	1/1	0.98	0.39	66,66,66,66	0
53	MG	2A	3390	1/1	0.98	0.11	45,45,45,45	0
53	MG	2a	1621	1/1	0.98	0.11	88,88,88,88	0
53	MG	1A	3298	1/1	0.98	0.38	22,22,22,22	0
53	MG	2A	3281	1/1	0.98	0.31	48,48,48,48	0
53	MG	1H	201	1/1	0.98	0.12	50,50,50,50	0
53	MG	2A	3302	1/1	0.98	0.15	38,38,38,38	0
53	MG	1a	3058	1/1	0.98	0.17	68,68,68,68	0
53	MG	2a	1610	1/1	0.98	0.21	74,74,74,74	0
53	MG	1A	3269	1/1	0.98	0.21	55,55,55,55	0
53	MG	1A	3284	1/1	0.98	0.30	28,28,28,28	0
53	MG	1A	3222	1/1	0.98	0.29	47,47,47,47	0
53	MG	1A	3665	1/1	0.98	0.25	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	3145	1/1	0.98	0.39	26,26,26,26	0
53	MG	2A	3174	1/1	0.98	0.20	23,23,23,23	0
53	MG	1A	3756	1/1	0.98	0.55	57,57,57,57	0
53	MG	1A	3735	1/1	0.98	0.13	54,54,54,54	0
55	ZN	1Y	201	1/1	0.98	0.33	80,80,80,80	0
53	MG	2A	3102	1/1	0.98	0.14	40,40,40,40	0
53	MG	2A	3284	1/1	0.98	0.22	56,56,56,56	0
53	MG	2A	3159	1/1	0.98	0.12	44,44,44,44	0
53	MG	2E	305	1/1	0.98	0.31	52,52,52,52	0
53	MG	1A	3671	1/1	0.98	0.11	60,60,60,60	0
53	MG	2A	3279	1/1	0.98	0.25	32,32,32,32	0
53	MG	1A	3156	1/1	0.98	0.49	43,43,43,43	0
53	MG	2A	3367	1/1	0.98	0.19	56,56,56,56	0
53	MG	1A	3668	1/1	0.98	0.13	26,26,26,26	0
53	MG	2A	3310	1/1	0.98	0.15	52,52,52,52	0
53	MG	1A	3203	1/1	0.98	0.26	25,25,25,25	0
53	MG	1A	3189	1/1	0.98	0.40	26,26,26,26	0
53	MG	1A	3300	1/1	0.98	0.27	47,47,47,47	0
53	MG	2A	3178	1/1	0.98	0.19	36,36,36,36	0
53	MG	1A	3716	1/1	0.98	0.11	57,57,57,57	0
53	MG	1A	3622	1/1	0.98	0.24	55,55,55,55	0
53	MG	1A	3192	1/1	0.98	0.31	26,26,26,26	0
53	MG	1A	3472	1/1	0.98	0.26	46,46,46,46	0
53	MG	1A	3683	1/1	0.98	0.09	61,61,61,61	0
53	MG	1A	3493	1/1	0.98	0.15	49,49,49,49	0
53	MG	1A	3148	1/1	0.98	0.40	35,35,35,35	0
53	MG	1A	3006	1/1	0.98	0.38	31,31,31,31	0
53	MG	1A	3204	1/1	0.99	0.27	57,57,57,57	0
53	MG	1A	3603	1/1	0.99	0.28	44,44,44,44	0
53	MG	1A	3165	1/1	0.99	0.41	29,29,29,29	0
53	MG	1a	3119	1/1	0.99	1.00	79,79,79,79	0
53	MG	1A	3386	1/1	0.99	0.17	70,70,70,70	0
53	MG	2a	1678	1/1	0.99	0.08	69,69,69,69	0
53	MG	1P	201	1/1	0.99	0.40	50,50,50,50	0
53	MG	1A	3645	1/1	0.99	0.45	39,39,39,39	0
53	MG	2A	3205	1/1	0.99	0.44	33,33,33,33	0
53	MG	1A	3186	1/1	0.99	0.33	21,21,21,21	0
53	MG	1a	3105	1/1	0.99	0.18	60,60,60,60	0
53	MG	1A	3462	1/1	0.99	0.17	53,53,53,53	0
53	MG	1A	3169	1/1	0.99	0.18	25,25,25,25	0
53	MG	1A	3324	1/1	0.99	0.28	34,34,34,34	0
53	MG	1A	3238	1/1	0.99	0.24	39,39,39,39	0

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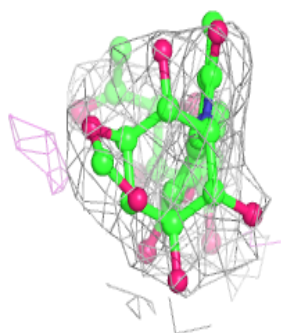
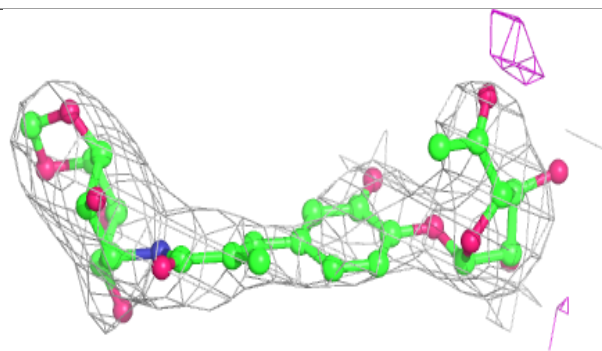
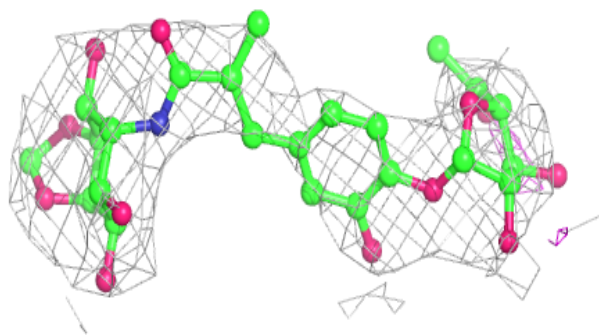
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	2A	3393	1/1	0.99	0.15	29,29,29,29	0
53	MG	1A	3670	1/1	0.99	0.09	48,48,48,48	0
53	MG	1A	3698	1/1	0.99	0.15	27,27,27,27	0
53	MG	2A	3261	1/1	0.99	0.19	43,43,43,43	0
53	MG	1A	3507	1/1	0.99	0.29	43,43,43,43	0
53	MG	1A	3143	1/1	0.99	0.24	20,20,20,20	0
55	ZN	16	501	1/1	0.99	0.26	65,65,65,65	0
53	MG	1A	3301	1/1	0.99	0.32	38,38,38,38	0
53	MG	1A	3045	1/1	0.99	0.29	32,32,32,32	0
53	MG	1A	3061	1/1	0.99	0.31	46,46,46,46	0
53	MG	2A	3183	1/1	0.99	0.30	32,32,32,32	0
53	MG	2A	3484	1/1	0.99	0.14	45,45,45,45	0
53	MG	1A	3575	1/1	0.99	0.26	83,83,83,83	0
53	MG	2A	3131	1/1	0.99	0.37	34,34,34,34	0
53	MG	2A	3054	1/1	0.99	0.21	63,63,63,63	0
53	MG	1A	3654	1/1	0.99	0.15	31,31,31,31	0
53	MG	1A	3438	1/1	0.99	0.15	33,33,33,33	0
53	MG	2A	3222	1/1	0.99	0.22	58,58,58,58	0
53	MG	15	102	1/1	0.99	0.23	26,26,26,26	0
53	MG	2A	3232	1/1	0.99	0.16	47,47,47,47	0
53	MG	2A	3359	1/1	0.99	0.09	54,54,54,54	0
53	MG	1A	3191	1/1	0.99	0.24	31,31,31,31	0
53	MG	2A	3148	1/1	0.99	0.18	60,60,60,60	0
55	ZN	25	501	1/1	0.99	0.29	66,66,66,66	0
53	MG	2A	3190	1/1	0.99	0.22	34,34,34,34	0
53	MG	1A	3610	1/1	0.99	0.16	40,40,40,40	0
53	MG	1A	3758	1/1	0.99	0.21	41,41,41,41	0
53	MG	2A	3197	1/1	0.99	0.20	41,41,41,41	0
53	MG	2A	3280	1/1	0.99	0.16	43,43,43,43	0
53	MG	1A	3457	1/1	0.99	0.19	30,30,30,30	0
53	MG	2A	3465	1/1	0.99	0.13	41,41,41,41	0
53	MG	2A	3243	1/1	0.99	0.32	35,35,35,35	0
53	MG	1A	3355	1/1	1.00	0.36	39,39,39,39	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.

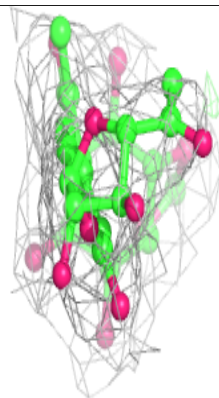
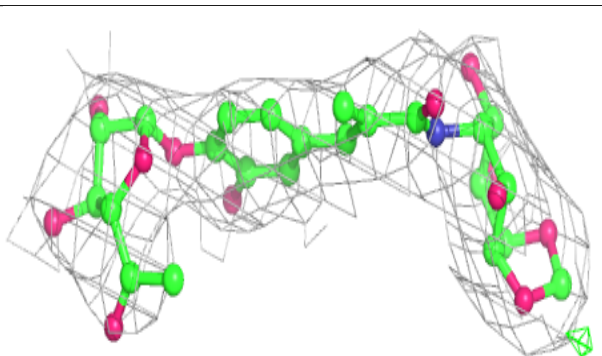
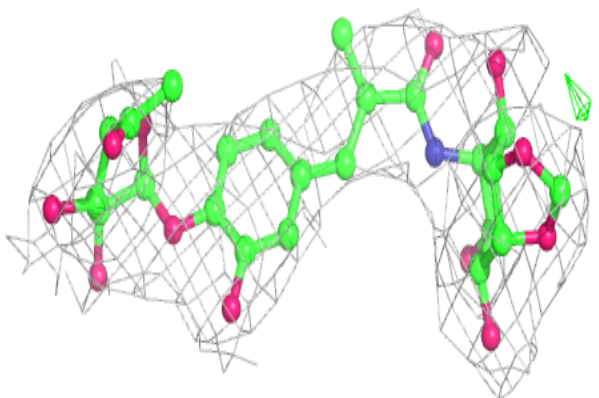


**Electron density around HGR 2A 3515:**

$2mF_o-DF_c$  (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.