Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 08:18 PM EST

PDB ID	:	6UO1
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with mRNA (containing pseudouridine at the first position of the codon) and deacylated A-, P-, and E-site tRNAs at 2.95A resolution
Authors	:	Batool, Z.; Dobosz-Bartoszek, M.; Polikanov, Y.S.
Deposited on	:	2019-10-14
Resolution	:	2.95 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

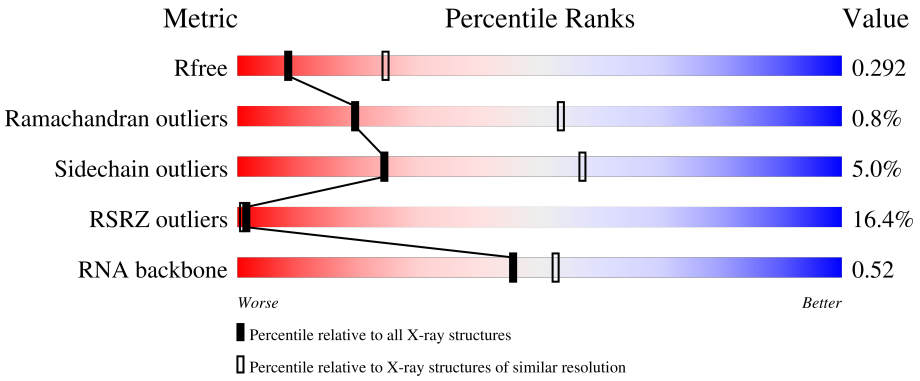
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 81% 17%
1	2A	2915	4% 77% 19%
2	1B	121	87% 12%
2	2B	121	83% 16%
3	1D	276	48% 96%

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Mol	Chain	Length	Quality of chain
3	2D	276	41% 96%
4	1E	206	41% 95%
4	2E	206	30% 94% 5%
5	1F	210	25% 94%
5	2F	210	27% 90% 6%
6	1G	182	3% 96%
6	2G	182	5% 95% 5%
7	1H	180	% 92%
7	2H	180	34% 92%
8	1I	148	14% 93% 5%
8	2I	148	24% 93% 6%
9	1N	140	48% 95% 5%
9	2N	140	73% 94% 6%
10	1O	122	53% 95% 5%
10	2O	122	37% 96%
11	1P	150	27% 96%
11	2P	150	43% 95% 5%
12	1Q	141	25% 99%
12	2Q	141	28% 96%
13	1R	118	39% 93% 7%
13	2R	118	26% 93% 7%
14	1S	112	% 96%
14	2S	112	95%
15	1T	146	32% 87% 10%
15	2T	146	22% 86% 10%

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Mol	Chain	Length	Quality of chain
16	1U	118	47% 94%
16	2U	118	46% 94%
17	1V	101	23% 92% 8%
17	2V	101	26% 95% 5%
18	1W	113	29% 97%
18	2W	113	41% 96%
19	1X	96	18% 99%
19	2X	96	21% 96%
20	1Y	110	6% 86% 11%
20	2Y	110	42% 93% 5%
21	1Z	206	% 70% 25%
21	2Z	206	76% 22%
22	10	85	15% 98%
22	20	85	29% 95%
23	11	98	61% 96%
23	21	98	45% 97%
24	12	72	8% 94%
24	22	72	6% 96%
25	13	60	5% 95%
25	23	60	37% 97%
26	14	71	89%
26	24	71	% 89% 8%
27	15	60	32% 90% 8%
27	25	60	30% 93% 5%
28	16	54	11% 85% 13%

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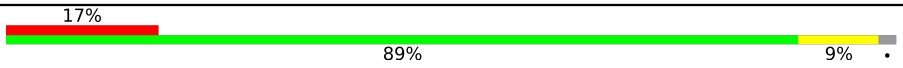
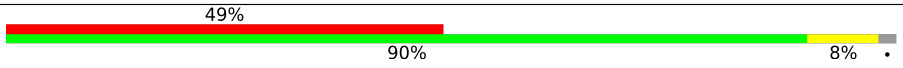
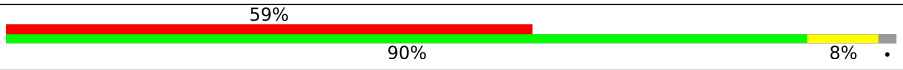
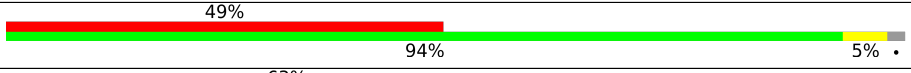
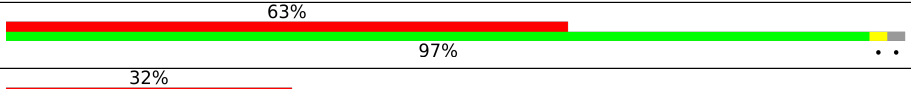
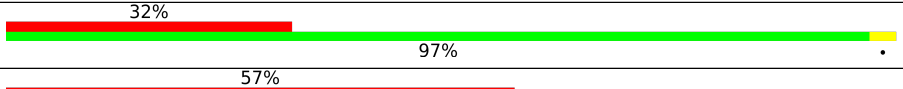
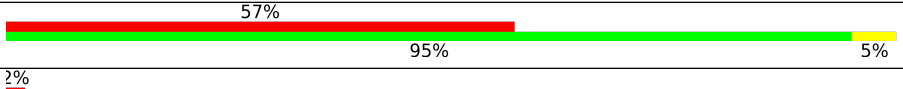
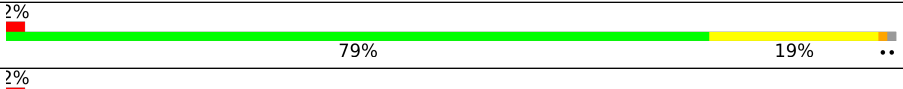
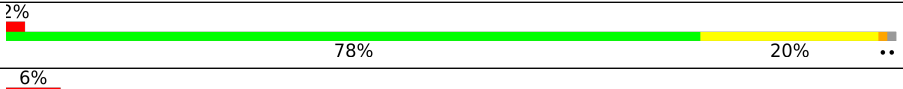
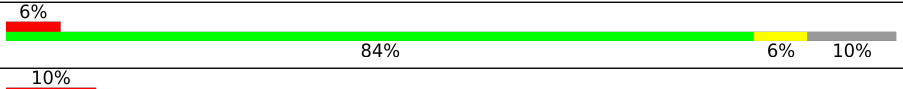
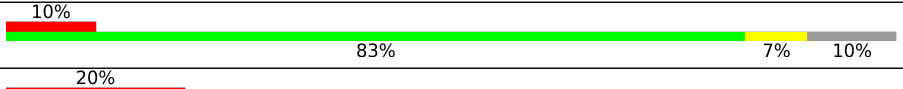
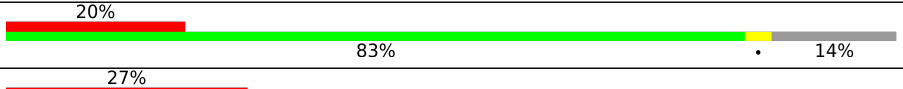
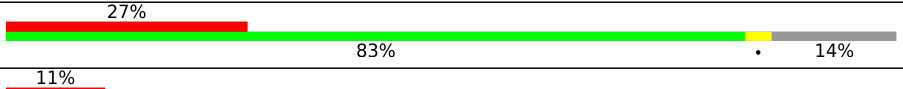
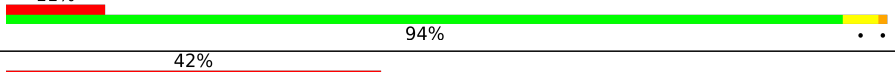
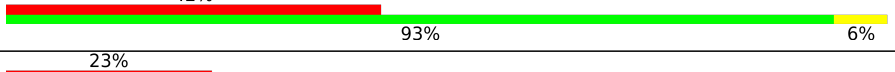
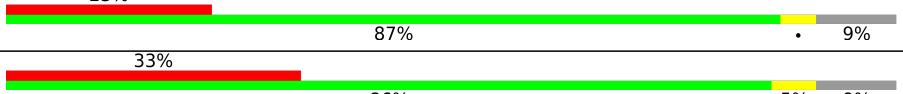
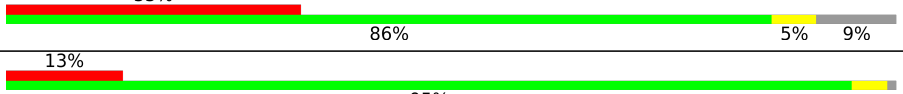
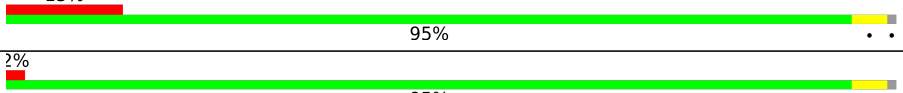
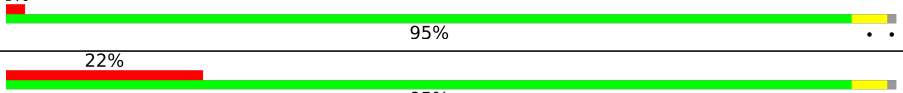
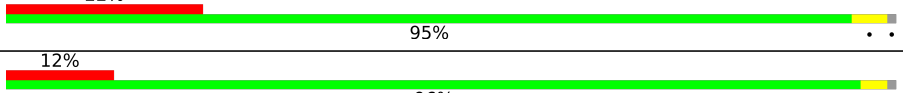
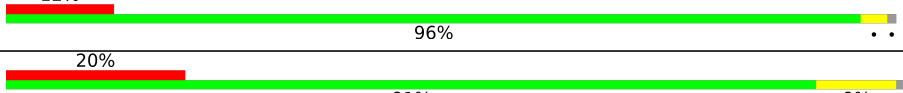
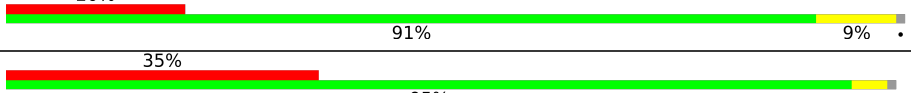
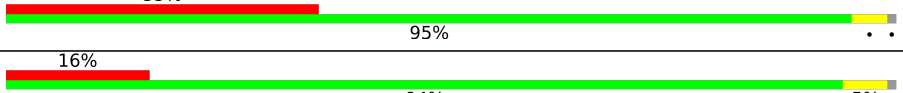
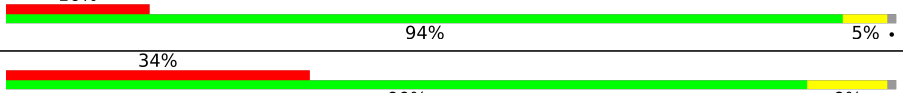
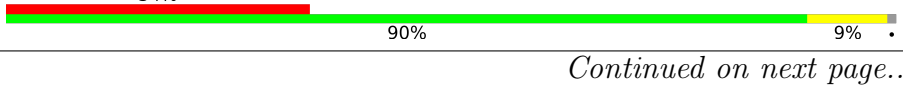
Mol	Chain	Length	Quality of chain
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	
40	2i	128	

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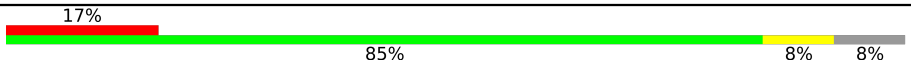
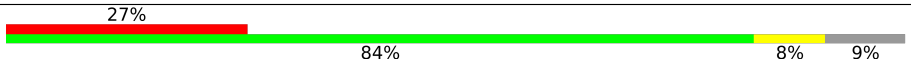
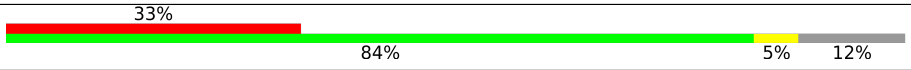
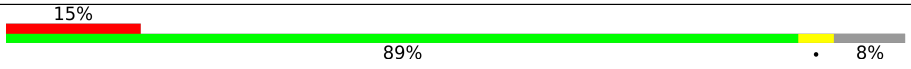
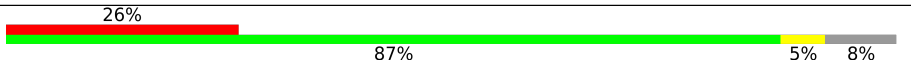
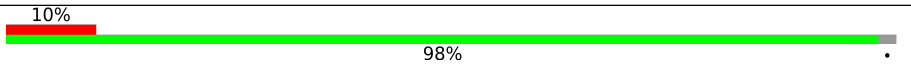
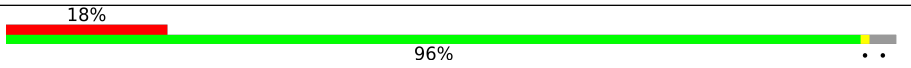
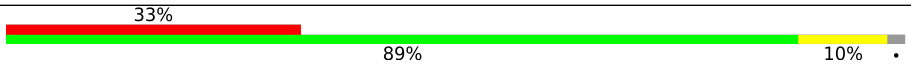
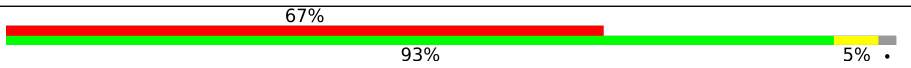
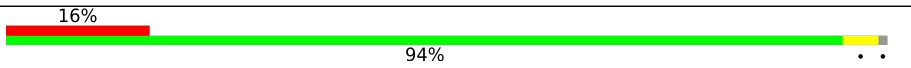
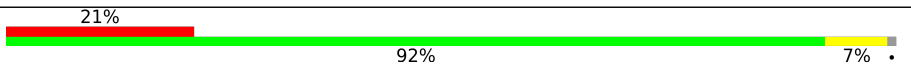
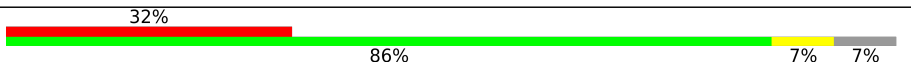
Mol	Chain	Length	Quality of chain
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
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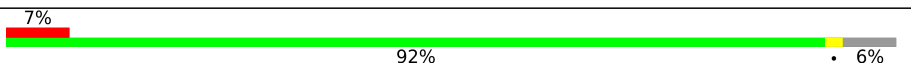
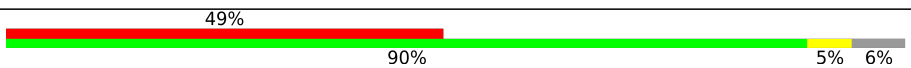
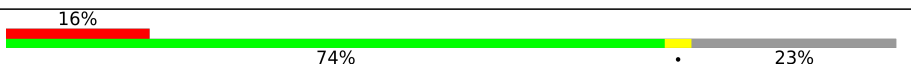
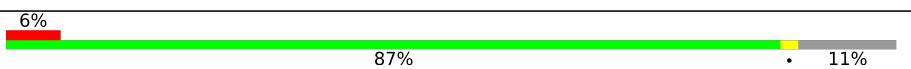
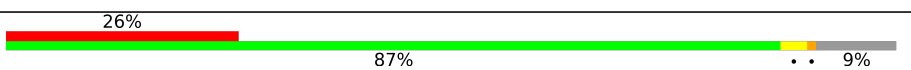
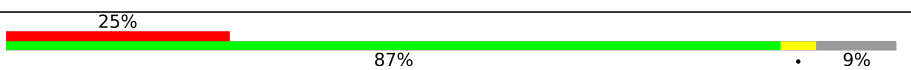
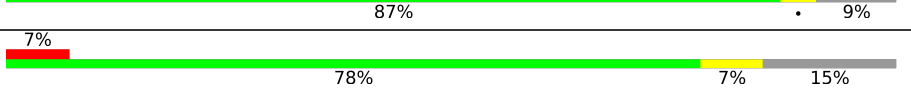
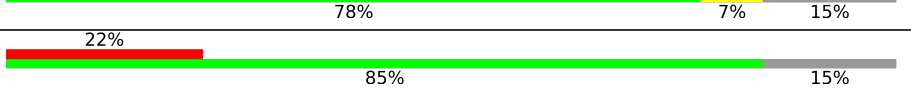
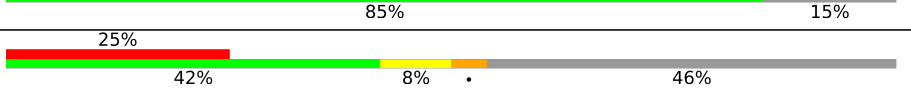
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	
53	1v	24	

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Mol	Chain	Length	Quality of chain
53	2v	24	8% 21% 8% 67%
54	1w	76	28% 62% 28% 7%
54	1y	76	24% 51% 43%
54	2w	76	8% 61% 26% 9%
54	2y	76	12% 53% 41%
55	1x	77	4% 78% 19%
55	2x	77	3% 78% 19%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3036	-	-	-	X
56	MG	1A	3098	-	-	-	X
56	MG	1A	3104	-	-	-	X
56	MG	1A	3114	-	-	-	X
56	MG	1A	3121	-	-	-	X
56	MG	1A	3123	-	-	-	X
56	MG	1A	3142	-	-	-	X
56	MG	1A	3148	-	-	-	X
56	MG	1A	3149	-	-	-	X
56	MG	1A	3190	-	-	-	X
56	MG	1A	3318	-	-	-	X
56	MG	1A	3359	-	-	-	X
56	MG	1A	3368	-	-	-	X
56	MG	1A	3377	-	-	-	X
56	MG	1A	3394	-	-	-	X
56	MG	1A	3433	-	-	-	X
56	MG	1A	3506	-	-	-	X
56	MG	1A	3513	-	-	-	X
56	MG	1a	3016	-	-	-	X
56	MG	1a	3037	-	-	-	X
56	MG	1a	3043	-	-	-	X
56	MG	1a	3053	-	-	-	X
56	MG	1a	3082	-	-	-	X
56	MG	1a	3092	-	-	-	X
56	MG	1a	3094	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	3111	-	-	-	X
56	MG	1a	3116	-	-	-	X
56	MG	1a	3122	-	-	-	X
56	MG	1a	3163	-	-	-	X
56	MG	1a	3167	-	-	-	X
56	MG	2A	3057	-	-	-	X
56	MG	2A	3092	-	-	-	X
56	MG	2A	3099	-	-	-	X
56	MG	2A	3101	-	-	-	X
56	MG	2A	3111	-	-	-	X
56	MG	2A	3142	-	-	-	X
56	MG	2A	3158	-	-	-	X
56	MG	2A	3234	-	-	-	X
56	MG	2A	3245	-	-	-	X
56	MG	2A	3315	-	-	-	X
56	MG	2A	3316	-	-	-	X
56	MG	2A	3317	-	-	-	X
56	MG	2a	3007	-	-	-	X
56	MG	2a	3017	-	-	-	X
56	MG	2a	3031	-	-	-	X
56	MG	2a	3053	-	-	-	X
56	MG	2a	3058	-	-	-	X
56	MG	2a	3059	-	-	-	X
56	MG	2a	3060	-	-	-	X
56	MG	2a	3087	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 295398 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	50	89	13			
53	2v	8	Total	C	N	O	P	0	0	0
			167	75	25	59	8			

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	71	Total	C	N	O	P	S	0	0	0
			1530	685	274	498	71	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	69	Total	C	N	O	P	S	0	0	0
			1482	662	267	482	69	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	680	Total	Mg	0	0
			680	680		
56	1a	238	Total	Mg	0	0
			238	238		
56	2A	351	Total	Mg	0	0
			351	351		
56	2a	183	Total	Mg	0	0
			183	183		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		

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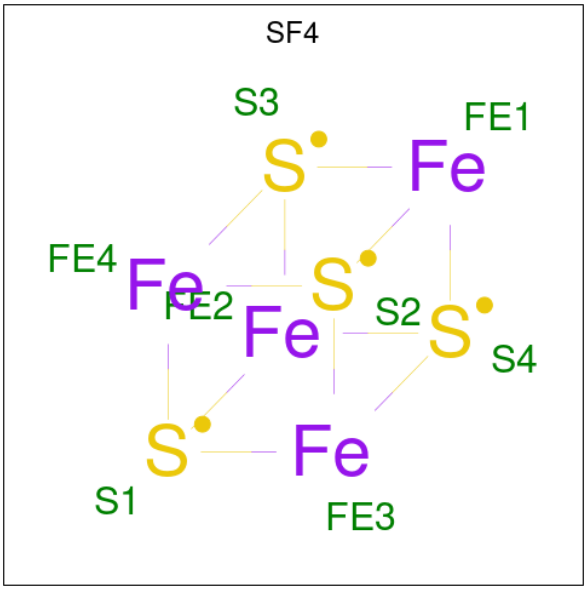
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	14	1	Total Zn 1 1	0	0
57	15	1	Total Zn 1 1	0	0
57	16	1	Total Zn 1 1	0	0
57	19	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	2Y	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0
57	25	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0
57	29	1	Total Zn 1 1	0	0
57	2n	1	Total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

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 59 is water.

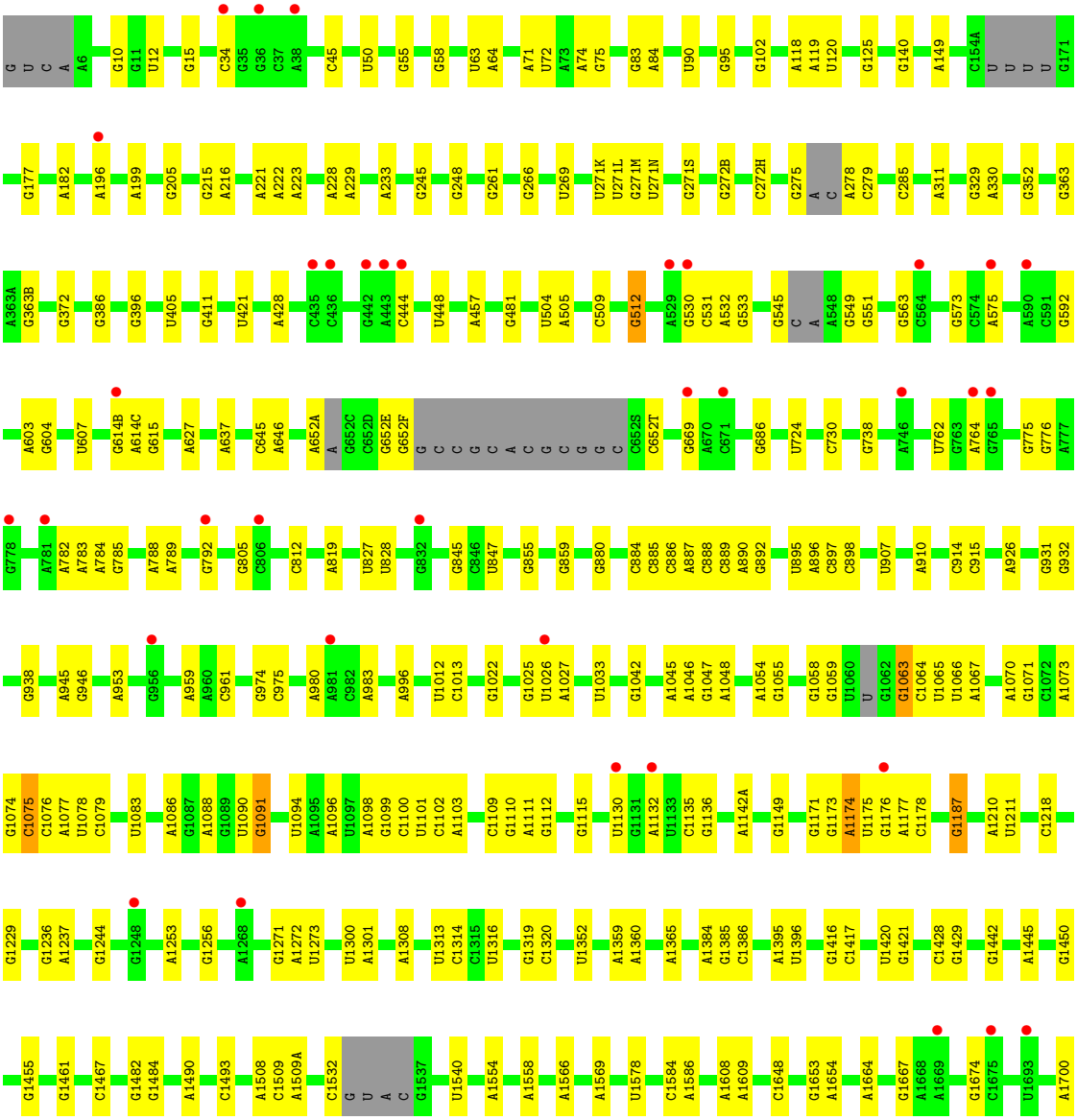
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	585	Total O 585 585	0	0
59	1a	181	Total O 181 181	0	0
59	2A	234	Total O 234 234	0	0
59	2a	167	Total O 167 167	0	0

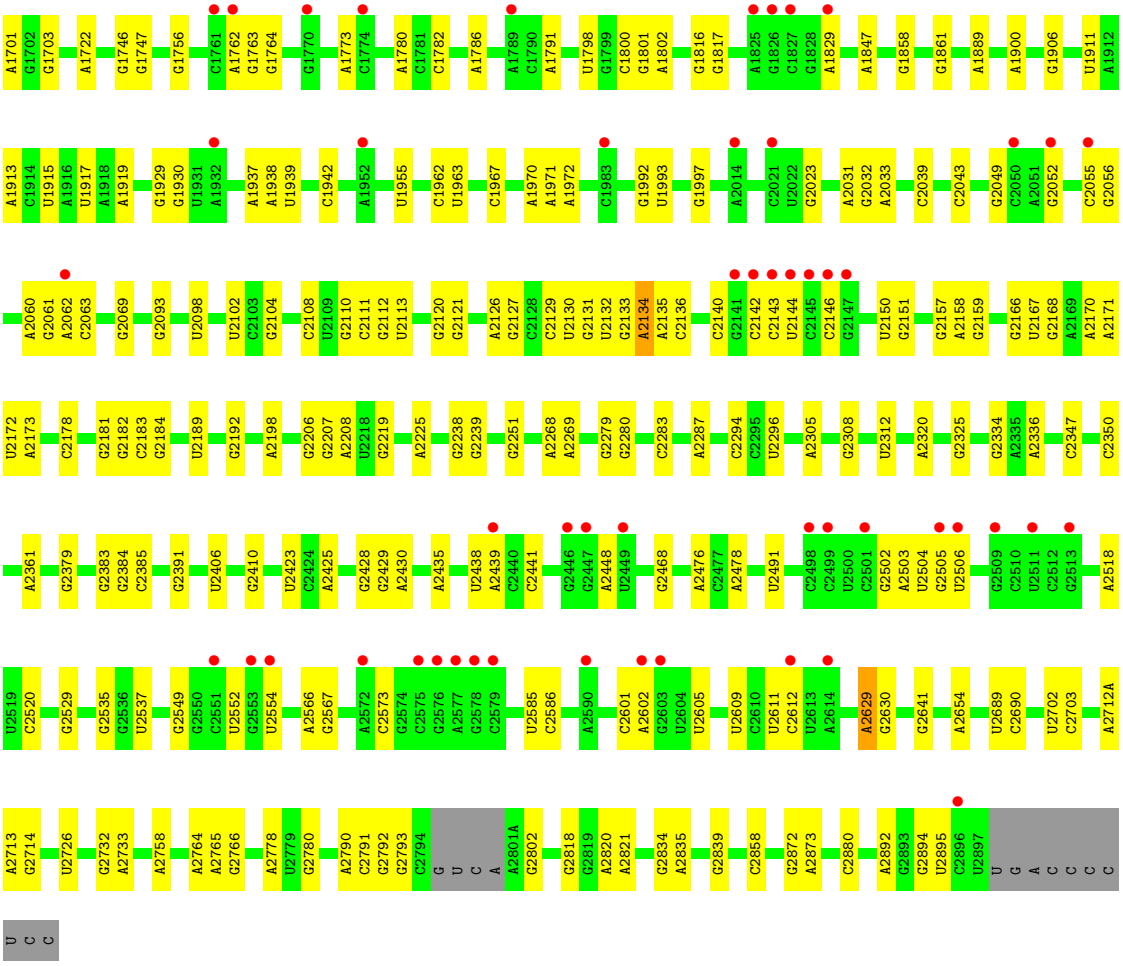
3 Residue-property plots (i)

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

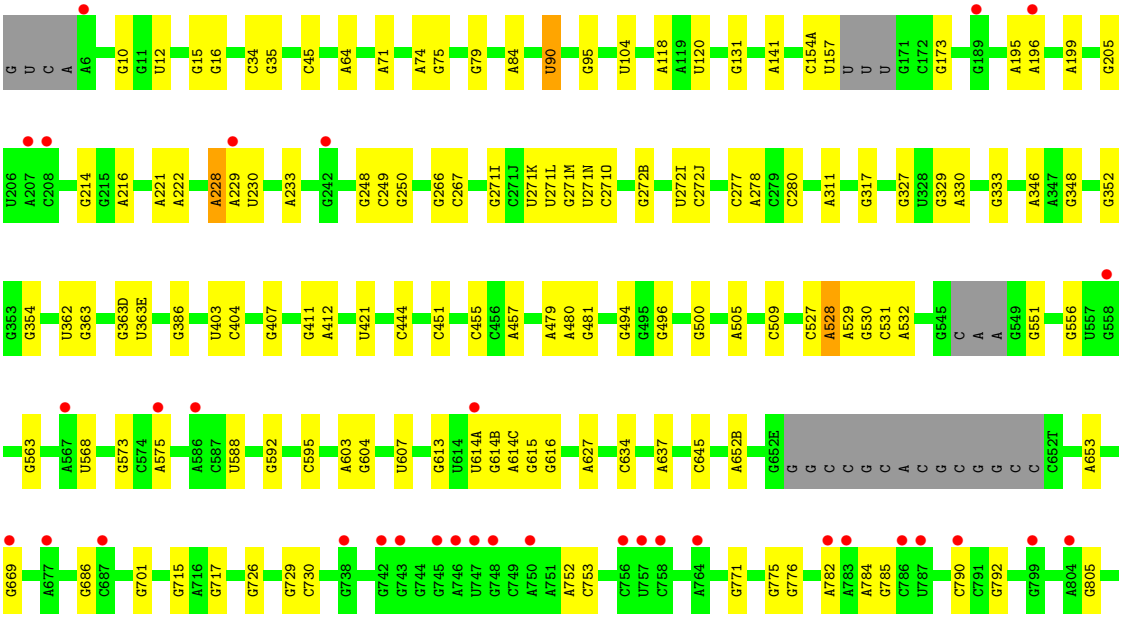
Chain 1A:

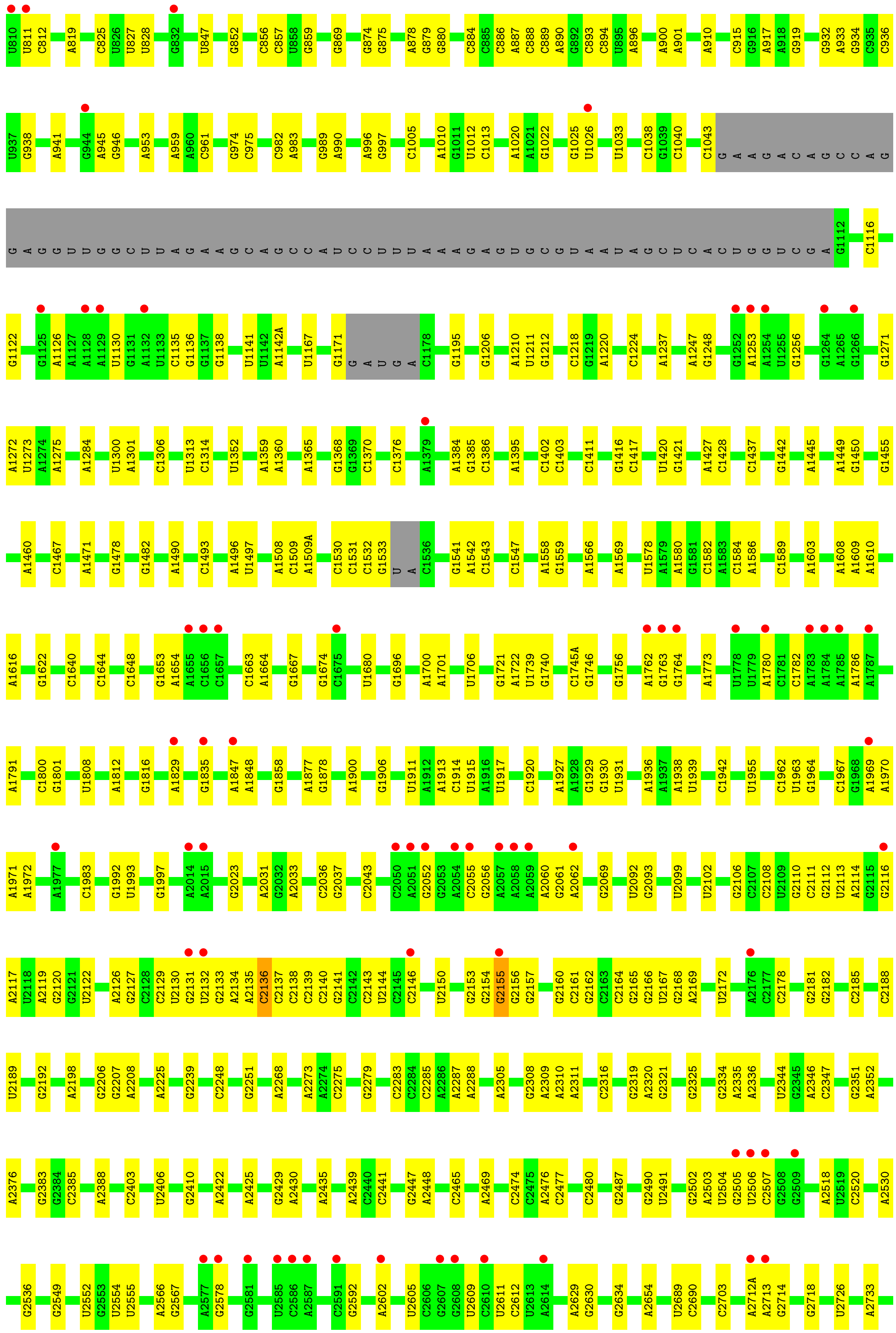




• Molecule 1: 23S Ribosomal RNA

Chain 2A:

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U937 G938 A941 G944 A945 G946 A953 A959 A960 C961 G974 C975 C982 A983 G989 A990 A996 G997 C1005 A1010 G1011 U1012 C1013 A1020 A1021 G1022 G1025 U1026 U1033 C1038 G1039 C1040 C1043 G A A G A C A G C C A G
G A G G U U G G C U U A G A A G C A G C C A U C C U U U A A A G A G U G C G U A A U A G C U C A C U G G U C G A G1112 C1116
G1122 G1125 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1137 G1138 U1141 U1142 A1142A U1167 G1171 G A U G A C1178 G1195 G1206 A1210 U1211 G1212 C1218 G1219 A1220 C1224 A1237 A1247 G1248 G1252 A1253 A1254 U1255 G1256 G1264 A1265 G1266 G1271
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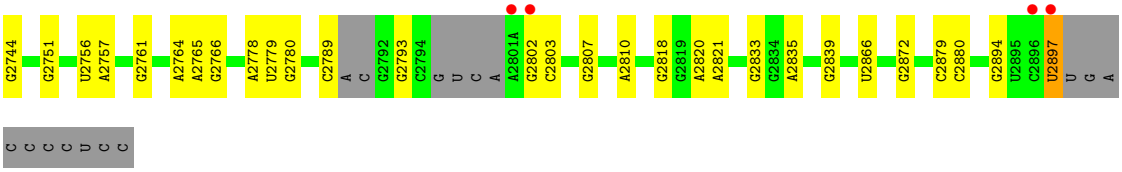
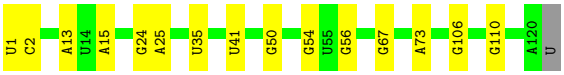
A1460 C1467 A1471 G1478 G1482 A1490 C1493 A1496 U1497 A1508 C1509 A1509A C1530 C1531 C1532 G1533 U A C1536 G1541 A1542 C1543 C1547 A1558 G1559 A1566 A1569 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 C1589 A1603 A1608 A1609 A1610
A1616 G1622 C1640 C1644 C1648 G1653 A1654 A1655 C1656 C1657 C1663 A1664 G1667 G1674 C1675 U1680 G1696 A1700 A1701 U1706 G1721 A1722 U1739 G1740 C1745A G1746 G1756 A1762 G1763 G1764 A1773 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787
A1791 C1800 G1801 U1808 A1812 G1816 A1829 G1835 A1847 A1848 G1858 A1877 G1878 A1900 G1906 U1911 A1912 A1913 C1914 U1915 A1916 U1917 C1920 A1927 A1928 G1929 G1930 U1931 A1936 A1937 A1938 U1939 C1942 U1955 C1962 U1963 G1964 C1967 G1968 A1969 A1970
A1971 A1972 A1977 C1983 G1992 U1993 G1997 A2014 A2015 G2023 A2031 G2032 A2033 C2036 G2037 C2043 C2050 A2051 G2052 G2053 A2054 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 G2069 U2092 G2093 U2099 U2102 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116
A2117 U2118 A2119 G2120 G2121 U2122 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 U2150 G2153 C2154 G2155 G2156 G2157 G2160 C2161 G2162 C2163 C2164 G2165 C2166 U2167 G2168 A2169 U2172 A2176 C2177 C2178 G2181 G2182 C2185 C2188
U2189 G2192 A2198 G2206 G2207 A2208 A2225 G2239 C2248 G2251 A2268 A2273 A2274 C2275 G2279 C2283 C2284 C2285 A2286 A2287 A2288 A2305 G2308 A2309 A2310 A2311 C2316 G2319 A2320 G2321 G2325 G2334 A2335 A2336 U2344 G2345 A2346 C2347 G2351 A2352
A2376 G2383 G2384 C2385 A2388 C2403 U2406 G2410 A2422 A2425 G2429 A2430 A2435 A2439 C2440 C2441 G2447 A2448 C2465 A2469 C2474 C2475 A2476 C2477 C2480 G2487 G2490 U2491 G2502 A2503 U2504 G2505 U2506 C2507 G2508 G2509 A2518 U2519 C2520 A2530
G2536 G2549 U2552 G2553 U2554 U2555 A2566 G2567 A2577 G2578 G2581 U2585 C2586 A2587 C2591 G2592 A2602 U2605 C2606 G2607 G2608 U2609 C2610 U2611 C2612 U2613 A2614 A2629 G2630 G2634 A2654 U2689 C2690 C2703 A2712A A2713 G2714 G2718 U2726 A2733



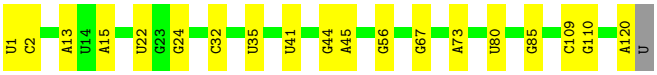
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



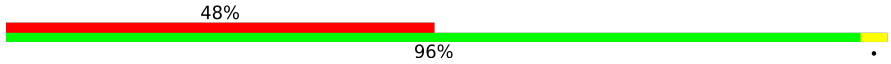
• Molecule 2: 5S Ribosomal RNA

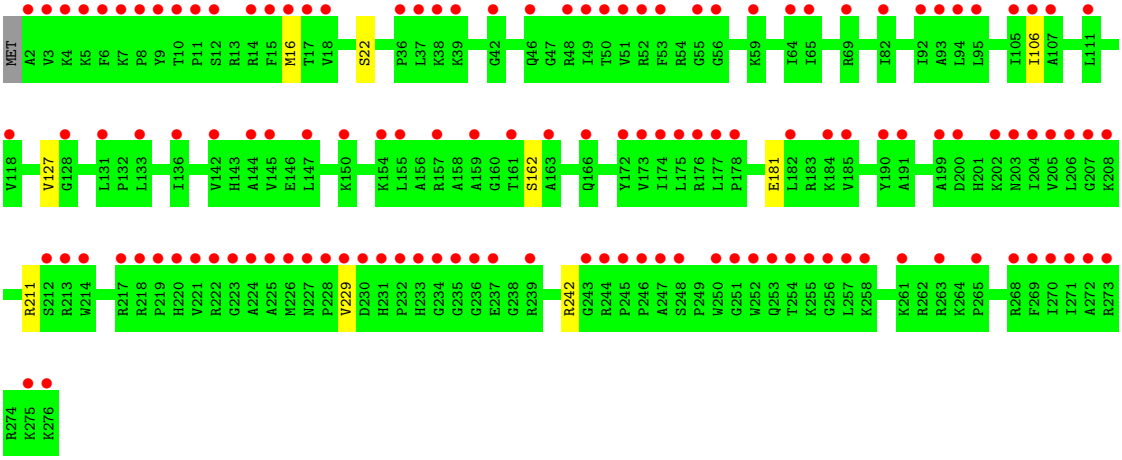
Chain 2B:



• Molecule 3: 50S ribosomal protein L2

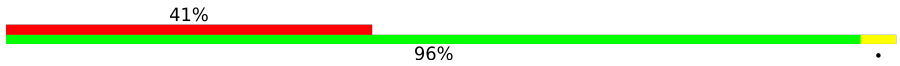
Chain 1D:

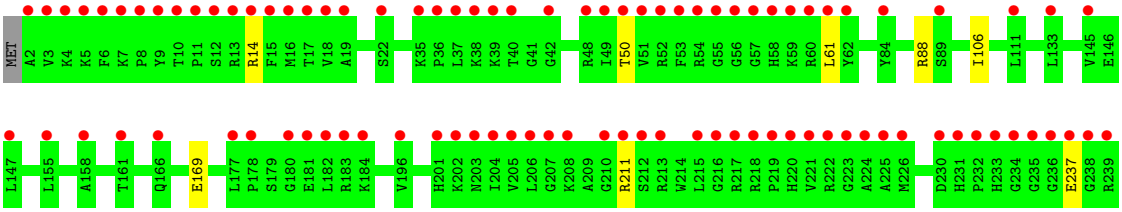


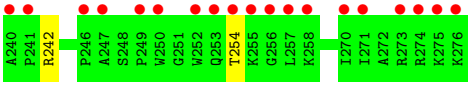


• Molecule 3: 50S ribosomal protein L2

Chain 2D:

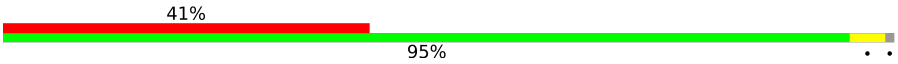


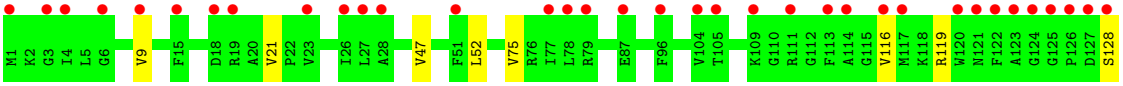


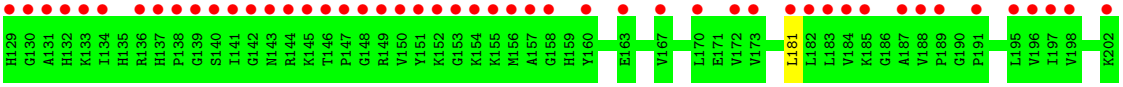


• Molecule 4: 50S ribosomal protein L3

Chain 1E:

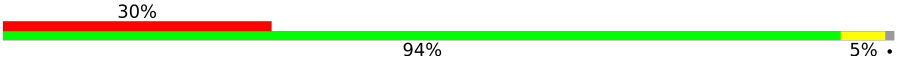


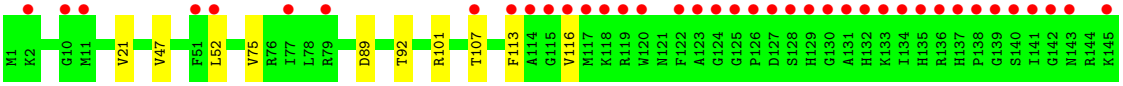


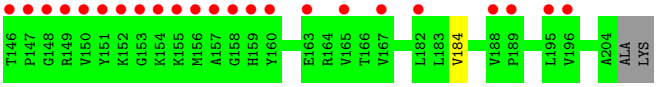


• Molecule 4: 50S ribosomal protein L3

Chain 2E:

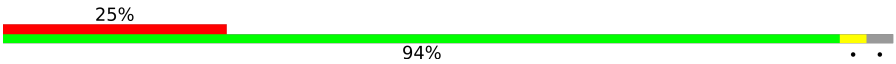


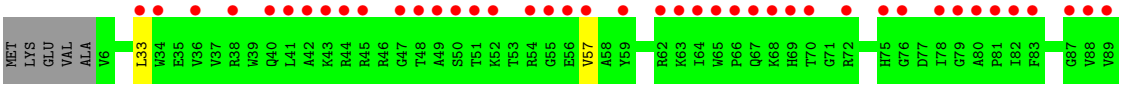


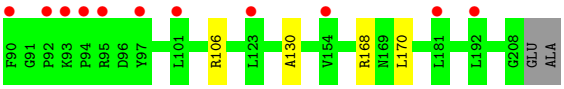


• Molecule 5: 50S ribosomal protein L4

Chain 1F:

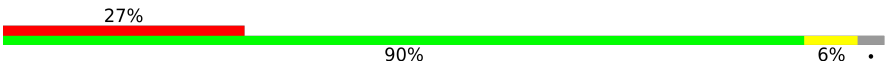


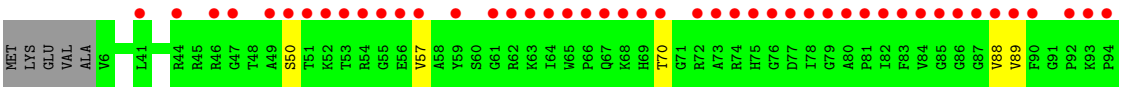


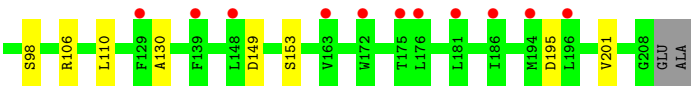


• Molecule 5: 50S ribosomal protein L4

Chain 2F:

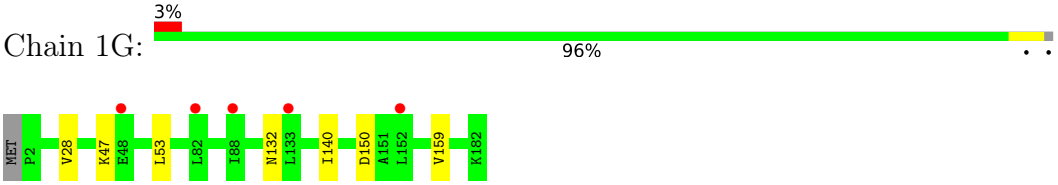






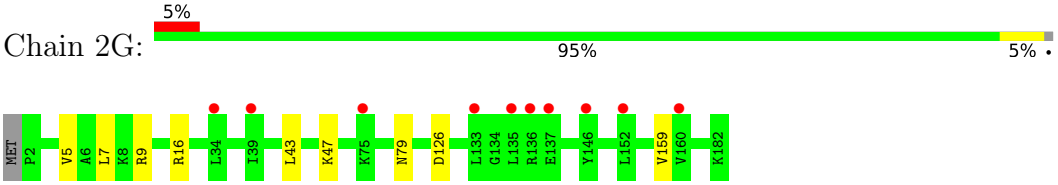
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



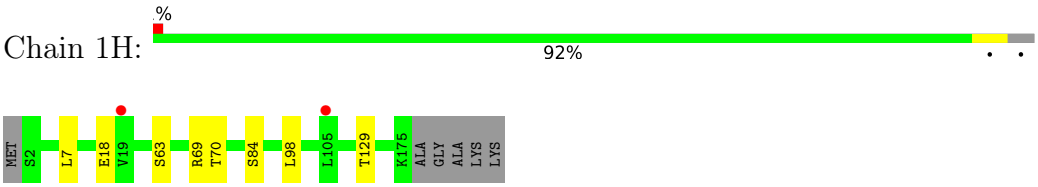
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



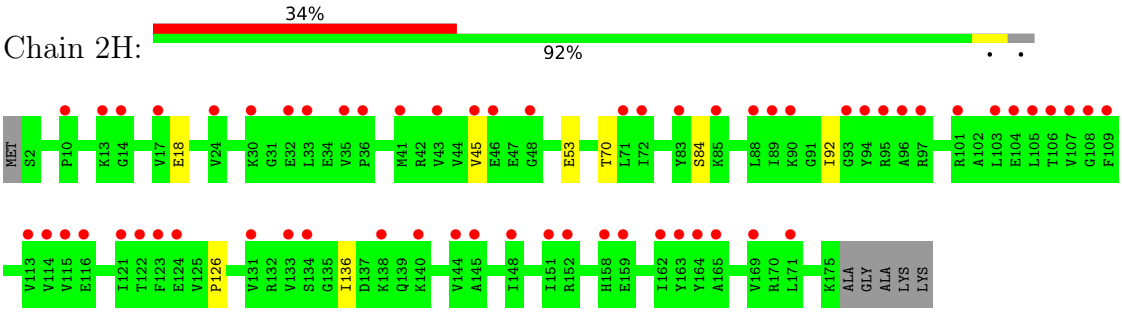
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



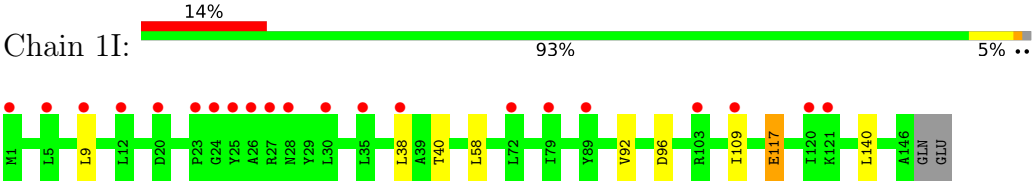
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



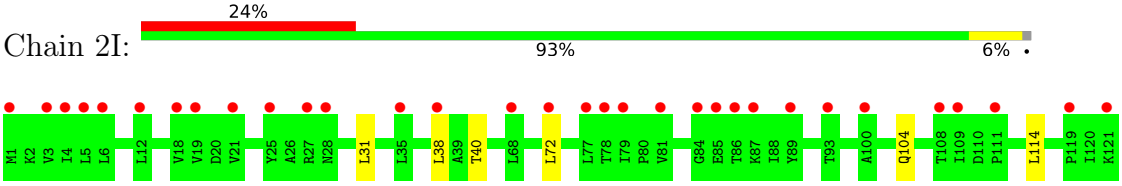
• Molecule 8: 50S ribosomal protein L9

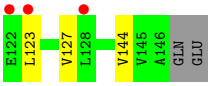
Chain 1I:



• Molecule 8: 50S ribosomal protein L9

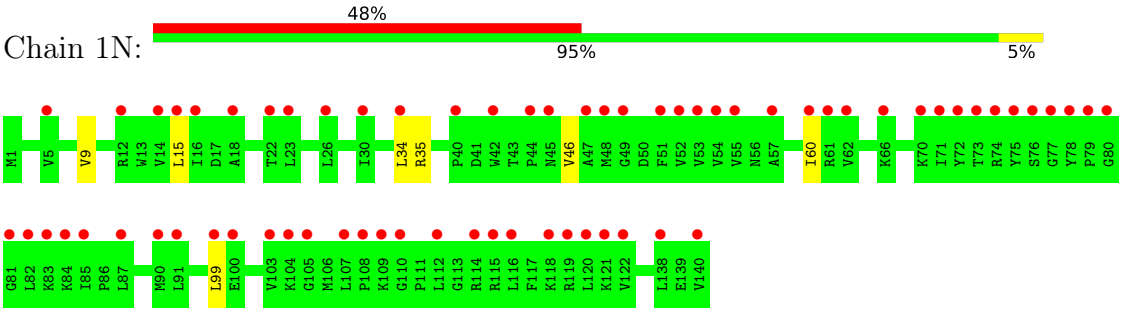
Chain 2I:





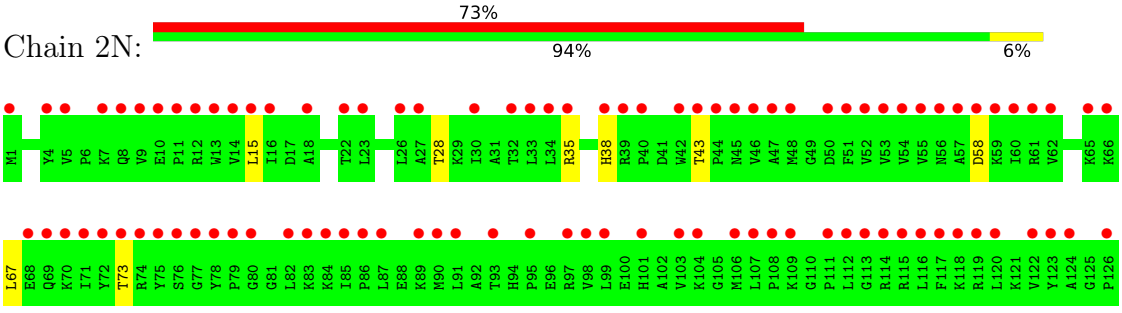
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



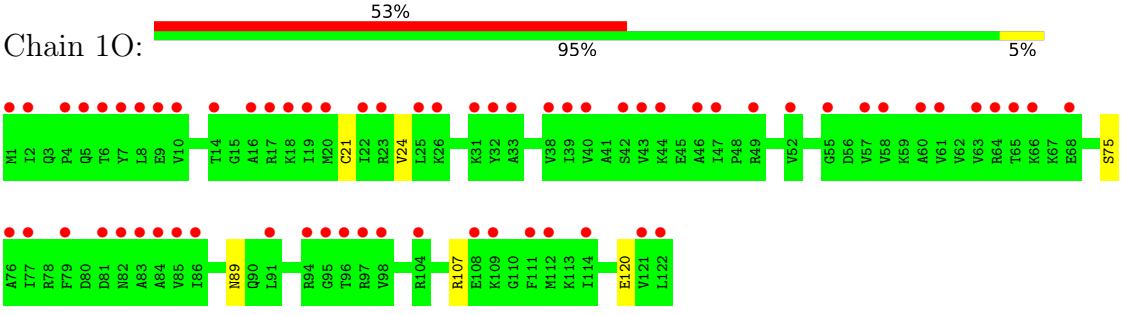
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



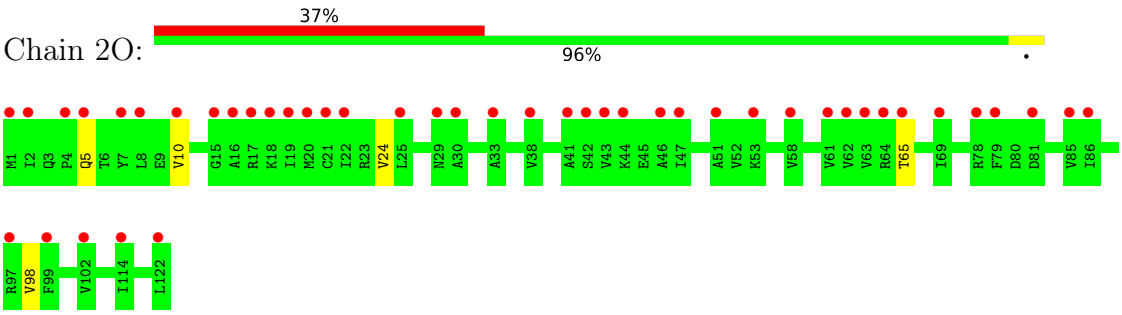
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



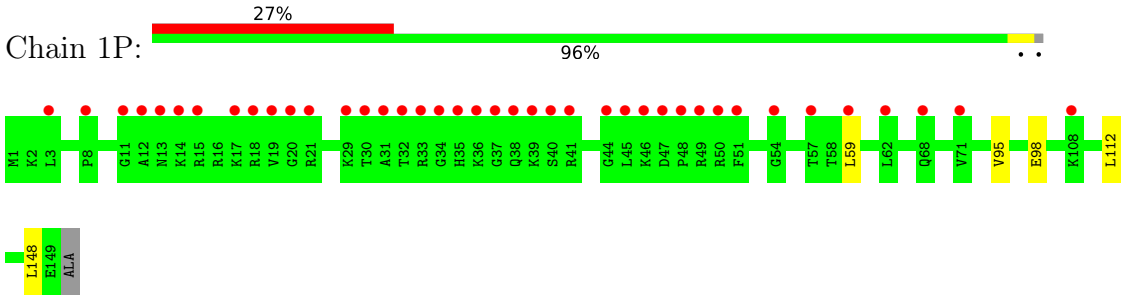
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



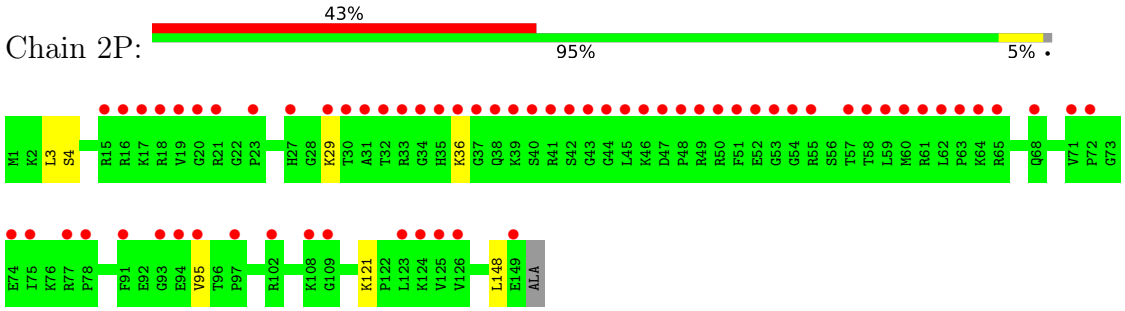
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



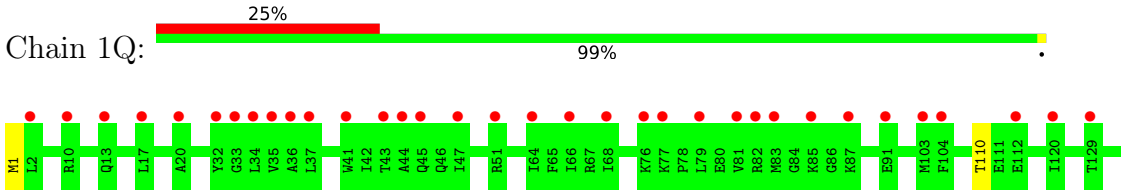
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



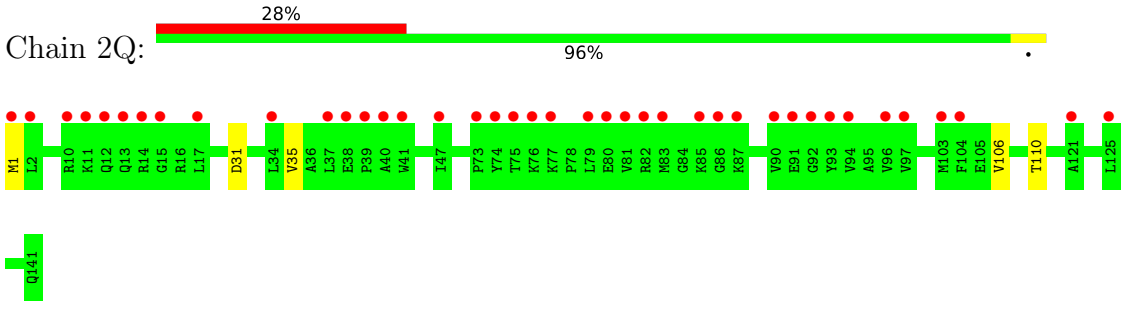
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



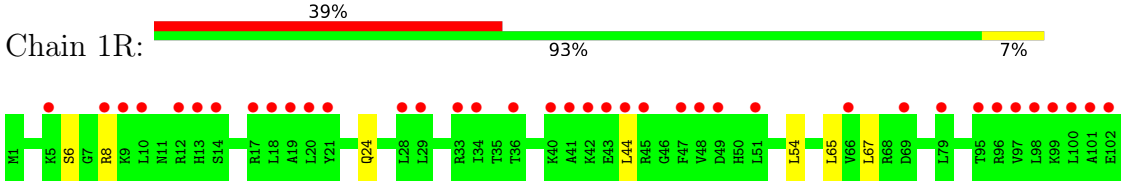
• Molecule 12: 50S ribosomal protein L16

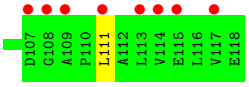
Chain 2Q:



• Molecule 13: 50S ribosomal protein L17

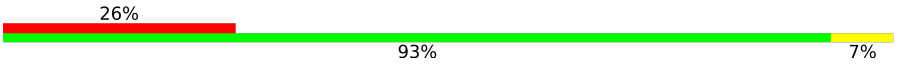
Chain 1R:

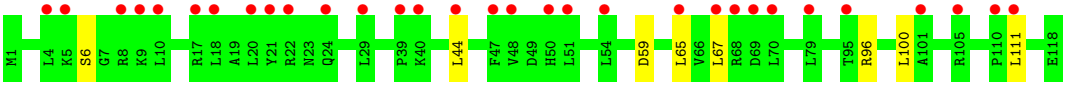




• Molecule 13: 50S ribosomal protein L17

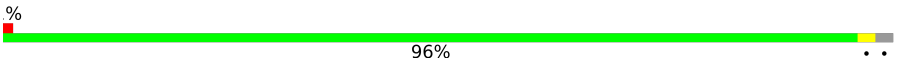
Chain 2R:





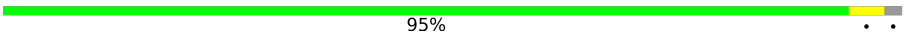
• Molecule 14: 50S ribosomal protein L18

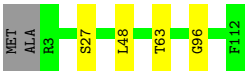
Chain 1S:



• Molecule 14: 50S ribosomal protein L18

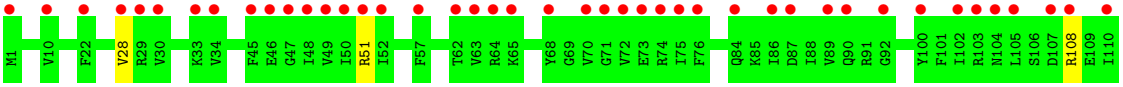
Chain 2S:

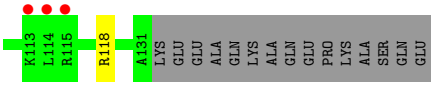




• Molecule 15: 50S ribosomal protein L19

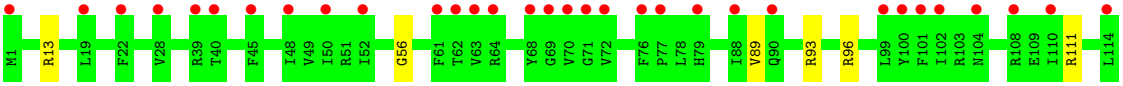
Chain 1T:

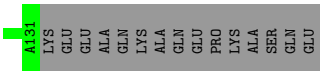




• Molecule 15: 50S ribosomal protein L19

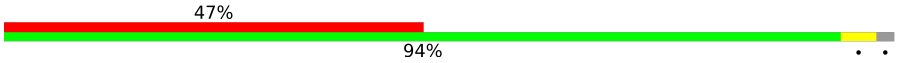
Chain 2T:

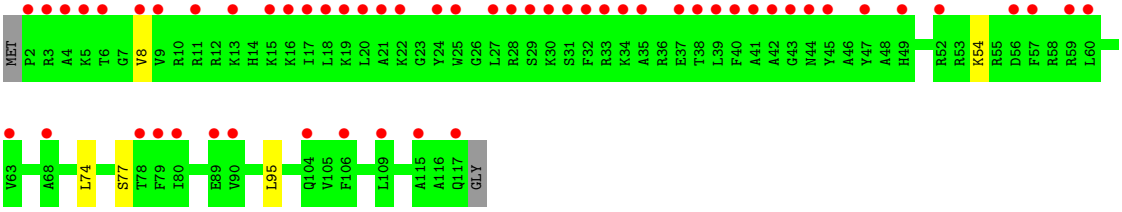




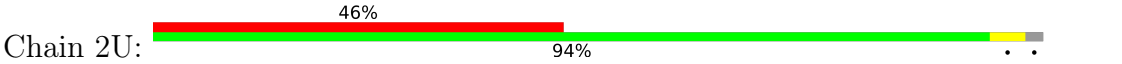
• Molecule 16: 50S ribosomal protein L20

Chain 1U:

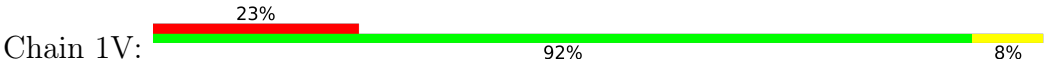


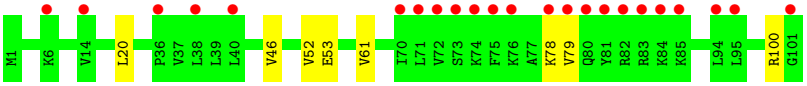


• Molecule 16: 50S ribosomal protein L20

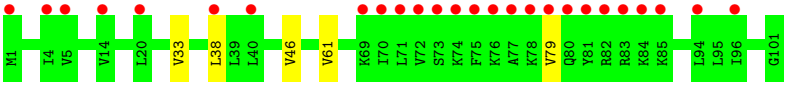


• Molecule 17: 50S ribosomal protein L21

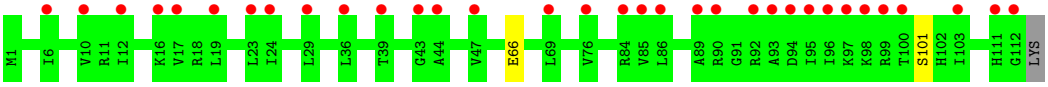




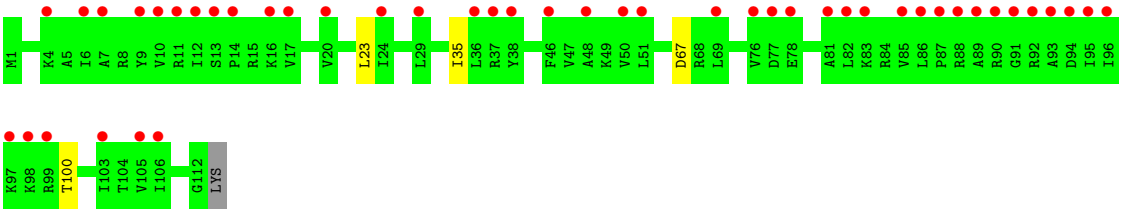
• Molecule 17: 50S ribosomal protein L21



• Molecule 18: 50S ribosomal protein L22

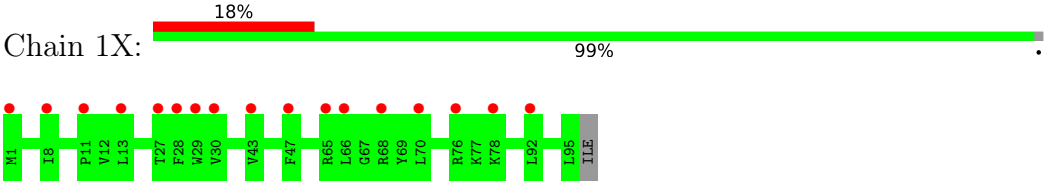


• Molecule 18: 50S ribosomal protein L22



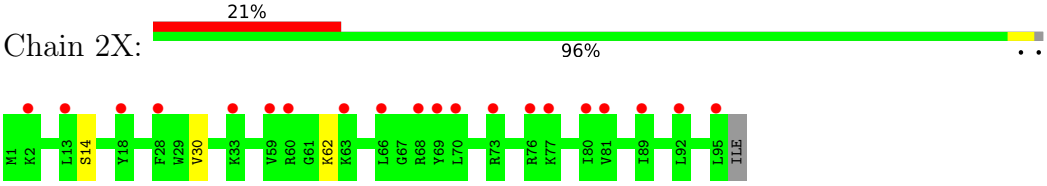
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



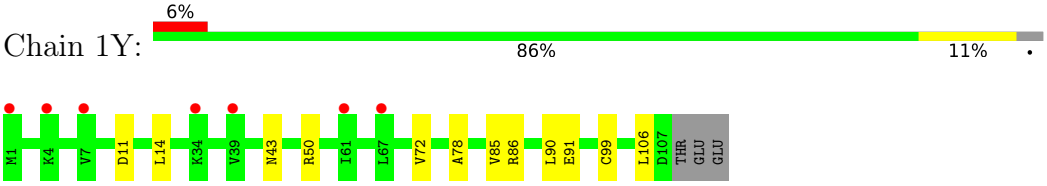
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



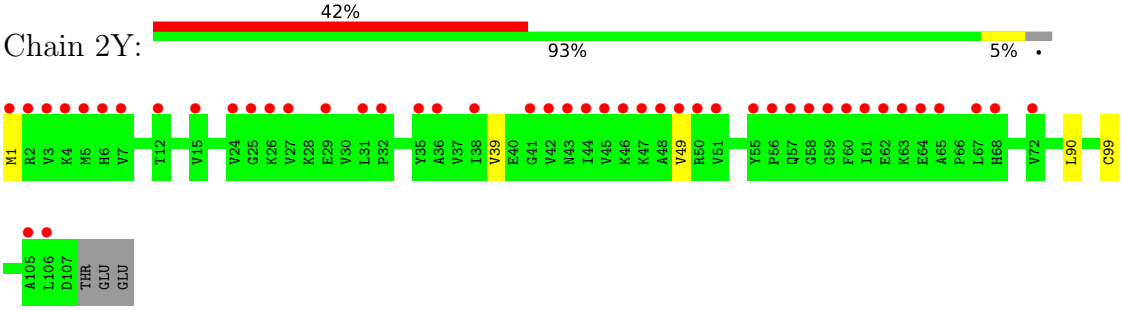
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



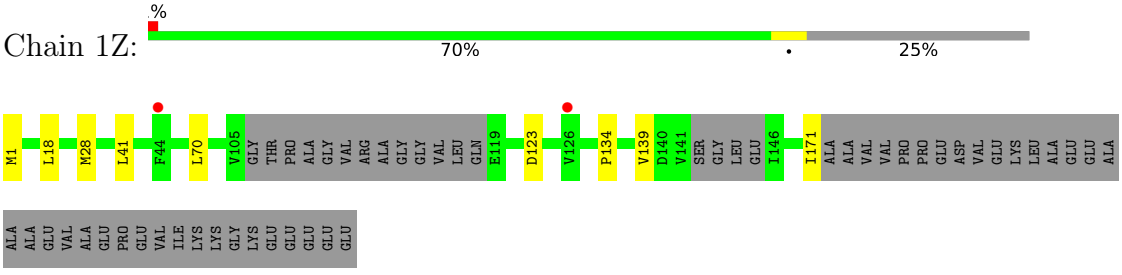
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



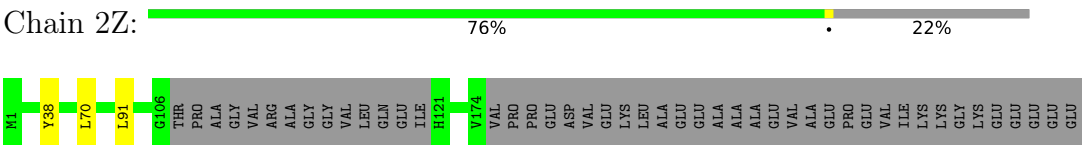
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



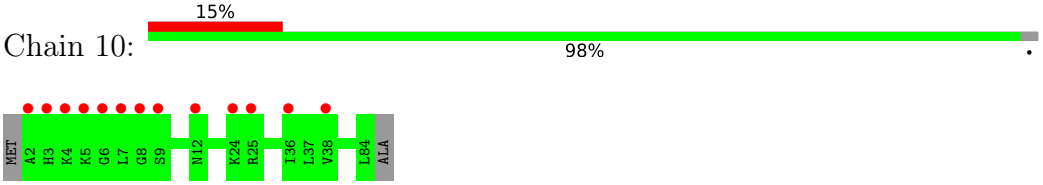
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



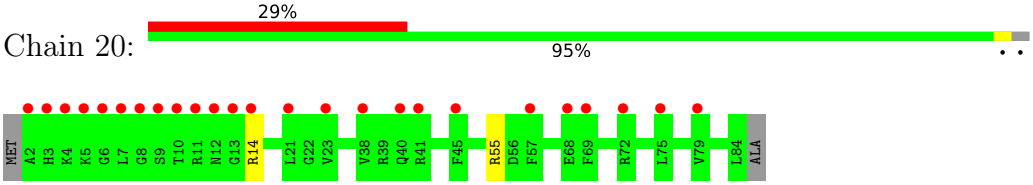
• Molecule 22: 50S ribosomal protein L27

Chain 10:



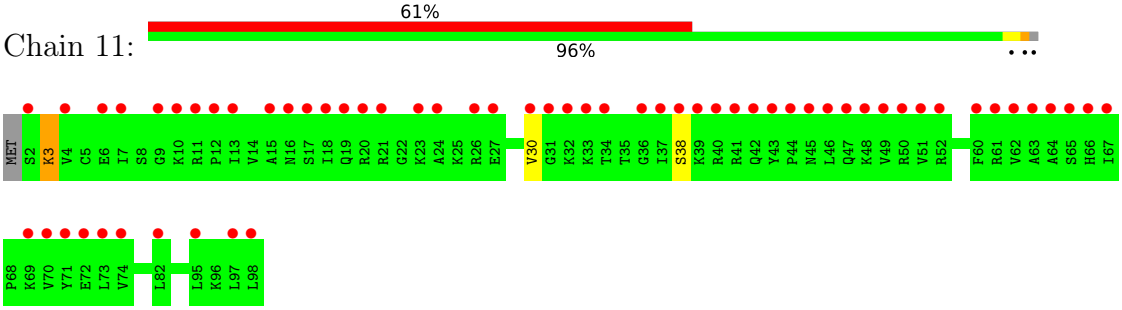
• Molecule 22: 50S ribosomal protein L27

Chain 20:



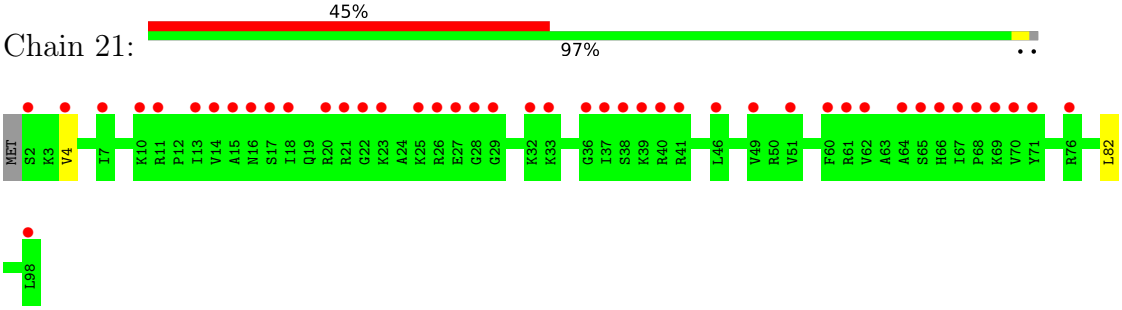
• Molecule 23: 50S ribosomal protein L28

Chain 11:



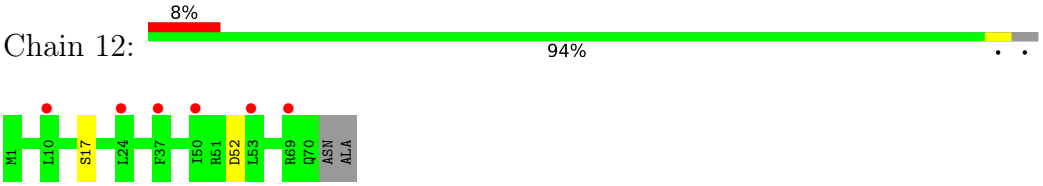
• Molecule 23: 50S ribosomal protein L28

Chain 21:



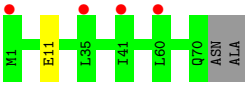
• Molecule 24: 50S ribosomal protein L29

Chain 12:



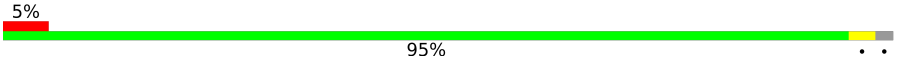
• Molecule 24: 50S ribosomal protein L29

Chain 22:



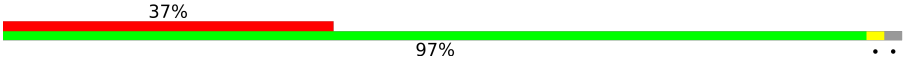
• Molecule 25: 50S ribosomal protein L30

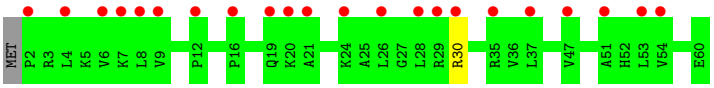
Chain 13:



• Molecule 25: 50S ribosomal protein L30

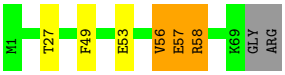
Chain 23:





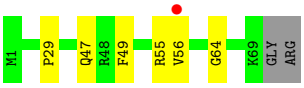
• Molecule 26: 50S ribosomal protein L31

Chain 14:



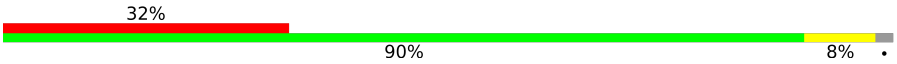
• Molecule 26: 50S ribosomal protein L31

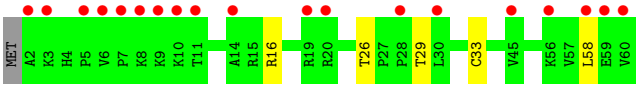
Chain 24:



• Molecule 27: 50S ribosomal protein L32

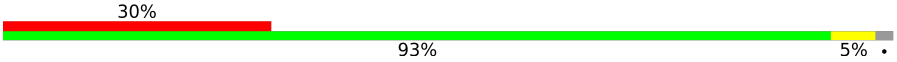
Chain 15:

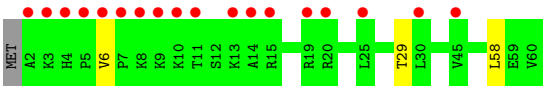




• Molecule 27: 50S ribosomal protein L32

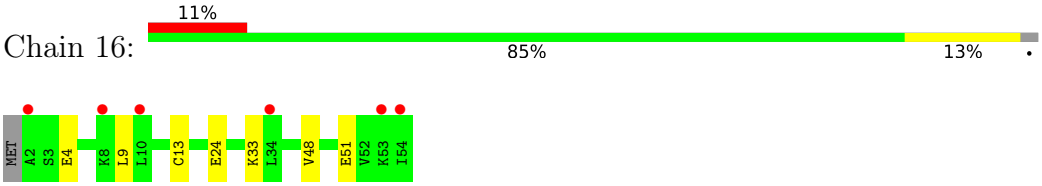
Chain 25:





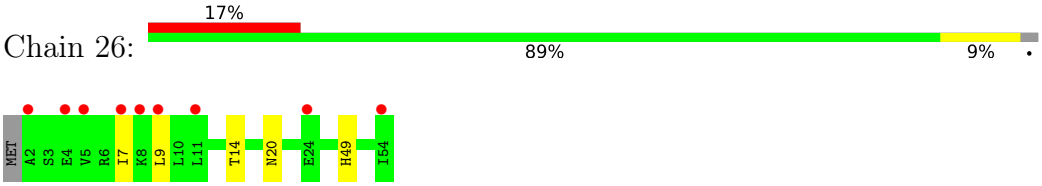
• Molecule 28: 50S ribosomal protein L33

Chain 16:



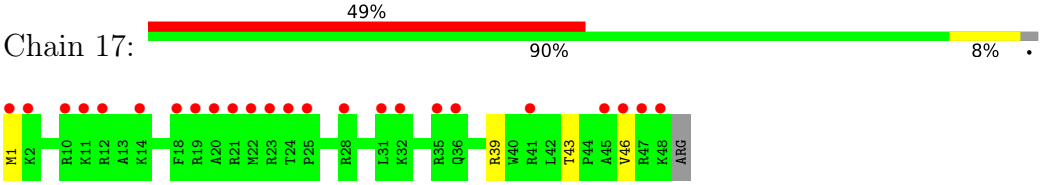
• Molecule 28: 50S ribosomal protein L33

Chain 26:



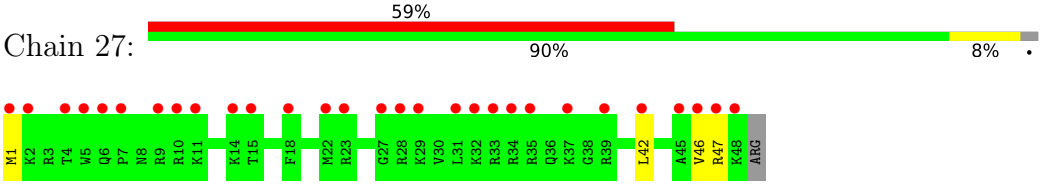
• Molecule 29: 50S ribosomal protein L34

Chain 17:



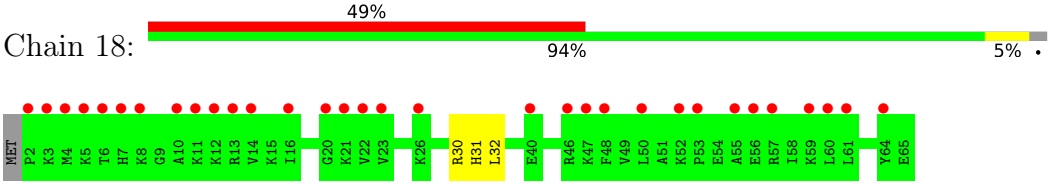
• Molecule 29: 50S ribosomal protein L34

Chain 27:



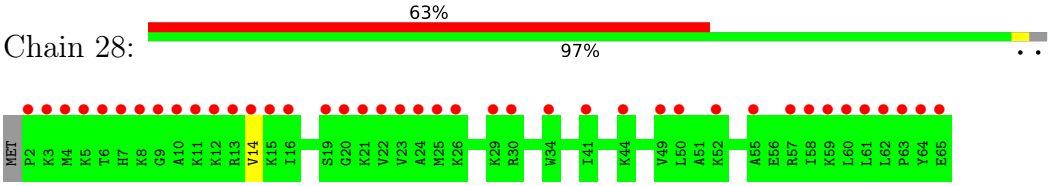
• Molecule 30: 50S ribosomal protein L35

Chain 18:



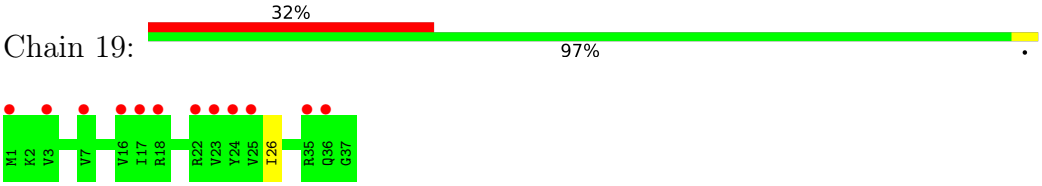
• Molecule 30: 50S ribosomal protein L35

Chain 28:



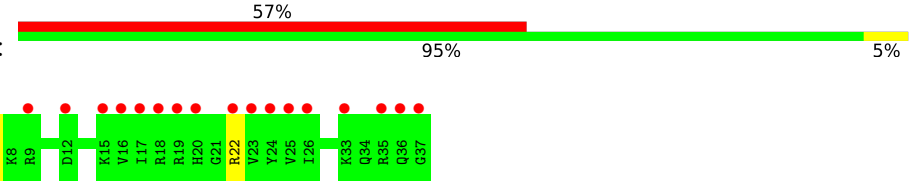
• Molecule 31: 50S ribosomal protein L36

Chain 19:



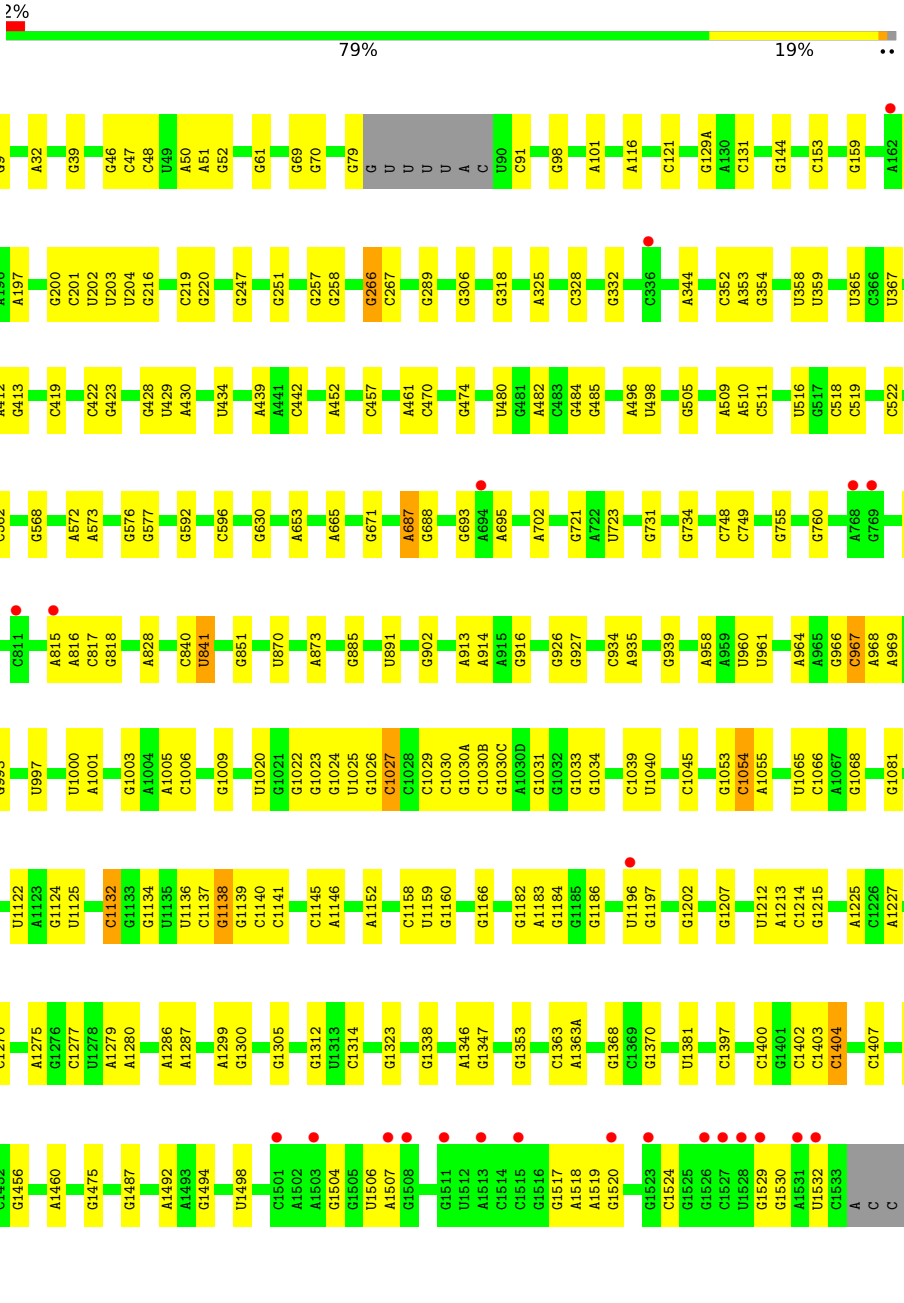
• Molecule 31: 50S ribosomal protein L36

Chain 29:



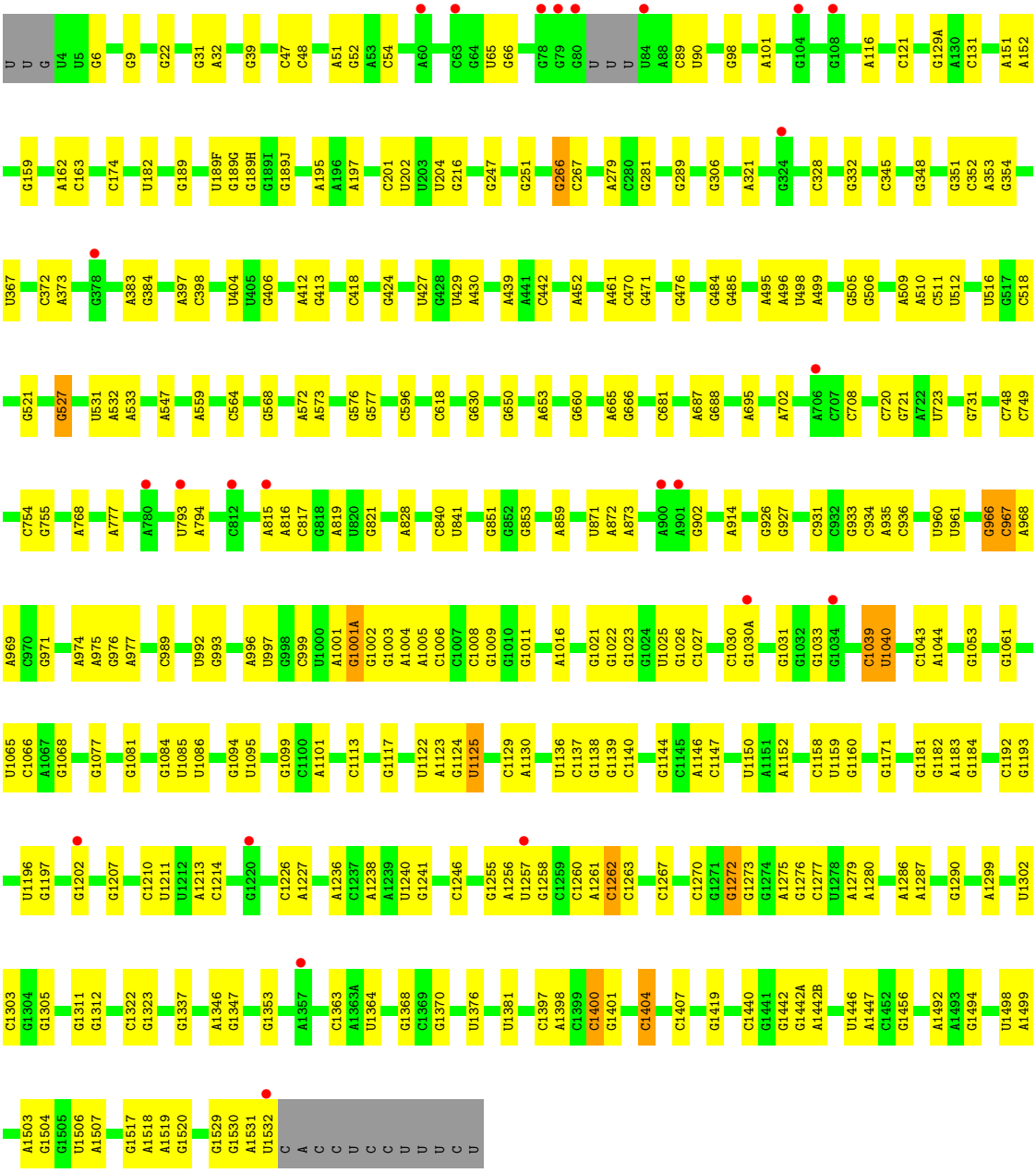
• Molecule 32: 16S Ribosomal RNA

Chain 1a:



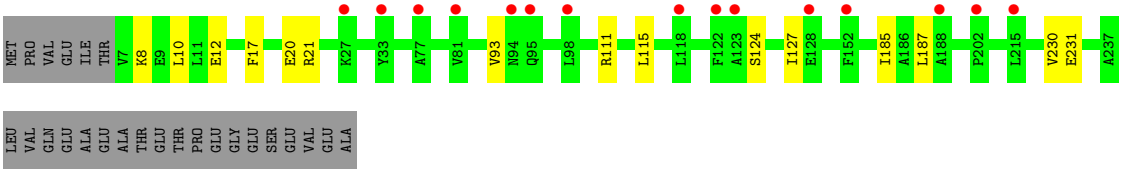
• Molecule 32: 16S Ribosomal RNA

Chain 2a:



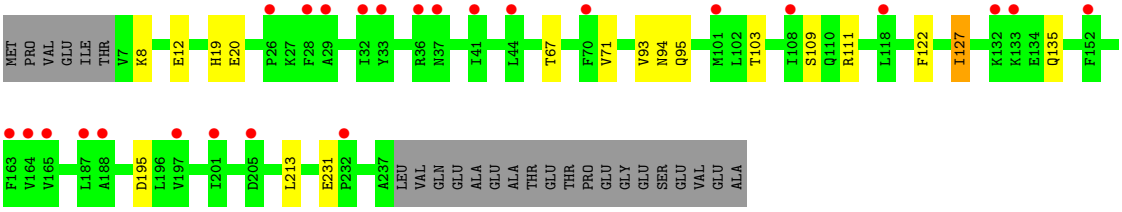
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



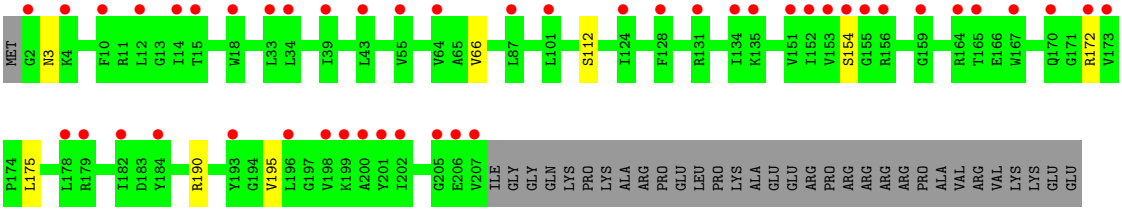
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



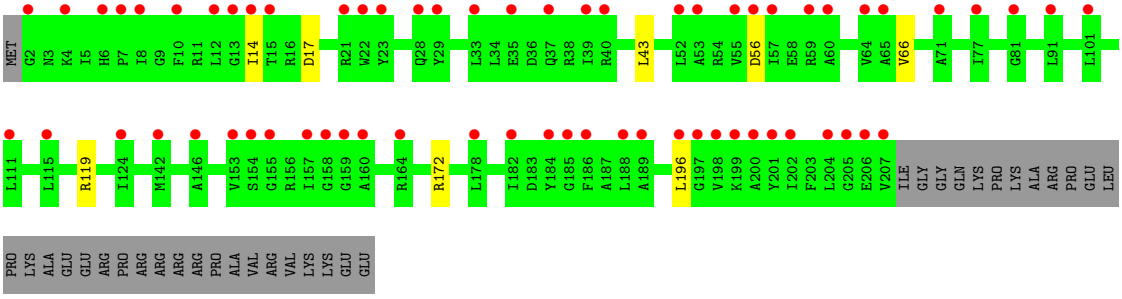
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



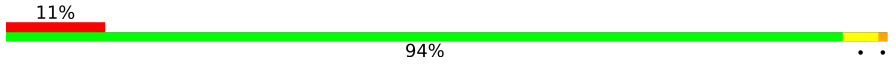
• Molecule 34: 30S ribosomal protein S3

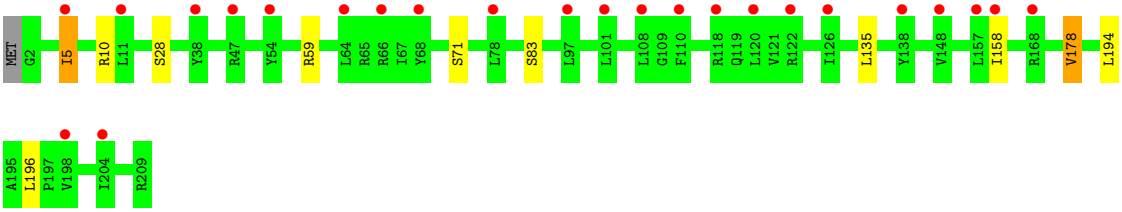
Chain 2c:



• Molecule 35: 30S ribosomal protein S4

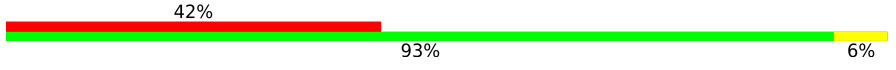
Chain 1d:

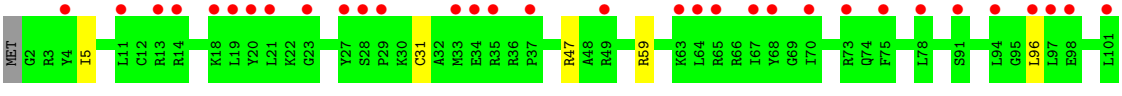


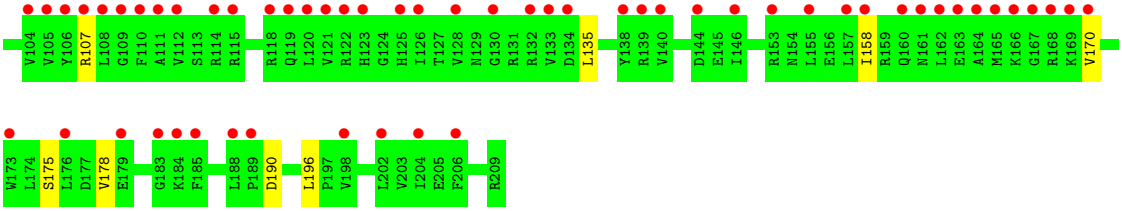


• Molecule 35: 30S ribosomal protein S4

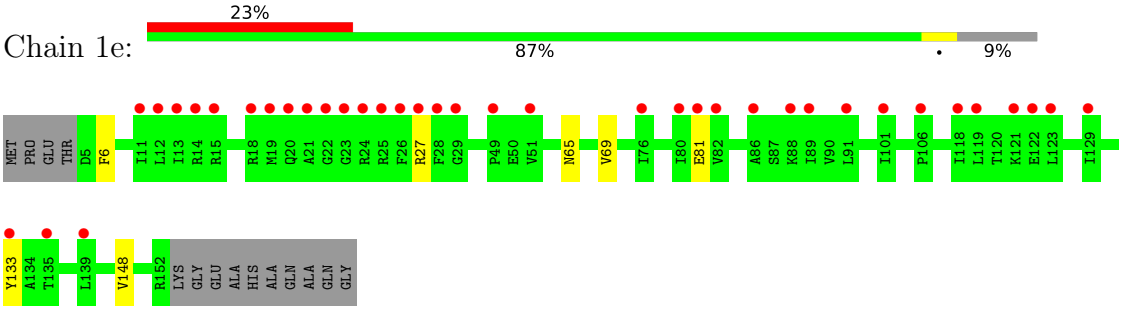
Chain 2d:



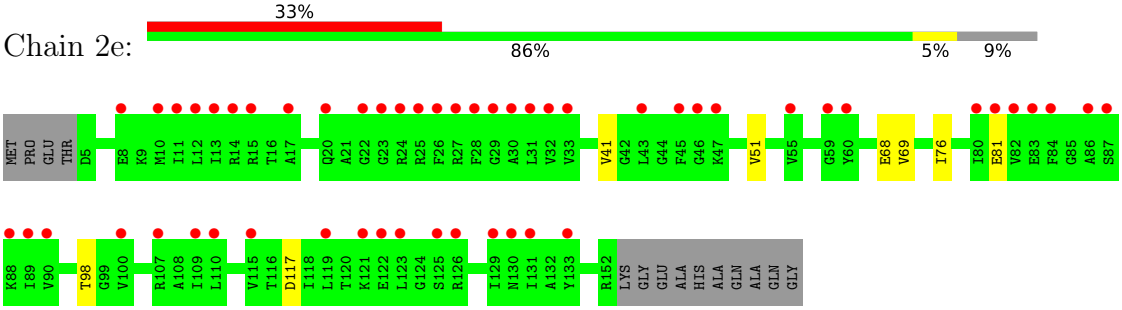




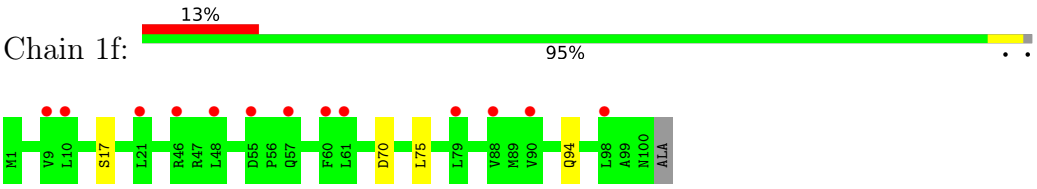
• Molecule 36: 30S ribosomal protein S5



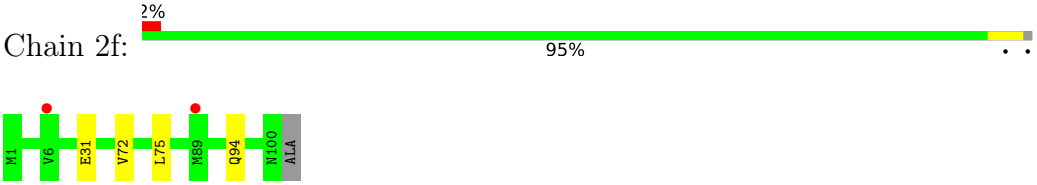
• Molecule 36: 30S ribosomal protein S5



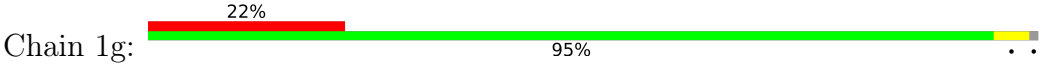
• Molecule 37: 30S ribosomal protein S6

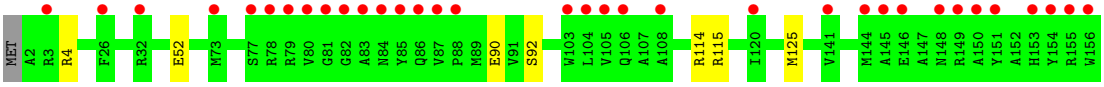


• Molecule 37: 30S ribosomal protein S6

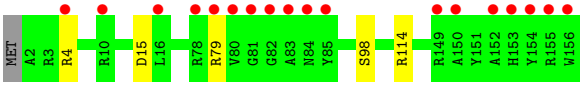


• Molecule 38: 30S ribosomal protein S7

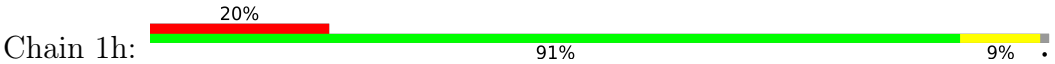


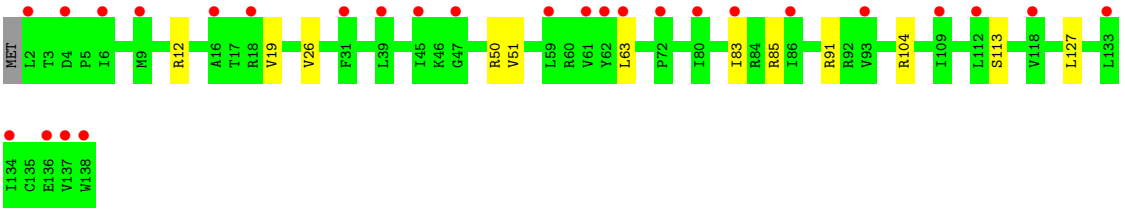


• Molecule 38: 30S ribosomal protein S7

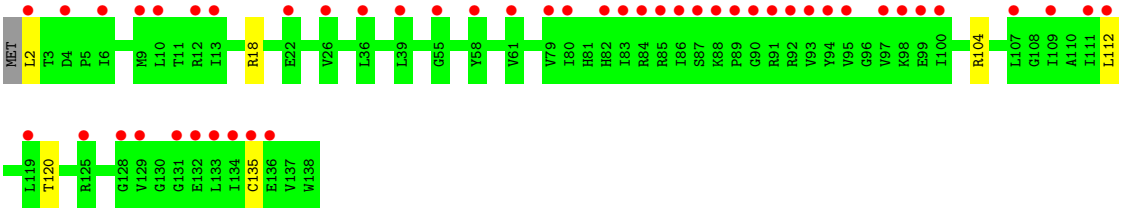


• Molecule 39: 30S ribosomal protein S8

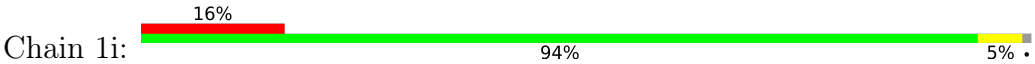


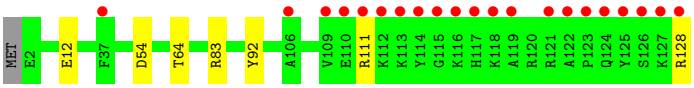


• Molecule 39: 30S ribosomal protein S8

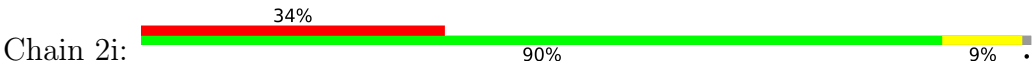


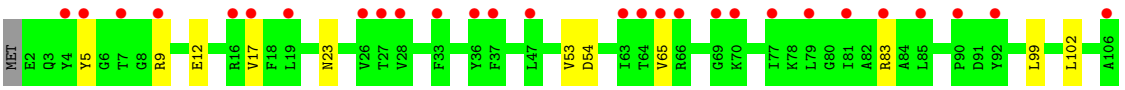
• Molecule 40: 30S ribosomal protein S9

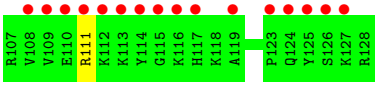




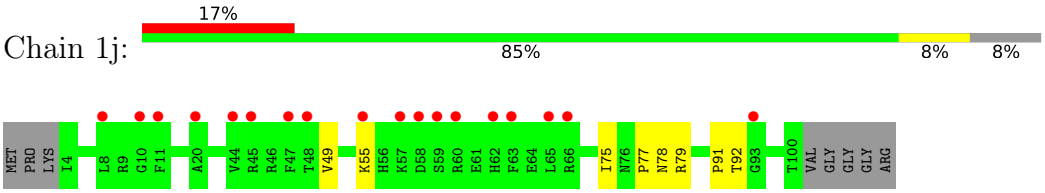
• Molecule 40: 30S ribosomal protein S9



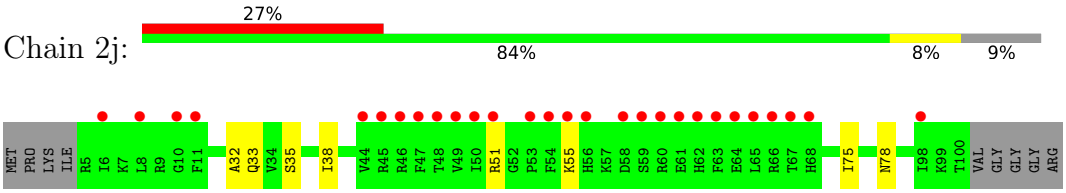




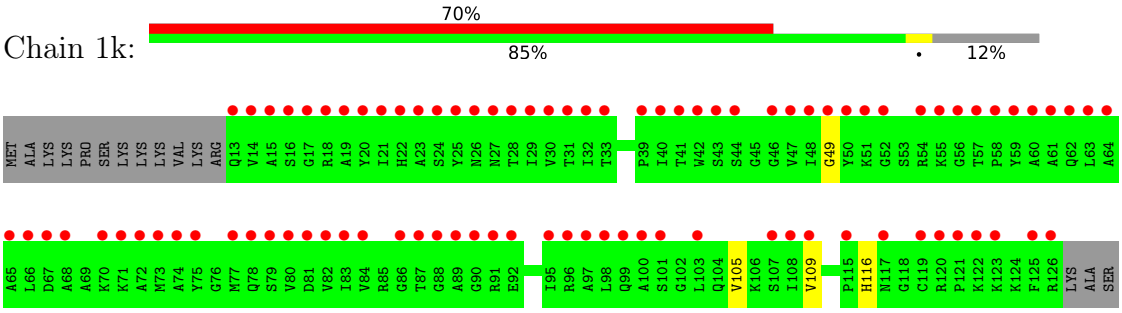
• Molecule 41: 30S ribosomal protein S10



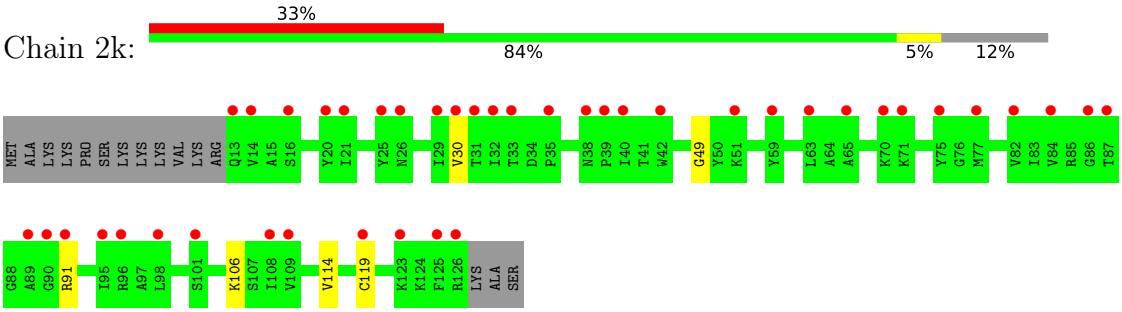
• Molecule 41: 30S ribosomal protein S10



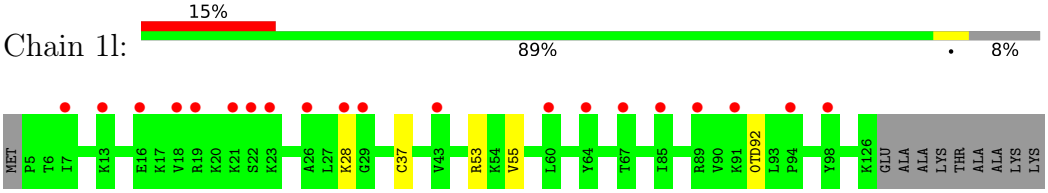
• Molecule 42: 30S ribosomal protein S11



• Molecule 42: 30S ribosomal protein S11

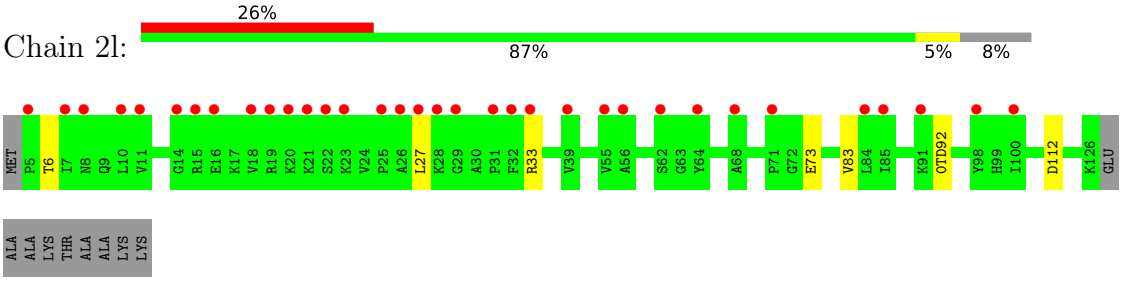


• Molecule 43: 30S ribosomal protein S12



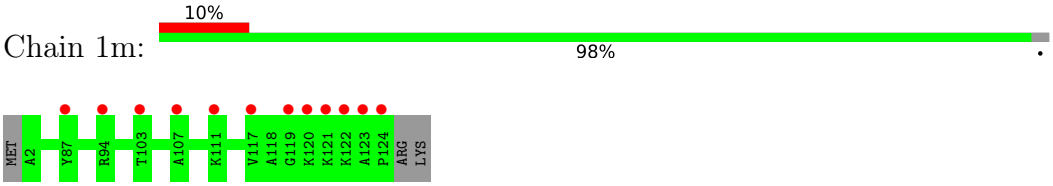
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



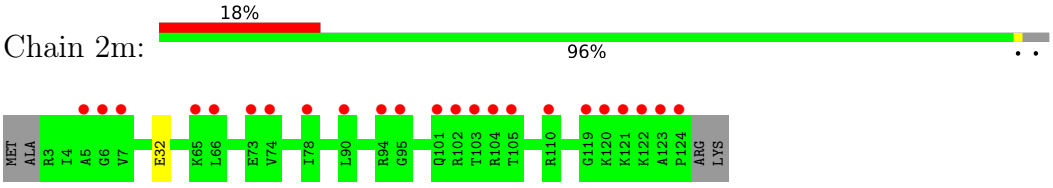
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



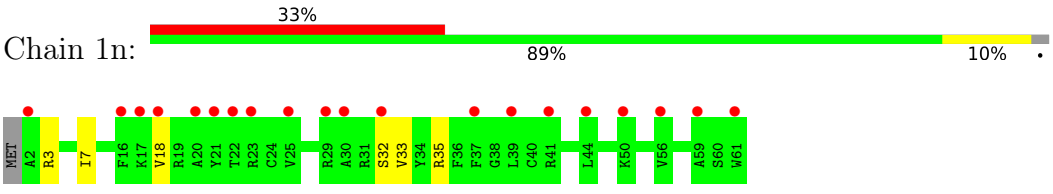
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



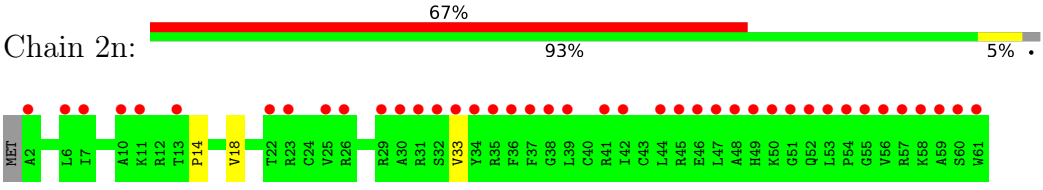
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



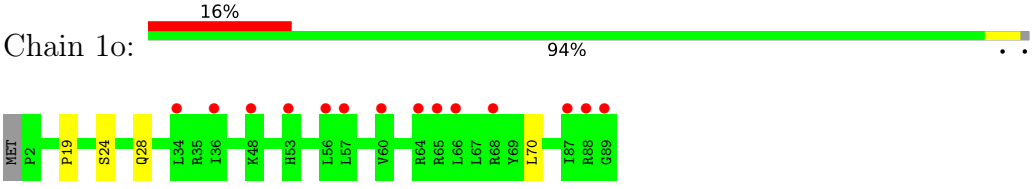
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



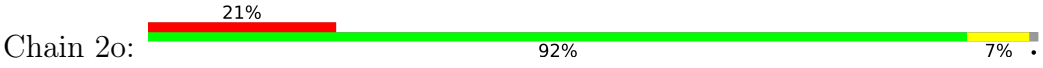
• Molecule 46: 30S ribosomal protein S15

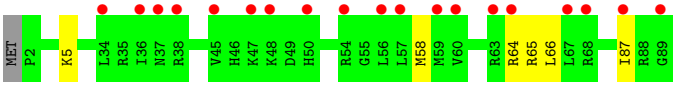
Chain 1o:



• Molecule 46: 30S ribosomal protein S15

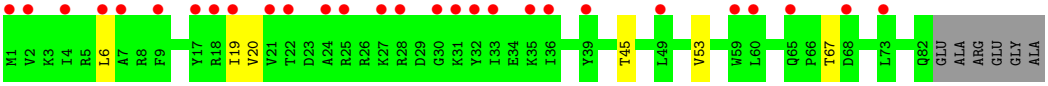
Chain 2o:





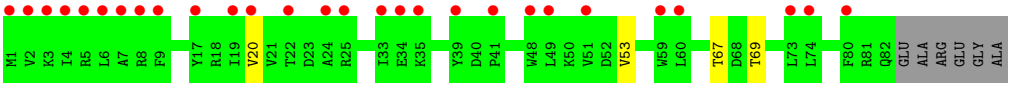
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



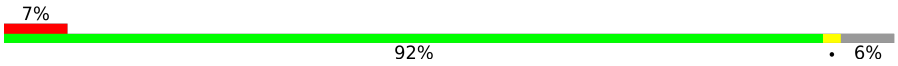
• Molecule 47: 30S ribosomal protein S16

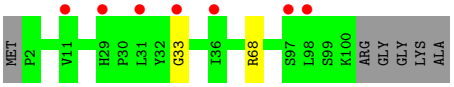
Chain 2p:



• Molecule 48: 30S ribosomal protein S17

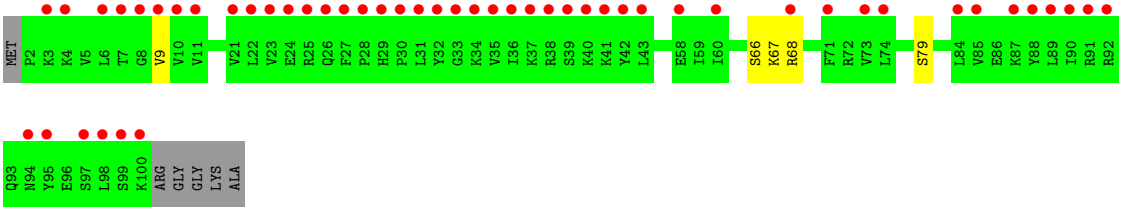
Chain 1q:





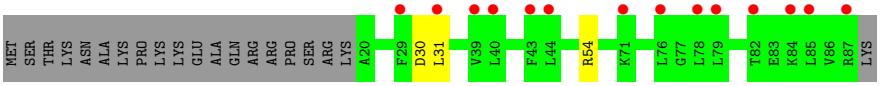
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



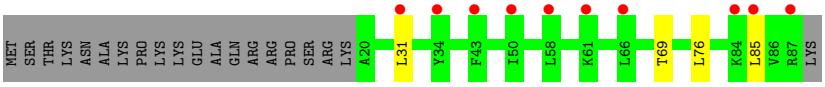
• Molecule 49: 30S ribosomal protein S18

Chain 1r:

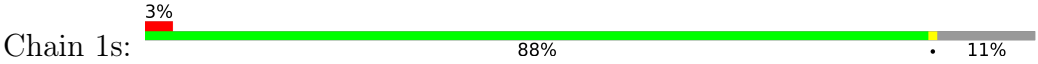


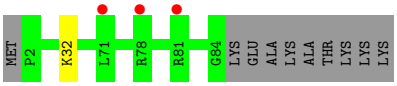
• Molecule 49: 30S ribosomal protein S18

Chain 2r:

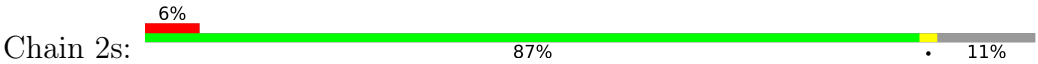


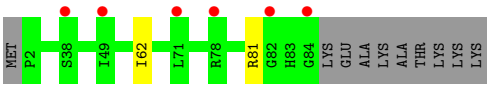
• Molecule 50: 30S ribosomal protein S19



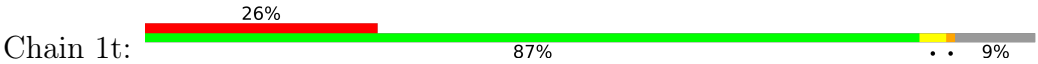


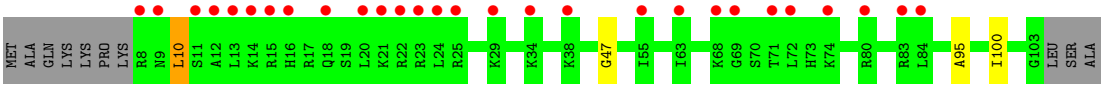
• Molecule 50: 30S ribosomal protein S19



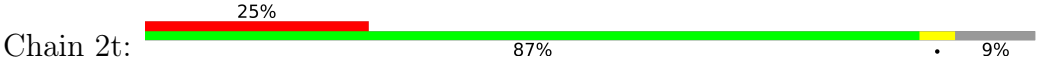


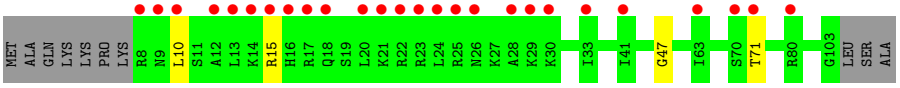
• Molecule 51: 30S ribosomal protein S20



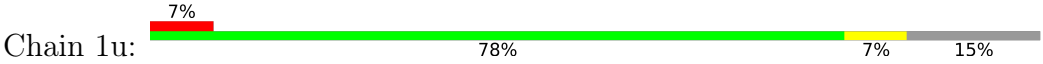


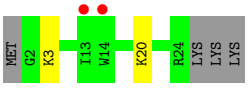
• Molecule 51: 30S ribosomal protein S20



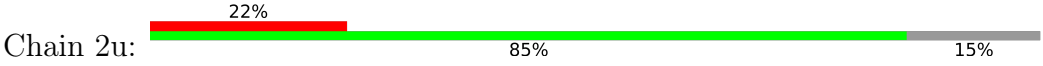


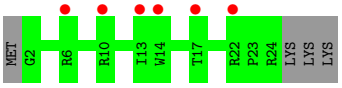
• Molecule 52: 30S ribosomal protein Thx





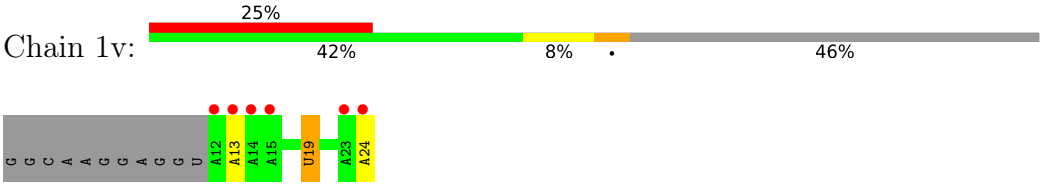
• Molecule 52: 30S ribosomal protein Thx





• Molecule 53: mRNA

Chain 1v:

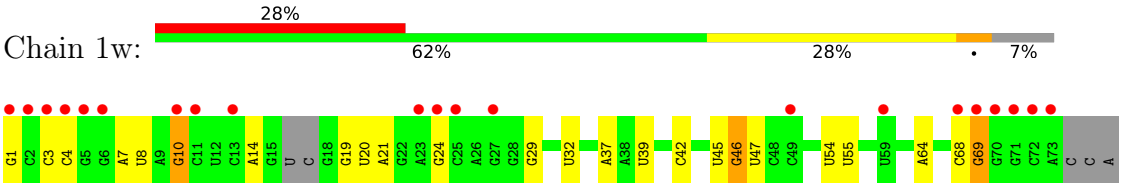


• Molecule 53: mRNA

Chain 2v:

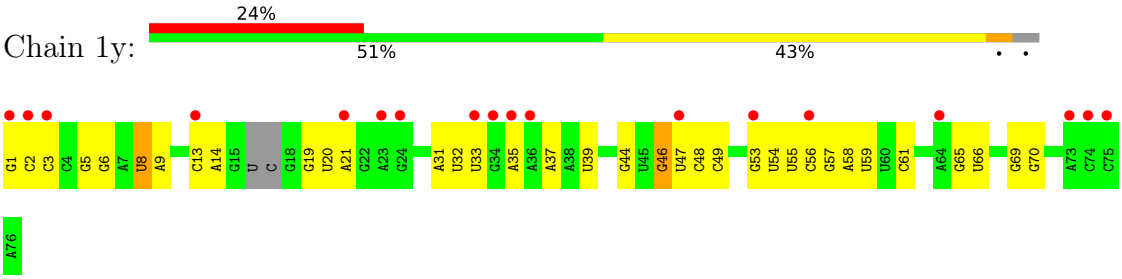
• Molecule 54: A-site and E-site tRNAs

Chain 1w:



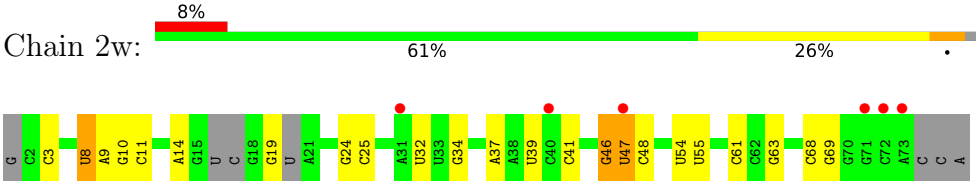
• Molecule 54: A-site and E-site tRNAs

Chain 1y:



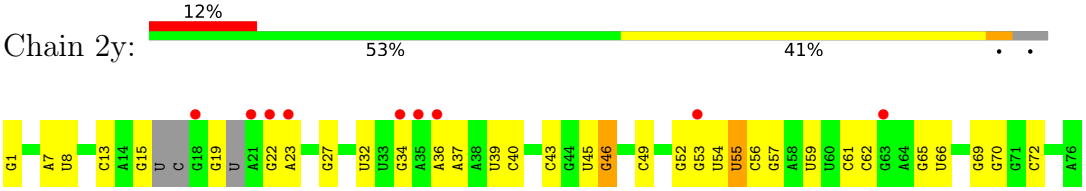
• Molecule 54: A-site and E-site tRNAs

Chain 2w:



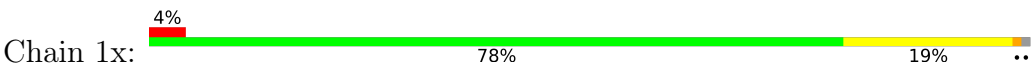
• Molecule 54: A-site and E-site tRNAs

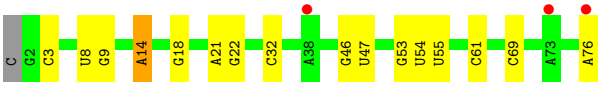
Chain 2y:



• Molecule 55: P-site tRNA

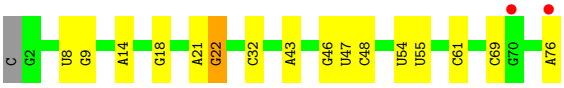
Chain 1x:





• Molecule 55: P-site tRNA

Chain 2x:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.73Å 445.10Å 613.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	360.30 – 2.95 360.30 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (360.30-2.95) 99.7 (360.30-2.95)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.238 , 0.292 0.238 , 0.292	Depositor DCC
R_{free} test set	59210 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	104.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	295398	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: OMG, 2MU, SF4, 2MA, 4SU, 7MG, M2G, 0TD, MIA, MA6, 5MU, 2MG, MG, UR3, PSU, ZN, 5MC, 4OC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.30	0/69009	0.79	27/107712 (0.0%)
1	2A	0.26	0/67293	0.79	22/105034 (0.0%)
2	1B	0.31	1/2882 (0.0%)	0.74	0/4494
2	2B	0.30	1/2879 (0.0%)	0.80	1/4487 (0.0%)
3	1D	0.28	0/2186	0.48	0/2944
3	2D	0.27	0/2186	0.48	0/2944
4	1E	0.27	0/1592	0.47	0/2149
4	2E	0.26	0/1592	0.47	0/2149
5	1F	0.27	0/1619	0.45	0/2193
5	2F	0.27	0/1615	0.43	0/2188
6	1G	0.26	0/1448	0.45	0/1957
6	2G	0.26	0/1453	0.44	0/1963
7	1H	0.28	0/1356	0.46	0/1834
7	2H	0.26	0/1356	0.45	0/1834
8	1I	0.25	0/1112	0.45	0/1514
8	2I	0.26	0/1079	0.47	0/1475
9	1N	0.27	0/1144	0.45	0/1543
9	2N	0.25	0/1144	0.43	0/1543
10	1O	0.29	0/943	0.49	0/1269
10	2O	0.28	0/943	0.49	0/1269
11	1P	0.29	0/1152	0.51	0/1533
11	2P	0.27	0/1152	0.49	0/1533
12	1Q	0.29	0/1143	0.45	0/1527
12	2Q	0.26	0/1143	0.44	0/1527
13	1R	0.25	0/982	0.45	0/1312
13	2R	0.24	0/982	0.44	0/1312
14	1S	0.26	0/883	0.42	0/1176
14	2S	0.27	0/880	0.45	0/1172
15	1T	0.26	0/1105	0.46	0/1477
15	2T	0.26	0/1097	0.46	0/1468
16	1U	0.26	0/977	0.41	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.25	0/977	0.40	0/1301
17	1V	0.30	0/782	0.51	0/1049
17	2V	0.27	0/782	0.50	0/1049
18	1W	0.28	0/897	0.45	0/1205
18	2W	0.26	0/897	0.43	0/1205
19	1X	0.29	0/764	0.50	0/1025
19	2X	0.25	0/764	0.44	0/1025
20	1Y	0.29	0/819	0.47	0/1095
20	2Y	0.28	0/819	0.47	0/1095
21	1Z	0.26	0/1267	0.46	0/1717
21	2Z	0.26	0/1299	0.47	0/1763
22	10	0.27	0/662	0.46	0/881
22	20	0.27	0/662	0.47	0/881
23	11	0.29	0/762	0.47	0/1014
23	21	0.27	0/762	0.48	0/1014
24	12	0.25	0/590	0.40	0/781
24	22	0.25	0/590	0.38	0/781
25	13	0.26	0/474	0.45	0/635
25	23	0.25	0/469	0.42	0/630
26	14	0.28	0/565	0.51	0/761
26	24	0.30	0/545	0.51	0/737
27	15	0.26	0/469	0.47	0/635
27	25	0.29	0/469	0.44	0/635
28	16	0.29	0/460	0.46	0/613
28	26	0.25	0/456	0.46	0/608
29	17	0.25	0/426	0.43	0/561
29	27	0.24	0/426	0.46	0/561
30	18	0.27	0/525	0.45	0/691
30	28	0.25	0/525	0.44	0/691
31	19	0.31	0/310	0.49	0/407
31	29	0.28	0/310	0.51	0/407
32	1a	0.26	0/35795	0.82	25/55864 (0.0%)
32	2a	0.27	2/35886 (0.0%)	0.85	31/56005 (0.1%)
33	1b	0.26	0/1881	0.46	0/2542
33	2b	0.26	0/1860	0.46	0/2518
34	1c	0.28	0/1572	0.44	0/2126
34	2c	0.25	0/1566	0.45	0/2119
35	1d	0.26	0/1685	0.43	0/2262
35	2d	0.25	0/1704	0.43	0/2284
36	1e	0.26	0/1145	0.48	0/1543
36	2e	0.27	0/1149	0.48	0/1548
37	1f	0.27	0/823	0.47	0/1115
37	2f	0.27	0/829	0.45	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.25	0/1250	0.43	0/1679
38	2g	0.25	0/1254	0.41	0/1683
39	1h	0.26	0/1108	0.45	0/1494
39	2h	0.26	0/1108	0.44	0/1494
40	1i	0.27	0/1002	0.47	0/1346
40	2i	0.26	0/997	0.49	0/1343
41	1j	0.25	0/722	0.48	0/982
41	2j	0.26	0/727	0.47	0/988
42	1k	0.25	0/844	0.44	0/1145
42	2k	0.28	0/848	0.45	0/1149
43	1l	0.27	0/937	0.48	0/1260
43	2l	0.28	0/937	0.48	0/1260
44	1m	0.26	0/969	0.46	0/1302
44	2m	0.25	0/961	0.47	0/1291
45	1n	0.28	0/501	0.42	0/664
45	2n	0.26	0/501	0.44	0/664
46	1o	0.24	0/739	0.41	0/985
46	2o	0.24	0/739	0.42	0/985
47	1p	0.25	0/697	0.46	0/939
47	2p	0.25	0/693	0.45	0/935
48	1q	0.26	0/836	0.46	0/1117
48	2q	0.26	0/836	0.46	0/1117
49	1r	0.25	0/560	0.48	0/746
49	2r	0.24	0/560	0.45	0/746
50	1s	0.25	0/667	0.50	0/900
50	2s	0.27	0/661	0.50	0/893
51	1t	0.26	0/730	0.41	0/965
51	2t	0.24	0/729	0.39	0/965
52	1u	0.23	0/203	0.43	0/266
52	2u	0.24	0/203	0.43	0/266
53	1v	0.27	0/288	0.85	0/446
53	2v	0.33	0/163	0.84	0/251
54	1w	0.46	1/1537 (0.1%)	1.06	6/2390 (0.3%)
54	1y	0.44	1/1606 (0.1%)	1.06	5/2497 (0.2%)
54	2w	0.36	0/1487	1.05	1/2311 (0.0%)
54	2y	0.50	1/1583 (0.1%)	1.15	7/2459 (0.3%)
55	1x	0.40	0/1725	1.05	9/2689 (0.3%)
55	2x	0.36	0/1725	0.99	9/2689 (0.3%)
All	All	0.28	7/316379 (0.0%)	0.74	143/473636 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	24	0	1
41	2j	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2B	1	U	OP3-P	-10.52	1.48	1.61
54	2y	1	G	OP3-P	-10.49	1.48	1.61
54	1w	1	G	OP3-P	-10.38	1.48	1.61
2	1B	1	U	OP3-P	-10.34	1.48	1.61
54	1y	1	G	OP3-P	-10.27	1.48	1.61
32	2a	1272	G	N1-C2	-7.83	1.31	1.37
32	2a	1272	G	C6-N1	-7.12	1.34	1.39

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1272	G	N3-C2-N2	18.40	132.78	119.90
32	2a	1263	C	N1-C2-O2	17.88	129.63	118.90
32	2a	1272	G	C5-C6-O6	16.95	138.77	128.60
32	2a	1272	G	N1-C2-N2	-14.73	102.94	116.20
2	2B	80	U	O4'-C1'-N1	12.03	117.82	108.20
32	2a	1272	G	C6-N1-C2	11.72	132.13	125.10
1	2A	2136	C	N1-C2-O2	11.38	125.73	118.90
32	2a	1263	C	C2-N3-C4	11.06	125.43	119.90
1	1A	1075	C	N1-C2-O2	10.66	125.30	118.90
32	2a	1263	C	N3-C2-O2	-10.08	114.84	121.90
1	1A	1086	A	N1-C6-N6	-9.58	112.85	118.60
32	2a	1263	C	C5-C6-N1	9.55	125.77	121.00
32	2a	1272	G	C5-C6-N1	-9.50	106.75	111.50
32	2a	1272	G	N1-C6-O6	-9.08	114.45	119.90
1	1A	1187	G	O5'-P-OP2	8.73	121.18	110.70
32	1a	1034	G	C6-N1-C2	8.19	130.01	125.10
54	2y	66	U	C5-C4-O4	-8.04	121.08	125.90
1	1A	1063	G	C5-C6-O6	7.78	133.27	128.60
54	1y	56	C	N1-C2-O2	7.75	123.55	118.90
1	2A	2155	G	N3-C4-N9	7.71	130.62	126.00
32	2a	1263	C	C6-N1-C2	-7.70	117.22	120.30
32	2a	754	C	C2-N1-C1'	7.69	127.26	118.80
1	1A	1063	G	N3-C2-N2	7.51	125.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2136	C	N3-C2-O2	-7.46	116.68	121.90
1	2A	2155	G	C6-C5-N7	-7.46	125.93	130.40
55	1x	22	G	N1-C6-O6	-7.43	115.44	119.90
55	1x	46	G	C6-N1-C2	-7.39	120.67	125.10
1	1A	847	U	C2-N1-C1'	7.14	126.27	117.70
32	2a	1272	G	C4-N9-C1'	7.12	135.75	126.50
1	1A	1063	G	C6-N1-C2	7.10	129.36	125.10
32	2a	1263	C	C2-N1-C1'	7.10	126.61	118.80
1	2A	2155	G	N3-C2-N2	7.03	124.82	119.90
32	2a	754	C	N1-C2-O2	7.01	123.10	118.90
54	1y	33	U	N1-C2-O2	6.96	127.67	122.80
32	2a	1001(A)	G	N3-C4-N9	6.95	130.17	126.00
1	1A	1075	C	C2-N3-C4	6.90	123.35	119.90
1	2A	2155	G	N9-C4-C5	-6.90	102.64	105.40
54	2y	7	A	C6-N1-C2	-6.89	114.47	118.60
32	2a	1272	G	C8-N9-C1'	-6.88	118.05	127.00
32	1a	266	G	P-O3'-C3'	6.81	127.87	119.70
1	2A	2155	G	C4-C5-N7	6.79	113.52	110.80
55	2x	14	A	C4-C5-C6	6.76	120.38	117.00
54	1y	33	U	C2-N1-C1'	6.75	125.80	117.70
54	1w	4	C	C5-C4-N4	6.75	124.92	120.20
54	1y	33	U	N3-C2-O2	-6.70	117.51	122.20
55	2x	22	G	C8-N9-C1'	6.68	135.68	127.00
55	1x	22	G	C6-C5-N7	6.66	134.40	130.40
55	1x	22	G	C4-C5-C6	-6.63	114.82	118.80
1	1A	1187	G	N1-C6-O6	-6.57	115.96	119.90
1	1A	2629	A	P-O3'-C3'	6.51	127.52	119.70
1	1A	1075	C	C2-N1-C1'	6.51	125.96	118.80
1	1A	2167	U	C2-N1-C1'	6.47	125.46	117.70
55	1x	22	G	C8-N9-C1'	6.42	135.34	127.00
32	1a	1065	U	P-O3'-C3'	6.41	127.39	119.70
55	2x	22	G	N1-C6-O6	-6.35	116.09	119.90
55	1x	22	G	N3-C4-N9	-6.33	122.20	126.00
32	2a	1158	C	C2-N1-C1'	6.29	125.72	118.80
32	1a	1132	C	N1-C2-O2	6.27	122.66	118.90
32	1a	1030	C	N1-C2-O2	6.24	122.65	118.90
1	2A	2897	U	C2-N1-C1'	6.22	125.16	117.70
54	2w	47	U	C2-N1-C1'	6.16	125.09	117.70
1	1A	1091	G	N3-C4-N9	6.13	129.68	126.00
1	1A	512	G	O4'-C1'-N9	6.12	113.10	108.20
55	2x	22	G	C4-N9-C1'	-6.10	118.57	126.50
32	2a	1039	C	C5-C4-N4	-6.09	115.94	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	847	U	N1-C2-O2	6.00	127.00	122.80
1	1A	1075	C	N3-C2-O2	-5.97	117.72	121.90
32	1a	1001	A	C5-C6-N6	5.96	128.47	123.70
55	2x	46	G	N3-C2-N2	-5.95	115.73	119.90
32	1a	1065	U	OP2-P-O3'	5.92	118.22	105.20
1	1A	2134	A	P-O3'-C3'	5.91	126.80	119.70
32	2a	1263	C	C4-C5-C6	-5.88	114.46	117.40
1	2A	2136	C	C2-N1-C1'	5.85	125.24	118.80
1	2A	1313	U	C2-N1-C1'	5.85	124.72	117.70
54	2y	7	A	N3-C4-N9	5.84	132.07	127.40
32	1a	1034	G	N3-C2-N2	5.83	123.98	119.90
54	1w	4	C	N3-C4-N4	-5.81	113.93	118.00
55	1x	22	G	C4-N9-C1'	-5.79	118.98	126.50
55	2x	22	G	N3-C4-N9	-5.74	122.55	126.00
55	2x	22	G	C6-C5-N7	5.74	133.84	130.40
32	2a	754	C	C6-N1-C1'	-5.73	113.92	120.80
55	1x	14	A	C4-C5-C6	5.69	119.85	117.00
32	1a	1001	A	N1-C6-N6	-5.62	115.23	118.60
32	1a	1027	C	C6-N1-C1'	5.60	127.52	120.80
32	1a	841	U	C2-N1-C1'	5.56	124.37	117.70
32	1a	1027	C	C2-N1-C1'	-5.54	112.70	118.80
1	1A	847	U	N3-C2-O2	-5.54	118.32	122.20
54	2y	66	U	C2-N3-C4	-5.53	123.68	127.00
1	1A	1100	C	C2-N1-C1'	5.49	124.84	118.80
32	1a	748	C	P-O3'-C3'	5.49	126.28	119.70
1	1A	2167	U	N1-C2-O2	5.48	126.64	122.80
32	2a	1150	U	C5-C4-O4	5.46	129.18	125.90
32	1a	1030(B)	C	C2-N1-C1'	5.45	124.79	118.80
32	2a	1272	G	C2-N3-C4	-5.42	109.19	111.90
54	1y	56	C	C2-N3-C4	5.42	122.61	119.90
1	2A	2866	U	C2-N1-C1'	5.42	124.20	117.70
32	2a	1123	A	C5-C6-N6	5.39	128.02	123.70
1	1A	1174	A	OP1-P-O3'	5.38	117.05	105.20
32	1a	1158	C	C2-N1-C1'	5.38	124.71	118.80
1	2A	2155	G	C4-N9-C1'	5.37	133.49	126.50
1	1A	1313	U	C2-N1-C1'	5.35	124.12	117.70
32	1a	1040	U	C2-N3-C4	5.34	130.21	127.00
32	2a	1263	C	N1-C2-N3	-5.33	115.47	119.20
54	1w	64	A	N1-C6-N6	5.32	121.79	118.60
32	2a	266	G	P-O3'-C3'	5.32	126.08	119.70
54	1w	64	A	C5-C6-N6	-5.31	119.45	123.70
32	2a	1262	C	N1-C2-O2	5.31	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2134	A	OP1-P-O3'	5.30	116.85	105.20
54	2y	7	A	C5-C6-N1	5.27	120.34	117.70
54	1w	10	G	N3-C2-N2	-5.26	116.22	119.90
55	1x	14	A	C5-N7-C8	5.26	106.53	103.90
1	1A	1099	G	N3-C4-N9	5.26	129.16	126.00
1	2A	528	A	OP1-P-O3'	5.25	116.76	105.20
32	1a	266	G	OP2-P-O3'	5.25	116.74	105.20
32	1a	841	U	C5-C6-N1	5.24	125.32	122.70
32	2a	1158	C	N1-C2-O2	5.24	122.05	118.90
1	2A	2136	C	C6-N1-C1'	-5.22	114.53	120.80
32	2a	1001(A)	G	C4-N9-C1'	5.21	133.28	126.50
1	1A	1187	G	C5-C6-O6	5.18	131.71	128.60
1	2A	90	U	C2-N1-C1'	5.16	123.90	117.70
32	1a	913	A	P-O3'-C3'	5.14	125.87	119.70
32	1a	1138	G	C4-N9-C1'	5.14	133.18	126.50
1	1A	1187	G	OP1-P-OP2	-5.14	111.89	119.60
55	2x	22	G	C4-C5-C6	-5.13	115.72	118.80
1	2A	2897	U	N1-C2-O2	5.13	126.39	122.80
1	2A	847	U	C2-N1-C1'	5.11	123.83	117.70
1	1A	1063	G	C5-C6-N1	-5.10	108.95	111.50
32	1a	1158	C	N1-C2-O2	5.09	121.95	118.90
54	1w	69	G	C5-C6-O6	5.09	131.65	128.60
32	2a	1125	U	C2-N1-C1'	5.09	123.81	117.70
1	2A	2321	G	C4-N9-C1'	5.09	133.12	126.50
54	2y	22	G	C6-C5-N7	-5.09	127.35	130.40
1	2A	1644	C	N1-C2-O2	5.08	121.95	118.90
32	1a	1030	C	N3-C2-O2	-5.08	118.34	121.90
32	1a	1054	C	C2-N1-C1'	5.07	124.37	118.80
32	1a	1034	G	C5-C6-O6	5.06	131.64	128.60
32	1a	687	A	P-O3'-C3'	5.05	125.76	119.70
32	2a	1040	U	C5-C4-O4	5.05	128.93	125.90
54	2y	22	G	N1-C6-O6	5.04	122.93	119.90
55	2x	14	A	C5-C6-N1	-5.04	115.18	117.70
1	2A	228	A	P-O3'-C3'	5.02	125.73	119.70
1	2A	2155	G	C8-N9-C1'	-5.02	120.47	127.00
1	2A	2139	C	C2-N1-C1'	5.02	124.32	118.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	24	56	VAL	Peptide

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Mol	Chain	Res	Type	Group
41	2j	32	ALA	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	262 (96%)	10 (4%)	1 (0%)	34 69
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100 100
4	1E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	29 64
4	2E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	15 48
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29 64
5	2F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	15 48
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	25 60
6	2G	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	25 60
7	1H	172/180 (96%)	159 (92%)	13 (8%)	0	100 100
7	2H	172/180 (96%)	162 (94%)	8 (5%)	2 (1%)	13 43
8	1I	144/148 (97%)	128 (89%)	15 (10%)	1 (1%)	22 56
8	2I	144/148 (97%)	127 (88%)	16 (11%)	1 (1%)	22 56
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100 100
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100 100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19 53
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	2P	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	11 39
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100 100
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100 100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100 100
14	2S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17 51
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100 100
15	2T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19 53
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100 100
17	1V	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	4 20
17	2V	99/101 (98%)	94 (95%)	5 (5%)	0	100 100
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
18	2W	110/113 (97%)	104 (94%)	6 (6%)	0	100 100
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100 100
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	15 48
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100 100
21	1Z	148/206 (72%)	131 (88%)	16 (11%)	1 (1%)	22 56
21	2Z	156/206 (76%)	142 (91%)	14 (9%)	0	100 100
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100 100
22	20	81/85 (95%)	79 (98%)	2 (2%)	0	100 100
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14 46
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100 100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1 7
26	24	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	0	1 (2%)	6	28
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	202 (88%)	23 (10%)	4 (2%)	9	34
33	2b	229/256 (90%)	205 (90%)	20 (9%)	4 (2%)	9	34
34	1c	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	29	64
34	2c	204/239 (85%)	192 (94%)	10 (5%)	2 (1%)	15	48
35	1d	206/209 (99%)	200 (97%)	4 (2%)	2 (1%)	15	48
35	2d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	64
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	11	39
36	2e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	11	39
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	7	30
38	2g	153/156 (98%)	142 (93%)	10 (6%)	1 (1%)	22	56
39	1h	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	22	56
39	2h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
40	1i	125/128 (98%)	116 (93%)	7 (6%)	2 (2%)	9	36
40	2i	125/128 (98%)	113 (90%)	10 (8%)	2 (2%)	9	36
41	1j	95/105 (90%)	81 (85%)	8 (8%)	6 (6%)	1	6
41	2j	94/105 (90%)	83 (88%)	7 (7%)	4 (4%)	2	12
42	1k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	33
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8	33
43	1l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	110 (91%)	11 (9%)	0	100	100
44	2m	120/126 (95%)	110 (92%)	10 (8%)	0	100	100
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	34
46	1o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13	43
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12	41
47	2p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12	41
48	1q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	15	48
48	2q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	15	48
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	2s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	13	43
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	12
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	29
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11370/12128 (94%)	10654 (94%)	629 (6%)	87 (1%)	19	53

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
33	1b	17	PHE
35	1d	5	ILE
40	1i	54	ASP
5	2F	130	ALA
33	2b	127	ILE
40	2i	54	ASP
42	2k	106	LYS
5	1F	130	ALA
26	14	53	GLU
26	14	58	ARG

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Mol	Chain	Res	Type
38	1g	114	ARG
42	1k	49	GLY
47	1p	53	VAL
51	1t	95	ALA
5	2F	89	VAL
6	2G	47	LYS
14	2S	96	GLY
35	2d	5	ILE
36	2e	98	THR
41	2j	33	GLN
41	2j	75	ILE
47	2p	53	VAL
17	1V	53	GLU
17	1V	78	LYS
17	1V	100	ARG
21	1Z	134	PRO
23	11	3	LYS
33	1b	20	GLU
36	1e	6	PHE
38	1g	52	GLU
40	1i	12	GLU
41	1j	55	LYS
51	1t	10	LEU
4	2E	113	PHE
10	2O	5	GLN
15	2T	56	GLY
26	24	47	GLN
26	24	55	ARG
33	2b	95	GLN
40	2i	12	GLU
41	2j	78	ASN
48	2q	68	ARG
51	2t	10	LEU
51	2t	47	GLY
4	1E	52	LEU
8	1I	117	GLU
20	1Y	78	ALA
26	14	57	GLU
41	1j	78	ASN
51	1t	47	GLY
4	2E	52	LEU
7	2H	92	ILE

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Mol	Chain	Res	Type
7	2H	126	PRO
33	2b	20	GLU
36	2e	69	VAL
42	2k	49	GLY
50	2s	81	ARG
3	1D	127	VAL
26	14	56	VAL
38	1g	4	ARG
41	1j	79	ARG
46	1o	19	PRO
8	2I	104	GLN
11	2P	36	LYS
29	27	47	ARG
41	2j	55	LYS
51	1t	100	ILE
11	2P	29	LYS
26	24	29	PRO
38	2g	4	ARG
45	2n	14	PRO
34	1c	66	VAL
36	1e	69	VAL
34	2c	66	VAL
41	1j	77	PRO
42	1k	105	VAL
39	1h	83	ILE
41	1j	91	PRO
48	1q	33	GLY
34	2c	14	ILE
33	1b	231	GLU
35	1d	178	VAL
41	1j	75	ILE
33	2b	231	GLU
33	1b	124	SER
26	24	64	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	207 (96%)	8 (4%)	34	66
3	2D	215/218 (99%)	205 (95%)	10 (5%)	26	59
4	1E	164/166 (99%)	156 (95%)	8 (5%)	25	58
4	2E	164/166 (99%)	155 (94%)	9 (6%)	21	53
5	1F	160/166 (96%)	155 (97%)	5 (3%)	40	71
5	2F	159/166 (96%)	148 (93%)	11 (7%)	15	44
6	1G	143/156 (92%)	137 (96%)	6 (4%)	30	63
6	2G	143/156 (92%)	135 (94%)	8 (6%)	21	53
7	1H	144/148 (97%)	136 (94%)	8 (6%)	21	53
7	2H	144/148 (97%)	138 (96%)	6 (4%)	30	63
8	1I	113/124 (91%)	104 (92%)	9 (8%)	12	37
8	2I	105/124 (85%)	97 (92%)	8 (8%)	13	39
9	1N	118/119 (99%)	111 (94%)	7 (6%)	19	50
9	2N	118/119 (99%)	110 (93%)	8 (7%)	16	45
10	1O	100/100 (100%)	94 (94%)	6 (6%)	19	50
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31	64
11	1P	115/116 (99%)	110 (96%)	5 (4%)	29	62
11	2P	115/116 (99%)	110 (96%)	5 (4%)	29	62
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	59	82
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	27	61
13	1R	101/101 (100%)	93 (92%)	8 (8%)	12	37
13	2R	101/101 (100%)	93 (92%)	8 (8%)	12	37
14	1S	86/88 (98%)	84 (98%)	2 (2%)	50	78
14	2S	85/88 (97%)	82 (96%)	3 (4%)	36	68
15	1T	115/127 (91%)	111 (96%)	4 (4%)	36	68
15	2T	113/127 (89%)	108 (96%)	5 (4%)	28	62
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22	54
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	54
17	1V	80/82 (98%)	75 (94%)	5 (6%)	18	48
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18	48
18	1W	90/92 (98%)	88 (98%)	2 (2%)	52	79
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	1X	77/78 (99%)	77 (100%)	0	100 100
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32 65
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4 16
20	2Y	85/91 (93%)	80 (94%)	5 (6%)	19 50
21	1Z	135/179 (75%)	127 (94%)	8 (6%)	19 50
21	2Z	137/179 (76%)	134 (98%)	3 (2%)	52 79
22	10	65/67 (97%)	65 (100%)	0	100 100
22	20	65/67 (97%)	63 (97%)	2 (3%)	40 71
23	11	80/83 (96%)	77 (96%)	3 (4%)	33 66
23	21	80/83 (96%)	78 (98%)	2 (2%)	47 76
24	12	65/67 (97%)	63 (97%)	2 (3%)	40 71
24	22	65/67 (97%)	64 (98%)	1 (2%)	65 85
25	13	51/52 (98%)	49 (96%)	2 (4%)	32 65
25	23	50/52 (96%)	49 (98%)	1 (2%)	55 80
26	14	59/63 (94%)	54 (92%)	5 (8%)	10 34
26	24	53/63 (84%)	52 (98%)	1 (2%)	57 81
27	15	50/52 (96%)	45 (90%)	5 (10%)	7 26
27	25	50/52 (96%)	47 (94%)	3 (6%)	19 50
28	16	51/52 (98%)	44 (86%)	7 (14%)	3 15
28	26	50/52 (96%)	45 (90%)	5 (10%)	7 26
29	17	41/42 (98%)	37 (90%)	4 (10%)	8 27
29	27	41/42 (98%)	38 (93%)	3 (7%)	14 41
30	18	54/55 (98%)	51 (94%)	3 (6%)	21 53
30	28	54/55 (98%)	53 (98%)	1 (2%)	57 81
31	19	34/34 (100%)	33 (97%)	1 (3%)	42 73
31	29	34/34 (100%)	32 (94%)	2 (6%)	19 50
33	1b	192/220 (87%)	181 (94%)	11 (6%)	20 52
33	2b	187/220 (85%)	172 (92%)	15 (8%)	12 37
34	1c	142/188 (76%)	135 (95%)	7 (5%)	25 58
34	2c	140/188 (74%)	134 (96%)	6 (4%)	29 62
35	1d	169/181 (93%)	158 (94%)	11 (6%)	17 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	2d	173/181 (96%)	161 (93%)	12 (7%)	15 44
36	1e	113/123 (92%)	108 (96%)	5 (4%)	28 62
36	2e	114/123 (93%)	108 (95%)	6 (5%)	22 55
37	1f	84/90 (93%)	80 (95%)	4 (5%)	25 59
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26 59
38	1g	119/127 (94%)	115 (97%)	4 (3%)	37 69
38	2g	120/127 (94%)	116 (97%)	4 (3%)	38 70
39	1h	114/119 (96%)	103 (90%)	11 (10%)	8 28
39	2h	114/119 (96%)	108 (95%)	6 (5%)	22 55
40	1i	90/99 (91%)	85 (94%)	5 (6%)	21 53
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6 22
41	1j	66/92 (72%)	64 (97%)	2 (3%)	41 72
41	2j	69/92 (75%)	66 (96%)	3 (4%)	29 62
42	1k	82/99 (83%)	80 (98%)	2 (2%)	49 77
42	2k	83/99 (84%)	79 (95%)	4 (5%)	25 59
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30 63
43	2l	96/108 (89%)	90 (94%)	6 (6%)	18 48
44	1m	93/101 (92%)	93 (100%)	0	100 100
44	2m	92/101 (91%)	91 (99%)	1 (1%)	73 89
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5 19
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30 64
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33 66
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13 39
47	1p	69/74 (93%)	64 (93%)	5 (7%)	14 42
47	2p	68/74 (92%)	65 (96%)	3 (4%)	28 62
48	1q	94/97 (97%)	93 (99%)	1 (1%)	73 89
48	2q	94/97 (97%)	90 (96%)	4 (4%)	29 62
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24 56
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16 45
50	1s	69/80 (86%)	68 (99%)	1 (1%)	67 86
50	2s	67/80 (84%)	66 (98%)	1 (2%)	65 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	1t	70/82 (85%)	69 (99%)	1 (1%)	67 86
51	2t	70/82 (85%)	68 (97%)	2 (3%)	42 73
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6 22
52	2u	18/22 (82%)	18 (100%)	0	100 100
All	All	9303/10064 (92%)	8839 (95%)	464 (5%)	24 57

All (464) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	16	MET
3	1D	22	SER
3	1D	106	ILE
3	1D	162	SER
3	1D	181	GLU
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
4	1E	9	VAL
4	1E	21	VAL
4	1E	47	VAL
4	1E	75	VAL
4	1E	116	VAL
4	1E	119	ARG
4	1E	128	SER
4	1E	181	LEU
5	1F	33	LEU
5	1F	57	VAL
5	1F	106	ARG
5	1F	168	ARG
5	1F	170	LEU
6	1G	28	VAL
6	1G	53	LEU
6	1G	132	ASN
6	1G	140	ILE
6	1G	150	ASP
6	1G	159	VAL
7	1H	7	LEU
7	1H	18	GLU
7	1H	63	SER
7	1H	69	ARG
7	1H	70	THR

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Mol	Chain	Res	Type
7	1H	84	SER
7	1H	98	LEU
7	1H	129	THR
8	1I	9	LEU
8	1I	38	LEU
8	1I	40	THR
8	1I	58	LEU
8	1I	92	VAL
8	1I	96	ASP
8	1I	109	ILE
8	1I	117	GLU
8	1I	140	LEU
9	1N	9	VAL
9	1N	15	LEU
9	1N	34	LEU
9	1N	35	ARG
9	1N	46	VAL
9	1N	60	ILE
9	1N	99	LEU
10	1O	21	CYS
10	1O	24	VAL
10	1O	75	SER
10	1O	89	ASN
10	1O	107	ARG
10	1O	120	GLU
11	1P	59	LEU
11	1P	95	VAL
11	1P	98	GLU
11	1P	112	LEU
11	1P	148	LEU
12	1Q	1	MET
12	1Q	110	THR
13	1R	6	SER
13	1R	8	ARG
13	1R	24	GLN
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	111	LEU
14	1S	14	VAL
14	1S	71	ARG

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Mol	Chain	Res	Type
15	1T	28	VAL
15	1T	51	ARG
15	1T	108	ARG
15	1T	118	ARG
16	1U	8	VAL
16	1U	54	LYS
16	1U	74	LEU
16	1U	77	SER
16	1U	95	LEU
17	1V	20	LEU
17	1V	46	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	79	VAL
18	1W	66	GLU
18	1W	101	SER
20	1Y	11	ASP
20	1Y	14	LEU
20	1Y	43	ASN
20	1Y	50	ARG
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	86	ARG
20	1Y	90	LEU
20	1Y	91	GLU
20	1Y	99	CYS
20	1Y	106	LEU
21	1Z	1	MET
21	1Z	18	LEU
21	1Z	28	MET
21	1Z	41	LEU
21	1Z	70	LEU
21	1Z	123	ASP
21	1Z	139	VAL
21	1Z	171	ILE
23	11	3	LYS
23	11	30	VAL
23	11	38	SER
24	12	17	SER
24	12	52	ASP
25	13	34	GLU
25	13	58	VAL

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Mol	Chain	Res	Type
26	14	27	THR
26	14	49	PHE
26	14	56	VAL
26	14	57	GLU
26	14	58	ARG
27	15	16	ARG
27	15	26	THR
27	15	29	THR
27	15	33	CYS
27	15	58	LEU
28	16	4	GLU
28	16	9	LEU
28	16	13	CYS
28	16	24	GLU
28	16	33	LYS
28	16	48	VAL
28	16	51	GLU
29	17	1	MET
29	17	39	ARG
29	17	43	THR
29	17	46	VAL
30	18	30	ARG
30	18	31	HIS
30	18	32	LEU
31	19	26	ILE
33	1b	8	LYS
33	1b	10	LEU
33	1b	12	GLU
33	1b	21	ARG
33	1b	93	VAL
33	1b	111	ARG
33	1b	115	LEU
33	1b	127	ILE
33	1b	185	ILE
33	1b	187	LEU
33	1b	230	VAL
34	1c	3	ASN
34	1c	112	SER
34	1c	154	SER
34	1c	172	ARG
34	1c	175	LEU
34	1c	190	ARG

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Mol	Chain	Res	Type
34	1c	195	VAL
35	1d	5	ILE
35	1d	10	ARG
35	1d	28	SER
35	1d	59	ARG
35	1d	71	SER
35	1d	83	SER
35	1d	135	LEU
35	1d	158	ILE
35	1d	178	VAL
35	1d	194	LEU
35	1d	196	LEU
36	1e	27	ARG
36	1e	65	ASN
36	1e	81	GLU
36	1e	133	TYR
36	1e	148	VAL
37	1f	17	SER
37	1f	70	ASP
37	1f	75	LEU
37	1f	94	GLN
38	1g	90	GLU
38	1g	92	SER
38	1g	115	ARG
38	1g	125	MET
39	1h	12	ARG
39	1h	19	VAL
39	1h	26	VAL
39	1h	50	ARG
39	1h	51	VAL
39	1h	63	LEU
39	1h	85	ARG
39	1h	91	ARG
39	1h	104	ARG
39	1h	113	SER
39	1h	127	LEU
40	1i	64	THR
40	1i	83	ARG
40	1i	92	TYR
40	1i	111	ARG
40	1i	128	ARG
41	1j	49	VAL

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Mol	Chain	Res	Type
41	1j	92	THR
42	1k	109	VAL
42	1k	116	HIS
43	1l	28	LYS
43	1l	37	CYS
43	1l	53	ARG
43	1l	55	VAL
45	1n	3	ARG
45	1n	7	ILE
45	1n	18	VAL
45	1n	32	SER
45	1n	33	VAL
45	1n	35	ARG
46	1o	24	SER
46	1o	28	GLN
46	1o	70	LEU
47	1p	6	LEU
47	1p	19	ILE
47	1p	20	VAL
47	1p	45	THR
47	1p	67	THR
48	1q	68	ARG
49	1r	30	ASP
49	1r	31	LEU
49	1r	54	ARG
50	1s	32	LYS
51	1t	10	LEU
52	1u	3	LYS
52	1u	20	LYS
3	2D	14	ARG
3	2D	50	THR
3	2D	61	LEU
3	2D	88	ARG
3	2D	106	ILE
3	2D	169	GLU
3	2D	211	ARG
3	2D	237	GLU
3	2D	242	ARG
3	2D	254	THR
4	2E	21	VAL
4	2E	47	VAL
4	2E	75	VAL

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Mol	Chain	Res	Type
4	2E	89	ASP
4	2E	92	THR
4	2E	101	ARG
4	2E	107	THR
4	2E	116	VAL
4	2E	184	VAL
5	2F	50	SER
5	2F	57	VAL
5	2F	70	THR
5	2F	88	VAL
5	2F	98	SER
5	2F	106	ARG
5	2F	110	LEU
5	2F	149	ASP
5	2F	153	SER
5	2F	195	ASP
5	2F	201	VAL
6	2G	5	VAL
6	2G	7	LEU
6	2G	9	ARG
6	2G	16	ARG
6	2G	43	LEU
6	2G	79	ASN
6	2G	126	ASP
6	2G	159	VAL
7	2H	18	GLU
7	2H	45	VAL
7	2H	53	GLU
7	2H	70	THR
7	2H	84	SER
7	2H	136	ILE
8	2I	31	LEU
8	2I	38	LEU
8	2I	40	THR
8	2I	72	LEU
8	2I	114	LEU
8	2I	123	LEU
8	2I	127	VAL
8	2I	144	VAL
9	2N	15	LEU
9	2N	28	THR
9	2N	35	ARG

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Mol	Chain	Res	Type
9	2N	38	HIS
9	2N	43	THR
9	2N	58	ASP
9	2N	67	LEU
9	2N	73	THR
10	2O	10	VAL
10	2O	24	VAL
10	2O	65	THR
10	2O	98	VAL
11	2P	3	LEU
11	2P	4	SER
11	2P	95	VAL
11	2P	121	LYS
11	2P	148	LEU
12	2Q	1	MET
12	2Q	31	ASP
12	2Q	35	VAL
12	2Q	106	VAL
12	2Q	110	THR
13	2R	6	SER
13	2R	44	LEU
13	2R	59	ASP
13	2R	65	LEU
13	2R	67	LEU
13	2R	96	ARG
13	2R	100	LEU
13	2R	111	LEU
14	2S	27	SER
14	2S	48	LEU
14	2S	63	THR
15	2T	13	ARG
15	2T	89	VAL
15	2T	93	ARG
15	2T	96	ARG
15	2T	111	ARG
16	2U	8	VAL
16	2U	50	ARG
16	2U	74	LEU
16	2U	77	SER
16	2U	95	LEU
17	2V	33	VAL
17	2V	38	LEU

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Mol	Chain	Res	Type
17	2V	46	VAL
17	2V	61	VAL
17	2V	79	VAL
18	2W	23	LEU
18	2W	35	ILE
18	2W	67	ASP
18	2W	100	THR
19	2X	14	SER
19	2X	30	VAL
19	2X	62	LYS
20	2Y	1	MET
20	2Y	39	VAL
20	2Y	49	VAL
20	2Y	90	LEU
20	2Y	99	CYS
21	2Z	38	TYR
21	2Z	70	LEU
21	2Z	91	LEU
22	20	14	ARG
22	20	55	ARG
23	21	4	VAL
23	21	82	LEU
24	22	11	GLU
25	23	30	ARG
26	24	49	PHE
27	25	6	VAL
27	25	29	THR
27	25	58	LEU
28	26	7	ILE
28	26	9	LEU
28	26	14	THR
28	26	20	ASN
28	26	49	HIS
29	27	1	MET
29	27	42	LEU
29	27	46	VAL
30	28	14	VAL
31	29	7	VAL
31	29	22	ARG
33	2b	8	LYS
33	2b	12	GLU
33	2b	19	HIS

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Mol	Chain	Res	Type
33	2b	67	THR
33	2b	71	VAL
33	2b	93	VAL
33	2b	94	ASN
33	2b	103	THR
33	2b	109	SER
33	2b	111	ARG
33	2b	122	PHE
33	2b	127	ILE
33	2b	135	GLN
33	2b	195	ASP
33	2b	213	LEU
34	2c	17	ASP
34	2c	43	LEU
34	2c	56	ASP
34	2c	119	ARG
34	2c	172	ARG
34	2c	196	LEU
35	2d	31	CYS
35	2d	47	ARG
35	2d	59	ARG
35	2d	96	LEU
35	2d	107	ARG
35	2d	135	LEU
35	2d	158	ILE
35	2d	170	VAL
35	2d	175	SER
35	2d	178	VAL
35	2d	190	ASP
35	2d	196	LEU
36	2e	41	VAL
36	2e	51	VAL
36	2e	68	GLU
36	2e	76	ILE
36	2e	81	GLU
36	2e	117	ASP
37	2f	31	GLU
37	2f	72	VAL
37	2f	75	LEU
37	2f	94	GLN
38	2g	15	ASP
38	2g	79	ARG

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Mol	Chain	Res	Type
38	2g	98	SER
38	2g	114	ARG
39	2h	2	LEU
39	2h	18	ARG
39	2h	104	ARG
39	2h	112	LEU
39	2h	120	THR
39	2h	135	CYS
40	2i	5	TYR
40	2i	9	ARG
40	2i	17	VAL
40	2i	23	ASN
40	2i	53	VAL
40	2i	65	VAL
40	2i	83	ARG
40	2i	99	LEU
40	2i	102	LEU
40	2i	111	ARG
41	2j	35	SER
41	2j	38	ILE
41	2j	51	ARG
42	2k	30	VAL
42	2k	91	ARG
42	2k	114	VAL
42	2k	119	CYS
43	2l	6	THR
43	2l	27	LEU
43	2l	33	ARG
43	2l	73	GLU
43	2l	83	VAL
43	2l	112	ASP
44	2m	32	GLU
45	2n	18	VAL
45	2n	33	VAL
46	2o	5	LYS
46	2o	58	MET
46	2o	64	ARG
46	2o	65	ARG
46	2o	66	LEU
46	2o	87	ILE
47	2p	20	VAL
47	2p	67	THR

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Mol	Chain	Res	Type
47	2p	69	THR
48	2q	9	VAL
48	2q	66	SER
48	2q	67	LYS
48	2q	79	SER
49	2r	31	LEU
49	2r	69	THR
49	2r	76	LEU
49	2r	85	LEU
50	2s	62	ILE
51	2t	15	ARG
51	2t	71	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
5	1F	8	GLN
5	1F	40	GLN
5	1F	69	HIS
6	1G	58	GLN
6	1G	132	ASN
7	1H	147	ASN
8	1I	11	ASN
8	1I	74	ASN
10	1O	5	GLN
13	1R	13	HIS
16	1U	94	ASN
17	1V	64	HIS
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	32	HIS
21	1Z	34	ASN
21	1Z	55	HIS
22	10	3	HIS
22	10	29	GLN
24	12	65	ASN
33	1b	94	ASN
34	1c	6	HIS
34	1c	98	ASN
34	1c	162	GLN
34	1c	176	HIS

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Mol	Chain	Res	Type
35	1d	42	GLN
35	1d	43	HIS
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
35	1d	161	ASN
36	1e	78	HIS
38	1g	13	GLN
38	1g	28	ASN
38	1g	51	GLN
38	1g	148	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	58	HIS
40	1i	73	GLN
40	1i	124	GLN
41	1j	56	HIS
44	1m	77	ASN
46	1o	46	HIS
48	1q	26	GLN
49	1r	63	GLN
50	1s	83	HIS
3	2D	115	GLN
5	2F	69	HIS
5	2F	75	HIS
6	2G	41	GLN
10	2O	5	GLN
13	2R	13	HIS
15	2T	58	ASN
15	2T	79	HIS
16	2U	94	ASN
21	2Z	32	HIS
21	2Z	55	HIS
21	2Z	73	GLN
22	20	12	ASN
24	22	65	ASN
28	26	20	ASN
30	28	35	GLN
33	2b	37	ASN
33	2b	94	ASN
33	2b	212	GLN
34	2c	37	GLN

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Mol	Chain	Res	Type
34	2c	102	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	129	ASN
36	2e	65	ASN
38	2g	28	ASN
38	2g	37	ASN
38	2g	51	GLN
38	2g	64	GLN
38	2g	68	ASN
38	2g	148	ASN
40	2i	31	GLN
40	2i	58	HIS
41	2j	33	GLN
41	2j	56	HIS
42	2k	116	HIS
44	2m	77	ASN
46	2o	53	HIS
46	2o	62	GLN
47	2p	16	HIS
50	2s	69	HIS
50	2s	83	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2860/2915 (98%)	474 (16%)	22 (0%)
1	2A	2788/2915 (95%)	531 (19%)	22 (0%)
2	1B	119/121 (98%)	14 (11%)	0
2	2B	118/121 (97%)	17 (14%)	0
32	1a	1494/1521 (98%)	279 (18%)	0
32	2a	1498/1521 (98%)	311 (20%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	7/24 (29%)	3 (42%)	0
54	1w	68/76 (89%)	15 (22%)	0
54	1y	71/76 (93%)	27 (38%)	0
54	2w	65/76 (85%)	18 (27%)	0
54	2y	69/76 (90%)	24 (34%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	10 (13%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9319/9620 (96%)	1736 (18%)	44 (0%)

All (1736) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	50	U
1	1A	55	G
1	1A	58	G
1	1A	63	U
1	1A	64	A
1	1A	71	A
1	1A	72	U
1	1A	74	A
1	1A	75	G
1	1A	83	G
1	1A	84	A
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	140	G
1	1A	149	A
1	1A	177	G
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	221	A
1	1A	222	A
1	1A	223	A
1	1A	228	A
1	1A	229	A
1	1A	233	A

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Mol	Chain	Res	Type
1	1A	245	G
1	1A	248	G
1	1A	261	G
1	1A	269	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	275	G
1	1A	279	C
1	1A	285	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	372	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	421	U
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	512	G
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	551	G

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Mol	Chain	Res	Type
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	614(C)	A
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(A)	A
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	724	U
1	1A	730	C
1	1A	738	G
1	1A	762	U
1	1A	764	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	788	A
1	1A	789	A
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	845	G
1	1A	855	G
1	1A	859	G

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Mol	Chain	Res	Type
1	1A	880	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	892	G
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	914	C
1	1A	915	C
1	1A	926	A
1	1A	931	G
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	980	A
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1025	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1042	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G

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Mol	Chain	Res	Type
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1064	C
1	1A	1066	U
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1083	U
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
1	1A	1094	U
1	1A	1096	A
1	1A	1098	A
1	1A	1101	U
1	1A	1102	C
1	1A	1103	A
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1130	U
1	1A	1132	A
1	1A	1135	C
1	1A	1136	G
1	1A	1142(A)	A
1	1A	1149	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U

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Mol	Chain	Res	Type
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1187	G
1	1A	1211	U
1	1A	1218	C
1	1A	1229	G
1	1A	1236	G
1	1A	1237	A
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1308	A
1	1A	1314	C
1	1A	1316	U
1	1A	1319	G
1	1A	1320	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1429	G
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1461	G
1	1A	1467	C

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Mol	Chain	Res	Type
1	1A	1482	G
1	1A	1484	G
1	1A	1490	A
1	1A	1493	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1540	U
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1667	G
1	1A	1674	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1746	G
1	1A	1747	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1786	A
1	1A	1791	A
1	1A	1798	U
1	1A	1800	C
1	1A	1801	G
1	1A	1802	A

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Mol	Chain	Res	Type
1	1A	1816	G
1	1A	1817	G
1	1A	1829	A
1	1A	1847	A
1	1A	1858	G
1	1A	1861	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1919	A
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2049	G
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	2063	C
1	1A	2069	G
1	1A	2093	G
1	1A	2098	U
1	1A	2102	U
1	1A	2104	G

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Mol	Chain	Res	Type
1	1A	2108	C
1	1A	2110	G
1	1A	2112	G
1	1A	2113	U
1	1A	2120	G
1	1A	2121	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2150	U
1	1A	2151	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2166	G
1	1A	2168	G
1	1A	2170	A
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2178	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A

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Mol	Chain	Res	Type
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2294	C
1	1A	2296	U
1	1A	2305	A
1	1A	2308	G
1	1A	2312	U
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	2361	A
1	1A	2379	G
1	1A	2383	G
1	1A	2384	G
1	1A	2385	C
1	1A	2391	G
1	1A	2406	U
1	1A	2410	G
1	1A	2423	U
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2438	U
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A

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Mol	Chain	Res	Type
1	1A	2491	U
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2535	G
1	1A	2537	U
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2585	U
1	1A	2586	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2732	G
1	1A	2733	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2780	G
1	1A	2790	A

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Mol	Chain	Res	Type
1	1A	2791	C
1	1A	2792	G
1	1A	2793	G
1	1A	2802	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2834	G
1	1A	2835	A
1	1A	2839	G
1	1A	2858	C
1	1A	2872	G
1	1A	2873	A
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	13	A
2	1B	15	A
2	1B	24	G
2	1B	25	A
2	1B	35	U
2	1B	41	U
2	1B	50	G
2	1B	54	G
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	46	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	52	G
32	1a	61	G

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Mol	Chain	Res	Type
32	1a	69	G
32	1a	70	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	129(A)	G
32	1a	131	C
32	1a	144	G
32	1a	153	C
32	1a	159	G
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(G)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	200	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	219	C
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	257	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	306	G
32	1a	318	G
32	1a	325	A
32	1a	328	C
32	1a	332	G
32	1a	344	A
32	1a	352	C

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Mol	Chain	Res	Type
32	1a	353	A
32	1a	354	G
32	1a	358	U
32	1a	359	U
32	1a	365	U
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	419	C
32	1a	422	C
32	1a	423	G
32	1a	428	G
32	1a	429	U
32	1a	430	A
32	1a	434	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	461	A
32	1a	470	C
32	1a	474	G
32	1a	480	U
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	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	519	C
32	1a	522	C
32	1a	527	7MG

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Mol	Chain	Res	Type
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	C
32	1a	568	G
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	630	G
32	1a	653	A
32	1a	665	A
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	702	A
32	1a	721	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	749	C
32	1a	755	G
32	1a	760	G
32	1a	777	A
32	1a	786	G
32	1a	793	U
32	1a	794	A
32	1a	799	G
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	818	G
32	1a	828	A
32	1a	840	C
32	1a	841	U

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Mol	Chain	Res	Type
32	1a	851	G
32	1a	870	U
32	1a	873	A
32	1a	885	G
32	1a	891	U
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	939	G
32	1a	958	A
32	1a	960	U
32	1a	961	U
32	1a	964	A
32	1a	967	5MC
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1029	C

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Mol	Chain	Res	Type
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1045	C
32	1a	1053	G
32	1a	1054	C
32	1a	1055	A
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1087	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1117	G
32	1a	1122	U
32	1a	1124	G
32	1a	1125	U
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1145	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1160	G
32	1a	1166	G
32	1a	1182	G
32	1a	1183	A
32	1a	1184	G
32	1a	1186	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G

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Mol	Chain	Res	Type
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1215	G
32	1a	1225	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1277	C
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1305	G
32	1a	1312	G
32	1a	1314	C
32	1a	1323	G
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1368	G
32	1a	1370	G
32	1a	1381	U
32	1a	1397	C
32	1a	1403	C
32	1a	1404	5MC
32	1a	1419	G
32	1a	1436	U
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U

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Mol	Chain	Res	Type
32	1a	1447	A
32	1a	1456	G
32	1a	1460	A
32	1a	1475	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1520	G
32	1a	1524	C
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	19	PSU
53	1v	24	A
54	1w	3	C
54	1w	7	A
54	1w	10	G
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	24	G
54	1w	29	G
54	1w	42	C
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	68	C
54	1w	69	G
55	1x	3	C
55	1x	9	G
55	1x	14	A
55	1x	18	G
55	1x	21	A
55	1x	47	U
55	1x	53	G
55	1x	61	C

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Mol	Chain	Res	Type
55	1x	69	C
55	1x	76	A
54	1y	2	C
54	1y	3	C
54	1y	5	G
54	1y	6	G
54	1y	8	4SU
54	1y	9	A
54	1y	13	C
54	1y	14	A
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	31	A
54	1y	35	A
54	1y	44	G
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	53	G
54	1y	57	G
54	1y	58	A
54	1y	59	U
54	1y	61	C
54	1y	65	G
54	1y	66	U
54	1y	69	G
54	1y	70	G
1	2A	10	G
1	2A	12	U
1	2A	15	G
1	2A	16	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	64	A
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A

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Mol	Chain	Res	Type
1	2A	90	U
1	2A	95	G
1	2A	104	U
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	267	C
1	2A	271(I)	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	280	C
1	2A	311	A
1	2A	317	G
1	2A	327	G
1	2A	329	G
1	2A	330	A

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Mol	Chain	Res	Type
1	2A	333	G
1	2A	346	A
1	2A	348	G
1	2A	352	G
1	2A	354	G
1	2A	362	U
1	2A	363	G
1	2A	363(D)	G
1	2A	363(E)	U
1	2A	386	G
1	2A	403	U
1	2A	404	C
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	444	C
1	2A	451	C
1	2A	455	C
1	2A	457	A
1	2A	479	A
1	2A	480	A
1	2A	481	G
1	2A	494	G
1	2A	496	G
1	2A	500	G
1	2A	505	A
1	2A	509	C
1	2A	527	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	551	G
1	2A	556	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	592	G
1	2A	595	C

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Mol	Chain	Res	Type
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	613	G
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	715	G
1	2A	717	G
1	2A	726	G
1	2A	729	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	811	U
1	2A	812	C
1	2A	819	A
1	2A	825	C
1	2A	827	U
1	2A	828	U
1	2A	852	G
1	2A	857	C

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Mol	Chain	Res	Type
1	2A	859	G
1	2A	869	G
1	2A	874	G
1	2A	875	G
1	2A	878	A
1	2A	879	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	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	919	G
1	2A	932	G
1	2A	933	A
1	2A	934	G
1	2A	936	C
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	982	C
1	2A	983	A
1	2A	989	G
1	2A	990	A
1	2A	996	A
1	2A	997	G
1	2A	1005	C

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Mol	Chain	Res	Type
1	2A	1010	A
1	2A	1012	U
1	2A	1013	C
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1040	C
1	2A	1043	C
1	2A	1116	C
1	2A	1122	G
1	2A	1126	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1138	G
1	2A	1141	U
1	2A	1142(A)	A
1	2A	1167	U
1	2A	1171	G
1	2A	1195	G
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1218	C
1	2A	1220	A
1	2A	1224	C
1	2A	1237	A
1	2A	1247	A
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	1275	A
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A

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Mol	Chain	Res	Type
1	2A	1306	C
1	2A	1314	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1376	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1402	C
1	2A	1403	C
1	2A	1411	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	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G

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Mol	Chain	Res	Type
1	2A	1541	G
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1582	C
1	2A	1584	C
1	2A	1586	A
1	2A	1589	C
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1622	G
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1663	C
1	2A	1664	A
1	2A	1667	G
1	2A	1674	G
1	2A	1680	U
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1706	U
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1745(A)	C
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G

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Mol	Chain	Res	Type
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1808	U
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1967	C
1	2A	1969	A
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1983	C
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A

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Mol	Chain	Res	Type
1	2A	2036	C
1	2A	2037	G
1	2A	2043	C
1	2A	2052	G
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2092	U
1	2A	2093	G
1	2A	2099	U
1	2A	2102	U
1	2A	2106	G
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2113	U
1	2A	2114	A
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2141	G
1	2A	2143	C
1	2A	2144	U

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Mol	Chain	Res	Type
1	2A	2146	C
1	2A	2150	U
1	2A	2153	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2160	G
1	2A	2161	C
1	2A	2162	G
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2178	C
1	2A	2181	G
1	2A	2182	G
1	2A	2185	C
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2239	G
1	2A	2248	C
1	2A	2268	A
1	2A	2273	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2285	C
1	2A	2287	A
1	2A	2288	A
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A

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Mol	Chain	Res	Type
1	2A	2310	A
1	2A	2311	A
1	2A	2316	C
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2344	U
1	2A	2346	A
1	2A	2347	C
1	2A	2352	A
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2422	A
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2447	G
1	2A	2448	A
1	2A	2465	C
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2477	C
1	2A	2480	C
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U

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Mol	Chain	Res	Type
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2530	A
1	2A	2536	G
1	2A	2549	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2578	G
1	2A	2592	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2751	G
1	2A	2757	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2779	U
1	2A	2780	G
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G

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Mol	Chain	Res	Type
1	2A	2803	C
1	2A	2807	G
1	2A	2810	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	13	A
2	2B	15	A
2	2B	22	U
2	2B	24	G
2	2B	32	C
2	2B	35	U
2	2B	41	U
2	2B	44	G
2	2B	45	A
2	2B	56	G
2	2B	67	G
2	2B	73	A
2	2B	85	G
2	2B	109	C
2	2B	110	G
2	2B	120	A
32	2a	6	G
32	2a	9	G
32	2a	22	G
32	2a	31	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	52	G
32	2a	54	C

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Mol	Chain	Res	Type
32	2a	65	U
32	2a	66	G
32	2a	89	C
32	2a	90	U
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	151	A
32	2a	152	A
32	2a	159	G
32	2a	162	A
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189	G
32	2a	189(F)	U
32	2a	189(G)	G
32	2a	189(H)	G
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	279	A
32	2a	281	G
32	2a	289	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	348	G
32	2a	351	G

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Mol	Chain	Res	Type
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	383	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	404	U
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	418	C
32	2a	424	G
32	2a	427	U
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	476	G
32	2a	484	G
32	2a	485	G
32	2a	495	A
32	2a	496	A
32	2a	498	U
32	2a	499	A
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	512	U
32	2a	518	C
32	2a	521	G
32	2a	527	7MG
32	2a	531	U

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Mol	Chain	Res	Type
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	618	C
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	660	G
32	2a	665	A
32	2a	666	G
32	2a	681	C
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	708	C
32	2a	720	C
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	748	C
32	2a	749	C
32	2a	755	G
32	2a	768	A
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	816	A
32	2a	817	C
32	2a	819	A
32	2a	821	G
32	2a	828	A
32	2a	840	C

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Mol	Chain	Res	Type
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	871	U
32	2a	872	A
32	2a	873	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	936	C
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	967	5MC
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	996	A
32	2a	997	U
32	2a	999	C
32	2a	1001	A
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1009	G

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Mol	Chain	Res	Type
32	2a	1011	G
32	2a	1016	A
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1039	C
32	2a	1040	U
32	2a	1043	C
32	2a	1044	A
32	2a	1053	G
32	2a	1061	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1084	G
32	2a	1085	U
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1099	G
32	2a	1101	A
32	2a	1113	C
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C

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Mol	Chain	Res	Type
32	2a	1144	G
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1159	U
32	2a	1160	G
32	2a	1171	G
32	2a	1181	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1192	C
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1210	C
32	2a	1211	U
32	2a	1213	A
32	2a	1214	C
32	2a	1226	C
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1246	C
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1261	A
32	2a	1262	C
32	2a	1267	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1275	A
32	2a	1276	G
32	2a	1277	C
32	2a	1279	A

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Mol	Chain	Res	Type
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1290	G
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1311	G
32	2a	1312	G
32	2a	1322	C
32	2a	1323	G
32	2a	1337	G
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1364	U
32	2a	1368	G
32	2a	1370	G
32	2a	1376	U
32	2a	1381	U
32	2a	1397	C
32	2a	1398	A
32	2a	1400	5MC
32	2a	1401	G
32	2a	1404	5MC
32	2a	1419	G
32	2a	1440	C
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1446	U
32	2a	1447	A
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A

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Mol	Chain	Res	Type
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	19	PSU
53	2v	22	U
53	2v	23	A
54	2w	3	C
54	2w	8	4SU
54	2w	9	A
54	2w	10	G
54	2w	11	C
54	2w	14	A
54	2w	19	G
54	2w	24	G
54	2w	25	C
54	2w	34	G
54	2w	41	C
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	61	C
54	2w	63	G
54	2w	68	C
54	2w	69	G
55	2x	9	G
55	2x	18	G
55	2x	21	A
55	2x	22	G
55	2x	43	A
55	2x	47	U
55	2x	48	C
55	2x	61	C
55	2x	69	C
55	2x	76	A
54	2y	13	C
54	2y	15	G
54	2y	19	G
54	2y	23	A
54	2y	27	G

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Mol	Chain	Res	Type
54	2y	34	G
54	2y	36	A
54	2y	40	C
54	2y	43	C
54	2y	45	U
54	2y	46	7MG
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	59	U
54	2y	61	C
54	2y	62	C
54	2y	65	G
54	2y	69	G
54	2y	70	G
54	2y	72	C

All (44) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	90	U
1	1A	266	G
1	1A	278	A
1	1A	895	U
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A
1	1A	1175	U
1	1A	1210	A
1	1A	1442	G
1	1A	1508	A
1	1A	1653	G
1	1A	1992	G
1	1A	2111	C
1	1A	2126	A
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C

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Mol	Chain	Res	Type
1	1A	2601	C
1	1A	2629	A
1	1A	2689	U
1	2A	195	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2156	G
1	2A	2351	G
1	2A	2689	U
1	2A	2756	U

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

86 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	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.48	3 (11%)
55	4SU	2x	8	55,56	18,21,22	1.92	6 (33%)	26,30,33	1.71	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	5MU	2w	54	54	19,22,23	1.42	6 (31%)	28,32,35	1.87	6 (21%)
54	PSU	2w	39	54	18,21,22	1.27	2 (11%)	22,30,33	2.08	4 (18%)
32	5MC	2a	1400	32	18,22,23	1.01	1 (5%)	26,32,35	1.43	5 (19%)
1	5MU	2A	1939	1	19,22,23	1.39	5 (26%)	28,32,35	2.19	6 (21%)
1	5MC	2A	1962	1	18,22,23	0.95	2 (11%)	26,32,35	1.18	2 (7%)
54	5MU	1w	54	54	19,22,23	1.44	6 (31%)	28,32,35	1.81	8 (28%)
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
54	PSU	2y	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.82	3 (13%)
32	MA6	2a	1518	32	19,26,27	0.98	1 (5%)	18,38,41	1.68	4 (22%)
1	OMG	1A	2251	55,56,1	18,26,27	0.95	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	1A	1911	1	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
54	7MG	1y	46	54	22,26,27	1.36	3 (13%)	29,39,42	2.63	6 (20%)
54	4SU	2y	8	54,56	18,21,22	1.67	4 (22%)	26,30,33	2.31	6 (23%)
54	PSU	1w	32	54	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
54	7MG	2w	46	54	22,26,27	1.34	4 (18%)	29,39,42	2.49	7 (24%)
55	PSU	1x	55	55	18,21,22	1.33	2 (11%)	22,30,33	1.98	4 (18%)
43	0TD	1l	92	43	7,9,10	4.69	1 (14%)	6,11,13	7.22	2 (33%)
1	PSU	1A	2605	1	18,21,22	1.34	2 (11%)	22,30,33	1.83	4 (18%)
1	2MU	1A	2552	56,1	19,22,24	1.26	3 (15%)	26,31,36	1.85	6 (23%)
54	PSU	2w	55	54	18,21,22	1.37	2 (11%)	22,30,33	1.93	3 (13%)
1	2MA	2A	2503	1	17,25,26	0.99	1 (5%)	17,37,40	0.97	2 (11%)
32	5MC	1a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.11	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
54	PSU	1w	55	54	18,21,22	1.41	2 (11%)	22,30,33	1.94	3 (13%)
1	PSU	2A	1911	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
54	PSU	1y	39	54	18,21,22	1.30	2 (11%)	22,30,33	1.99	3 (13%)
32	MA6	2a	1519	32	19,26,27	0.99	1 (5%)	18,38,41	1.60	5 (27%)
32	7MG	2a	527	32	22,26,27	1.34	3 (13%)	29,39,42	2.50	6 (20%)
54	7MG	2y	46	54	22,26,27	1.41	3 (13%)	29,39,42	2.61	6 (20%)
32	4OC	1a	1402	32	20,23,24	0.75	0	26,32,35	0.92	1 (3%)
53	PSU	1v	19	53,54	18,21,22	1.44	3 (16%)	22,30,33	1.48	3 (13%)
32	5MC	2a	1404	32	18,22,23	0.97	1 (5%)	26,32,35	1.17	3 (11%)
54	PSU	2y	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.85	4 (18%)
32	MA6	1a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.72	6 (33%)
53	PSU	2v	19	53,54,56	18,21,22	1.38	2 (11%)	22,30,33	1.82	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	4SU	1w	8	54	18,21,22	1.70	4 (22%)	26,30,33	2.11	5 (19%)
32	7MG	1a	527	32,56	22,26,27	1.34	3 (13%)	29,39,42	2.51	6 (20%)
1	5MC	1A	1942	1	18,22,23	0.95	2 (11%)	26,32,35	1.17	3 (11%)
54	MIA	2w	37	54	20,27,32	1.84	2 (10%)	22,39,47	1.87	7 (31%)
54	PSU	1y	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.94	4 (18%)
1	PSU	2A	2605	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
32	M2G	2a	966	32	20,27,28	1.47	3 (15%)	22,40,43	0.93	2 (9%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	22,30,33	1.80	4 (18%)
1	2MA	1A	2503	56,1	17,25,26	1.00	1 (5%)	17,37,40	0.98	2 (11%)
32	5MC	2a	1407	32,56	18,22,23	0.94	2 (11%)	26,32,35	1.12	3 (11%)
1	5MU	2A	1915	1	19,22,23	1.46	5 (26%)	28,32,35	2.03	7 (25%)
54	MIA	1w	37	54	24,31,32	2.27	3 (12%)	26,44,47	2.54	10 (38%)
1	2MU	2A	2552	56,1	19,22,24	1.24	3 (15%)	26,31,36	1.79	6 (23%)
1	5MU	1A	1915	1	19,22,23	1.39	5 (26%)	28,32,35	2.03	7 (25%)
54	PSU	2y	39	54	18,21,22	1.36	2 (11%)	22,30,33	1.71	3 (13%)
54	4SU	1y	8	54	18,21,22	1.63	4 (22%)	26,30,33	2.11	4 (15%)
32	5MC	2a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.15	3 (11%)
32	UR3	2a	1498	32	19,22,23	1.05	2 (10%)	26,32,35	1.48	1 (3%)
1	5MU	1A	1939	1	19,22,23	1.44	5 (26%)	28,32,35	2.19	6 (21%)
32	5MC	1a	967	32	18,22,23	0.92	2 (11%)	26,32,35	1.11	2 (7%)
43	0TD	2l	92	43	7,9,10	4.71	1 (14%)	6,11,13	8.18	2 (33%)
54	4SU	2w	8	54	18,21,22	1.69	5 (27%)	26,30,33	2.06	4 (15%)
32	5MC	1a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.14	2 (7%)
1	5MC	1A	1962	1	18,22,23	0.95	2 (11%)	26,32,35	1.13	2 (7%)
1	4OC	2A	1920	1	19,22,24	0.81	0	26,31,35	0.88	1 (3%)
1	4OC	1A	1920	1	19,22,24	0.81	0	26,31,35	0.90	0
1	OMG	2A	2251	55,1	18,26,27	0.93	1 (5%)	19,38,41	1.10	3 (15%)
54	MIA	1y	37	54	18,24,32	1.12	2 (11%)	18,35,47	1.19	2 (11%)
54	5MU	2y	54	54	19,22,23	1.44	5 (26%)	28,32,35	2.02	5 (17%)
54	5MU	1y	54	54	19,22,23	1.37	4 (21%)	28,32,35	2.15	6 (21%)
54	PSU	1y	32	54	18,21,22	1.31	2 (11%)	22,30,33	1.87	4 (18%)
32	2MG	2a	1207	32,56	18,26,27	0.88	1 (5%)	16,38,41	1.04	2 (12%)
1	PSU	1A	1917	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
54	PSU	1w	39	54	18,21,22	1.24	1 (5%)	22,30,33	2.11	4 (18%)
55	5MC	1x	32	55	18,22,23	0.98	2 (11%)	26,32,35	1.14	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	MA6	1a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.65	4 (22%)
1	5MC	2A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.21	2 (7%)
55	5MU	2x	54	55	19,22,23	1.40	5 (26%)	28,32,35	2.10	6 (21%)
32	4OC	2a	1402	32,56	20,23,24	0.77	0	26,32,35	0.96	0
55	5MC	2x	32	55	18,22,23	1.01	2 (11%)	26,32,35	1.21	3 (11%)
32	M2G	1a	966	32	20,27,28	1.42	3 (15%)	22,40,43	0.96	2 (9%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
55	5MU	1x	54	55	19,22,23	1.37	5 (26%)	28,32,35	1.98	7 (25%)
55	4SU	1x	8	55,56	18,21,22	1.99	4 (22%)	26,30,33	1.63	5 (19%)
54	MIA	2y	37	54,32	18,24,32	1.13	2 (11%)	18,35,47	1.22	2 (11%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.07	2 (12%)
32	PSU	1a	516	32	18,21,22	1.35	2 (11%)	22,30,33	1.76	3 (13%)
32	5MC	1a	1407	32	18,22,23	0.95	2 (11%)	26,32,35	1.09	2 (7%)
54	7MG	1w	46	54	22,26,27	1.32	3 (13%)	29,39,42	2.54	7 (24%)

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	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	2/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	5/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	2/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	4/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/7/29/30	0/3/3/3
1	OMG	1A	2251	55,56,1	-	0/5/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
54	4SU	2y	8	54,56	-	1/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1	-	1/3/25/26	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	5/7/29/30	0/3/3/3
32	7MG	2a	527	32	-	3/7/37/38	0/3/3/3
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
53	PSU	1v	19	53,54	-	3/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	3/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
53	PSU	2v	19	53,54,56	-	2/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	1/7/29/34	0/3/3/3
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
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	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	56,1	-	2/3/25/26	0/3/3/3
32	5MC	2a	1407	32,56	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	2/11/33/34	0/3/3/3
1	2MU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	2/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	2/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
1	4OC	1A	1920	1	-	0/9/27/30	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
54	MIA	1y	37	54	-	2/3/25/34	0/3/3/3
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	2/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	1/5/27/28	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
55	PSU	2x	55	55	-	1/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55,56	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54,32	-	2/3/25/34	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	0/7/37/38	0/3/3/3

All (207) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.15	1.69	1.82
43	1l	92	0TD	CB-SB	-12.07	1.69	1.82
54	1w	37	MIA	C13-C14	7.24	1.53	1.32
54	1w	37	MIA	C2-S10	-7.02	1.69	1.75
54	2w	37	MIA	C2-S10	-6.89	1.69	1.75
32	2a	966	M2G	C2-N3	4.74	1.36	1.30
54	2y	8	4SU	C4-S4	-4.46	1.59	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	966	M2G	C2-N3	4.42	1.36	1.30
54	2w	8	4SU	C4-S4	-4.41	1.60	1.68
55	1x	8	4SU	C4-S4	-4.39	1.60	1.68
54	1w	8	4SU	C4-S4	-4.31	1.60	1.68
55	1x	8	4SU	C4-N3	-4.23	1.33	1.37
55	2x	8	4SU	C4-S4	-4.23	1.60	1.68
54	1y	8	4SU	C4-S4	-4.14	1.60	1.68
55	2x	8	4SU	C4-N3	-3.96	1.33	1.37
54	2w	55	PSU	C6-C5	3.82	1.39	1.35
54	1w	55	PSU	C6-C5	3.80	1.39	1.35
53	1v	19	PSU	C6-C5	3.68	1.39	1.35
54	2y	39	PSU	C6-C5	3.66	1.39	1.35
54	1y	55	PSU	C6-C5	3.58	1.39	1.35
54	2y	32	PSU	C6-C5	3.48	1.39	1.35
55	2x	55	PSU	C6-C5	3.40	1.39	1.35
54	1w	32	PSU	C6-C5	3.38	1.39	1.35
54	1y	32	PSU	C6-C5	3.37	1.39	1.35
55	1x	55	PSU	C6-C5	3.36	1.39	1.35
55	1x	8	4SU	C2-N3	-3.35	1.32	1.38
1	2A	1917	PSU	C6-C5	3.35	1.39	1.35
1	1A	2605	PSU	C6-C5	3.31	1.39	1.35
54	1y	39	PSU	C6-C5	3.27	1.39	1.35
54	2y	46	7MG	C5-C4	3.26	1.48	1.38
54	2w	46	7MG	C4-N9	-3.26	1.33	1.37
32	2a	516	PSU	C6-C5	3.22	1.39	1.35
32	1a	516	PSU	C6-C5	3.21	1.39	1.35
54	2w	32	PSU	C6-C5	3.21	1.39	1.35
1	1A	1917	PSU	C6-C5	3.21	1.39	1.35
54	2y	55	PSU	C6-C5	3.21	1.39	1.35
54	1y	46	7MG	C5-C4	3.20	1.48	1.38
54	2w	39	PSU	C6-C5	3.19	1.39	1.35
32	1a	527	7MG	C4-N9	-3.17	1.34	1.37
53	2v	19	PSU	C6-C5	3.14	1.39	1.35
1	2A	2605	PSU	C6-C5	3.14	1.39	1.35
55	1x	8	4SU	C5-C4	-3.13	1.38	1.42
32	2a	527	7MG	C4-N9	-3.12	1.34	1.37
1	2A	1911	PSU	C6-C5	3.11	1.38	1.35
1	1A	1911	PSU	C6-C5	3.10	1.38	1.35
55	2x	8	4SU	C5-C4	-3.07	1.38	1.42
54	1w	46	7MG	C5-C4	3.04	1.48	1.38
54	2w	46	7MG	C5-C4	3.03	1.48	1.38
54	1w	46	7MG	C4-N9	-3.02	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	8	4SU	C4-N3	-2.99	1.34	1.37
54	1w	39	PSU	C6-C5	2.99	1.38	1.35
32	2a	1404	5MC	C6-C5	2.98	1.39	1.34
32	1a	527	7MG	C5-C4	2.98	1.47	1.38
54	2y	54	5MU	C6-C5	2.95	1.39	1.34
53	1v	19	PSU	C4-N3	-2.95	1.33	1.38
32	1a	966	M2G	C2-N2	2.94	1.40	1.35
54	2w	54	5MU	C6-C5	2.93	1.39	1.34
32	2a	527	7MG	C5-C4	2.92	1.47	1.38
55	2x	32	5MC	C6-C5	2.90	1.39	1.34
54	1y	54	5MU	C6-C5	2.90	1.39	1.34
1	2A	1942	5MC	C6-C5	2.89	1.39	1.34
32	1a	1400	5MC	C6-C5	2.89	1.39	1.34
1	2A	1915	5MU	C6-C5	2.86	1.39	1.34
32	2a	966	M2G	C2-N2	2.84	1.40	1.35
55	1x	32	5MC	C6-C5	2.84	1.39	1.34
1	1A	1939	5MU	C6-C5	2.83	1.39	1.34
1	1A	2552	2MU	C4-N3	-2.79	1.33	1.38
1	1A	1939	5MU	C4-N3	-2.79	1.33	1.38
32	1a	1404	5MC	C6-C5	2.79	1.39	1.34
32	2a	1400	5MC	C6-C5	2.78	1.39	1.34
54	1w	8	4SU	C4-N3	-2.76	1.34	1.37
32	2a	967	5MC	C6-C5	2.76	1.39	1.34
54	1y	8	4SU	C4-N3	-2.75	1.34	1.37
55	2x	54	5MU	C6-C5	2.75	1.39	1.34
1	2A	1962	5MC	C6-C5	2.74	1.39	1.34
54	2y	37	MIA	C2-N3	2.73	1.36	1.32
1	1A	1911	PSU	C4-N3	-2.73	1.33	1.38
32	1a	1407	5MC	C6-C5	2.73	1.39	1.34
32	1a	1207	2MG	C6-N1	-2.73	1.33	1.37
1	1A	1915	5MU	C6-C5	2.73	1.39	1.34
1	2A	1939	5MU	C6-C5	2.72	1.39	1.34
54	1y	37	MIA	C5-C4	2.71	1.48	1.40
1	2A	1911	PSU	C4-N3	-2.70	1.33	1.38
54	1w	8	4SU	C5-C4	-2.70	1.39	1.42
1	1A	1942	5MC	C6-C5	2.70	1.39	1.34
54	1w	37	MIA	C5-C4	2.70	1.48	1.40
1	2A	1917	PSU	C4-N3	-2.69	1.33	1.38
54	2y	54	5MU	C4-N3	-2.68	1.33	1.38
54	1y	37	MIA	C2-N3	2.68	1.36	1.32
55	1x	54	5MU	C6-C5	2.67	1.39	1.34
54	2y	37	MIA	C5-C4	2.67	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	8	4SU	C4-N3	-2.67	1.34	1.37
1	2A	1939	5MU	C4-N3	-2.67	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.66	1.33	1.38
32	2a	1407	5MC	C6-C5	2.66	1.39	1.34
54	2y	55	PSU	C4-N3	-2.66	1.33	1.38
54	1w	54	5MU	C4-N3	-2.66	1.33	1.38
1	2A	2605	PSU	C4-N3	-2.66	1.33	1.38
54	2w	37	MIA	C5-C4	2.65	1.47	1.40
54	2y	46	7MG	C6-N1	-2.64	1.33	1.38
54	1w	54	5MU	C6-C5	2.63	1.38	1.34
1	1A	1962	5MC	C6-C5	2.61	1.38	1.34
1	1A	2605	PSU	C4-N3	-2.61	1.34	1.38
32	2a	1519	MA6	C5-C4	2.61	1.47	1.40
1	2A	1915	5MU	C4-C5	2.61	1.49	1.44
32	1a	1519	MA6	C5-C4	2.60	1.47	1.40
32	1a	967	5MC	C6-C5	2.60	1.38	1.34
54	1w	54	5MU	C2-N1	2.59	1.42	1.38
54	2y	39	PSU	C4-N3	-2.58	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.58	1.34	1.38
1	1A	2251	OMG	C6-N1	-2.58	1.34	1.37
32	2a	1518	MA6	C5-C4	2.57	1.47	1.40
1	1A	1917	PSU	C4-N3	-2.57	1.34	1.38
54	2w	54	5MU	C4-N3	-2.56	1.34	1.38
54	1w	32	PSU	C4-N3	-2.55	1.34	1.38
1	2A	2552	2MU	C4-N3	-2.55	1.34	1.38
53	2v	19	PSU	C4-N3	-2.55	1.34	1.38
54	1w	55	PSU	C4-N3	-2.54	1.34	1.38
32	1a	1518	MA6	C5-C4	2.54	1.47	1.40
54	2w	32	PSU	C4-N3	-2.53	1.34	1.38
55	2x	8	4SU	C2-N1	2.53	1.42	1.38
54	1y	32	PSU	C4-N3	-2.52	1.34	1.38
55	2x	55	PSU	C4-N3	-2.51	1.34	1.38
32	2a	516	PSU	C4-N3	-2.51	1.34	1.38
55	2x	54	5MU	C4-N3	-2.50	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.49	1.34	1.37
54	2w	8	4SU	C5-C4	-2.49	1.39	1.42
54	2y	8	4SU	C5-C4	-2.49	1.39	1.42
54	1y	54	5MU	C4-N3	-2.48	1.34	1.38
54	2y	46	7MG	C8-N9	2.48	1.47	1.46
32	1a	516	PSU	C4-N3	-2.47	1.34	1.38
55	1x	55	PSU	C4-N3	-2.46	1.34	1.38
54	2y	54	5MU	C2-N1	2.45	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C6-N1	-2.44	1.33	1.38
32	2a	966	M2G	C6-N1	-2.44	1.34	1.37
54	1y	46	7MG	C6-N1	-2.43	1.34	1.38
54	2y	32	PSU	C4-N3	-2.42	1.34	1.38
54	1w	8	4SU	C2-N1	2.41	1.42	1.38
55	2x	54	5MU	C2-N1	2.40	1.42	1.38
55	1x	54	5MU	C4-N3	-2.39	1.34	1.38
55	2x	8	4SU	C2-N3	-2.38	1.33	1.38
1	2A	1939	5MU	C6-N1	-2.37	1.34	1.38
1	1A	1915	5MU	C4-C5	2.37	1.48	1.44
32	2a	527	7MG	C6-N1	-2.36	1.34	1.38
55	1x	54	5MU	C4-C5	2.36	1.48	1.44
32	1a	966	M2G	C6-N1	-2.36	1.34	1.37
55	2x	54	5MU	C4-C5	2.35	1.48	1.44
54	1y	54	5MU	C4-C5	2.35	1.48	1.44
54	1y	55	PSU	C4-N3	-2.35	1.34	1.38
1	2A	1915	5MU	C2-N1	2.35	1.42	1.38
1	1A	1939	5MU	C4-C5	2.35	1.48	1.44
54	2w	54	5MU	C4-C5	2.35	1.48	1.44
54	1y	46	7MG	C8-N9	2.34	1.47	1.46
54	2w	55	PSU	C4-N3	-2.33	1.34	1.38
55	2x	8	4SU	O2-C2	2.32	1.27	1.23
55	1x	32	5MC	C6-N1	-2.32	1.34	1.38
1	1A	2503	2MA	C2-N3	2.29	1.36	1.31
1	1A	1962	5MC	C6-N1	-2.29	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.29	1.33	1.38
1	2A	1962	5MC	C6-N1	-2.29	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.28	1.34	1.38
1	1A	2552	2MU	C5-C4	2.27	1.48	1.43
1	2A	1939	5MU	C4-C5	2.27	1.48	1.44
1	2A	2552	2MU	C5-C4	2.25	1.48	1.43
54	1y	39	PSU	C4-N3	-2.25	1.34	1.38
32	1a	527	7MG	C6-N1	-2.25	1.34	1.38
54	2y	54	5MU	C4-C5	2.24	1.48	1.44
32	2a	1498	UR3	C2-N1	2.24	1.41	1.38
32	2a	1207	2MG	C6-N1	-2.22	1.34	1.37
32	1a	1404	5MC	C6-N1	-2.21	1.34	1.38
32	1a	967	5MC	C6-N1	-2.21	1.34	1.38
32	2a	967	5MC	C6-N1	-2.20	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.20	1.34	1.38
54	1y	8	4SU	C2-N1	2.20	1.42	1.38
1	1A	1915	5MU	C2-N1	2.19	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	54	5MU	C2-N1	2.18	1.41	1.38
54	1y	8	4SU	C5-C4	-2.17	1.39	1.42
32	1a	1498	UR3	C2-N1	2.16	1.41	1.38
54	2w	54	5MU	C2-N3	-2.16	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.16	1.34	1.38
54	1w	54	5MU	C4-C5	2.16	1.48	1.44
55	2x	32	5MC	C6-N1	-2.14	1.34	1.38
54	1y	54	5MU	C6-N1	-2.14	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.14	1.34	1.38
1	2A	2503	2MA	C2-N3	2.13	1.35	1.31
32	1a	1400	5MC	C6-N1	-2.13	1.34	1.38
54	1w	54	5MU	C2-N3	-2.13	1.34	1.38
54	2w	39	PSU	C4-C5	2.12	1.50	1.44
1	2A	1939	5MU	C2-N3	-2.11	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.11	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.10	1.34	1.38
54	2w	54	5MU	C6-N1	-2.09	1.34	1.38
53	1v	19	PSU	C2-N3	-2.09	1.33	1.37
32	2a	1498	UR3	C6-C5	2.08	1.39	1.35
55	1x	54	5MU	C6-N1	-2.07	1.34	1.38
54	2y	54	5MU	C2-N3	-2.07	1.34	1.38
54	2y	8	4SU	C2-N1	2.07	1.41	1.38
1	1A	2552	2MU	C2-N3	-2.07	1.34	1.38
54	2w	46	7MG	C6-N1	-2.06	1.35	1.38
54	2w	54	5MU	C2-N1	2.06	1.41	1.38
54	1w	46	7MG	C6-N1	-2.04	1.35	1.38
55	2x	54	5MU	C6-N1	-2.04	1.34	1.38
54	1w	54	5MU	C6-N1	-2.03	1.34	1.38
1	2A	2552	2MU	C2-N1	2.03	1.41	1.38
54	2w	46	7MG	C8-N9	2.03	1.47	1.46
54	2w	8	4SU	C2-N1	2.03	1.41	1.38
54	2w	8	4SU	C2-N3	-2.00	1.34	1.38

All (330) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-19.84	66.54	102.44
43	1l	92	0TD	CSB-SB-CB	-17.44	70.90	102.44
54	2y	46	7MG	N9-C4-N3	9.74	140.03	125.47
54	1y	46	7MG	N9-C4-N3	9.71	139.99	125.47
54	1w	46	7MG	N9-C4-N3	8.86	138.72	125.47
32	1a	527	7MG	N9-C4-N3	8.73	138.53	125.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	527	7MG	N9-C4-N3	8.70	138.49	125.47
54	2w	46	7MG	N9-C4-N3	8.48	138.16	125.47
54	1w	37	MIA	C12-C13-C14	-7.80	111.96	127.14
54	2y	8	4SU	C4-N3-C2	-7.07	120.47	127.34
54	1y	8	4SU	C4-N3-C2	-6.62	120.91	127.34
54	1w	39	PSU	N1-C2-N3	6.31	122.28	115.13
54	2w	8	4SU	C4-N3-C2	-6.24	121.28	127.34
1	2A	1917	PSU	N1-C2-N3	6.19	122.15	115.13
54	2y	8	4SU	C5-C4-N3	6.19	120.43	114.69
54	2w	39	PSU	N1-C2-N3	6.16	122.11	115.13
54	1y	39	PSU	N1-C2-N3	6.15	122.09	115.13
55	1x	55	PSU	N1-C2-N3	6.15	122.09	115.13
54	1y	55	PSU	N1-C2-N3	6.05	121.98	115.13
1	1A	1911	PSU	N1-C2-N3	6.00	121.92	115.13
54	2w	55	PSU	N1-C2-N3	5.99	121.92	115.13
32	2a	1498	UR3	C4-N3-C2	-5.97	118.94	124.56
1	1A	1917	PSU	N1-C2-N3	5.95	121.87	115.13
32	1a	1498	UR3	C4-N3-C2	-5.91	119.00	124.56
55	2x	55	PSU	N1-C2-N3	5.91	121.83	115.13
54	1w	8	4SU	C4-N3-C2	-5.91	121.60	127.34
54	1w	32	PSU	N1-C2-N3	5.90	121.82	115.13
1	2A	1911	PSU	N1-C2-N3	5.90	121.82	115.13
54	1w	55	PSU	N1-C2-N3	5.90	121.81	115.13
54	2w	32	PSU	N1-C2-N3	5.89	121.80	115.13
54	1y	32	PSU	N1-C2-N3	5.84	121.74	115.13
54	2y	46	7MG	C5-C4-N3	-5.81	117.06	128.13
53	2v	19	PSU	N1-C2-N3	5.79	121.69	115.13
54	2y	32	PSU	N1-C2-N3	5.78	121.68	115.13
1	2A	2605	PSU	N1-C2-N3	5.76	121.66	115.13
54	2w	8	4SU	C5-C4-N3	5.76	120.03	114.69
54	2y	55	PSU	N1-C2-N3	5.73	121.62	115.13
54	1y	46	7MG	C5-C4-N3	-5.70	117.27	128.13
32	2a	516	PSU	N1-C2-N3	5.67	121.55	115.13
54	1w	8	4SU	C5-C4-N3	5.60	119.88	114.69
32	1a	516	PSU	N1-C2-N3	5.58	121.45	115.13
54	2w	46	7MG	N9-C8-N7	-5.55	95.44	103.38
32	2a	527	7MG	N9-C8-N7	-5.50	95.51	103.38
1	1A	2605	PSU	N1-C2-N3	5.50	121.36	115.13
1	1A	1939	5MU	C4-N3-C2	-5.50	120.23	127.35
1	2A	1939	5MU	C4-N3-C2	-5.50	120.24	127.35
54	1y	54	5MU	C4-N3-C2	-5.47	120.27	127.35
32	1a	527	7MG	C5-C4-N3	-5.45	117.73	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	8	4SU	C5-C4-N3	5.44	119.74	114.69
54	2y	39	PSU	N1-C2-N3	5.41	121.25	115.13
1	1A	2552	2MU	N3-C2-N1	5.30	121.93	114.89
1	1A	1939	5MU	N3-C2-N1	5.30	121.93	114.89
54	1w	46	7MG	C5-C4-N3	-5.30	118.03	128.13
54	1y	54	5MU	N3-C2-N1	5.27	121.89	114.89
32	2a	527	7MG	C5-C4-N3	-5.27	118.09	128.13
55	2x	54	5MU	C4-N3-C2	-5.26	120.54	127.35
54	1w	46	7MG	N9-C8-N7	-5.23	95.90	103.38
32	1a	527	7MG	N9-C8-N7	-5.19	95.95	103.38
1	2A	2552	2MU	N3-C2-N1	5.19	121.78	114.89
1	2A	1915	5MU	C4-N3-C2	-5.13	120.72	127.35
1	2A	1915	5MU	N3-C2-N1	5.11	121.67	114.89
55	2x	54	5MU	N3-C2-N1	5.07	121.63	114.89
1	2A	1939	5MU	N3-C2-N1	5.03	121.57	114.89
1	1A	1915	5MU	C4-N3-C2	-5.03	120.84	127.35
55	1x	54	5MU	N3-C2-N1	4.96	121.48	114.89
54	2y	54	5MU	C4-N3-C2	-4.96	120.93	127.35
54	2w	46	7MG	C5-C4-N3	-4.88	118.83	128.13
1	1A	1915	5MU	N3-C2-N1	4.87	121.36	114.89
54	2y	54	5MU	N3-C2-N1	4.86	121.34	114.89
54	2w	39	PSU	C4-N3-C2	-4.86	119.33	126.34
53	1v	19	PSU	N1-C2-N3	4.84	120.61	115.13
54	1w	39	PSU	C4-N3-C2	-4.81	119.41	126.34
54	1y	46	7MG	N9-C8-N7	-4.80	96.51	103.38
55	1x	54	5MU	C4-N3-C2	-4.73	121.23	127.35
55	2x	8	4SU	C1'-N1-C2	4.69	126.06	117.57
1	1A	1939	5MU	C5-C6-N1	-4.61	118.60	123.34
54	2y	54	5MU	C5-C4-N3	4.60	119.24	115.31
1	2A	1939	5MU	C5-C4-N3	4.60	119.24	115.31
54	2w	54	5MU	N3-C2-N1	4.55	120.93	114.89
54	2w	54	5MU	C4-N3-C2	-4.53	121.49	127.35
55	1x	8	4SU	C5-C4-N3	4.52	118.88	114.69
54	1y	46	7MG	C2-N3-C4	4.51	120.34	112.30
54	1y	54	5MU	C5-C4-N3	4.50	119.15	115.31
54	2y	46	7MG	C2-N3-C4	4.50	120.32	112.30
1	1A	1915	5MU	C5-C4-N3	4.47	119.12	115.31
54	2y	46	7MG	N9-C8-N7	-4.45	97.02	103.38
55	2x	54	5MU	C5-C4-N3	4.43	119.09	115.31
32	1a	527	7MG	C2-N3-C4	4.43	120.19	112.30
1	1A	2552	2MU	C4-N3-C2	-4.41	120.76	126.58
1	2A	1939	5MU	C5-C6-N1	-4.41	118.80	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1939	5MU	C5-C4-N3	4.35	119.02	115.31
54	2w	37	MIA	C2-N3-C4	4.34	121.31	115.32
1	2A	2552	2MU	C4-N3-C2	-4.33	120.87	126.58
54	2y	8	4SU	C5-C4-S4	-4.31	118.91	124.47
1	2A	1915	5MU	C5-C4-N3	4.31	118.99	115.31
55	2x	8	4SU	C5-C4-N3	4.30	118.68	114.69
54	1w	46	7MG	C2-N3-C4	4.30	119.95	112.30
32	2a	527	7MG	C2-N3-C4	4.28	119.93	112.30
54	1y	39	PSU	C4-N3-C2	-4.17	120.33	126.34
1	2A	1939	5MU	O4-C4-C5	-4.14	120.10	124.90
1	1A	1911	PSU	C4-N3-C2	-4.14	120.38	126.34
54	1w	39	PSU	O2-C2-N1	-4.13	118.24	122.79
55	2x	54	5MU	O4-C4-C5	-4.13	120.12	124.90
54	2w	46	7MG	C2-N3-C4	4.10	119.60	112.30
54	1w	37	MIA	C15-C14-C13	-4.09	110.81	122.65
54	1y	39	PSU	O2-C2-N1	-4.08	118.29	122.79
1	2A	2605	PSU	C4-N3-C2	-4.06	120.48	126.34
54	1y	54	5MU	O4-C4-C5	-4.06	120.20	124.90
54	1w	37	MIA	C2-N3-C4	4.05	120.90	115.32
54	2w	54	5MU	C5-C4-N3	4.04	118.76	115.31
54	1w	8	4SU	C5-C4-S4	-4.03	119.27	124.47
55	1x	55	PSU	C4-N3-C2	-4.03	120.53	126.34
54	1y	8	4SU	N3-C2-N1	4.01	120.21	114.89
55	1x	54	5MU	O4-C4-C5	-3.99	120.28	124.90
55	2x	55	PSU	C4-N3-C2	-3.95	120.65	126.34
54	1w	54	5MU	C5-C4-N3	3.94	118.67	115.31
1	2A	1942	5MC	C5-C6-N1	-3.91	119.31	123.34
54	1y	32	PSU	C4-N3-C2	-3.91	120.70	126.34
54	2y	54	5MU	O4-C4-C5	-3.91	120.37	124.90
54	1w	37	MIA	C16-C14-C13	-3.87	111.45	122.65
1	1A	2605	PSU	C4-N3-C2	-3.87	120.76	126.34
1	2A	1911	PSU	C4-N3-C2	-3.87	120.77	126.34
1	2A	1917	PSU	C4-N3-C2	-3.87	120.77	126.34
54	1w	37	MIA	C5-C6-N1	-3.85	117.61	120.81
1	1A	1917	PSU	C4-N3-C2	-3.85	120.79	126.34
54	2y	8	4SU	N3-C2-N1	3.85	120.00	114.89
54	1y	55	PSU	C4-N3-C2	-3.84	120.81	126.34
55	1x	54	5MU	C5-C4-N3	3.83	118.58	115.31
54	1y	55	PSU	O2-C2-N1	-3.82	118.59	122.79
1	1A	1915	5MU	O4-C4-C5	-3.78	120.52	124.90
54	1w	32	PSU	C4-N3-C2	-3.76	120.91	126.34
54	2y	55	PSU	C4-N3-C2	-3.76	120.91	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	54	5MU	C5-C6-N1	-3.76	119.47	123.34
1	1A	1962	5MC	C5-C6-N1	-3.76	119.47	123.34
54	1w	54	5MU	C4-N3-C2	-3.75	122.50	127.35
54	2w	55	PSU	O2-C2-N1	-3.74	118.67	122.79
54	2w	32	PSU	C4-N3-C2	-3.74	120.95	126.34
54	1w	54	5MU	N3-C2-N1	3.72	119.83	114.89
32	1a	1404	5MC	C5-C6-N1	-3.72	119.51	123.34
54	2w	54	5MU	O4-C4-C5	-3.70	120.61	124.90
1	1A	1917	PSU	O2-C2-N1	-3.68	118.74	122.79
32	1a	1400	5MC	C5-C6-N1	-3.68	119.55	123.34
54	2w	55	PSU	C4-N3-C2	-3.67	121.06	126.34
32	2a	516	PSU	C4-N3-C2	-3.65	121.08	126.34
54	2y	32	PSU	C4-N3-C2	-3.64	121.09	126.34
1	1A	1939	5MU	O4-C4-C5	-3.63	120.69	124.90
54	1w	54	5MU	O4-C4-C5	-3.63	120.70	124.90
54	2w	8	4SU	N3-C2-N1	3.62	119.70	114.89
54	1w	55	PSU	C4-N3-C2	-3.62	121.12	126.34
55	1x	55	PSU	O2-C2-N1	-3.62	118.81	122.79
54	1w	55	PSU	O2-C2-N1	-3.61	118.82	122.79
54	1y	8	4SU	C5-C4-S4	-3.58	119.86	124.47
54	2w	39	PSU	O2-C2-N1	-3.57	118.86	122.79
54	1w	32	PSU	O2-C2-N1	-3.57	118.86	122.79
53	2v	19	PSU	O2-C2-N1	-3.56	118.87	122.79
53	2v	19	PSU	C4-N3-C2	-3.55	121.22	126.34
54	2w	8	4SU	C5-C4-S4	-3.54	119.91	124.47
54	2w	37	MIA	C5-C6-N1	-3.52	117.89	120.81
54	2y	54	5MU	C5-C6-N1	-3.52	119.72	123.34
32	2a	1400	5MC	O2-C2-N3	-3.52	116.61	122.33
32	2a	1518	MA6	C9-N6-C6	-3.49	108.94	119.51
54	1w	8	4SU	N3-C2-N1	3.49	119.52	114.89
54	2y	39	PSU	C4-N3-C2	-3.48	121.32	126.34
55	2x	54	5MU	C5-C6-N1	-3.48	119.76	123.34
1	1A	1942	5MC	C5-C6-N1	-3.47	119.77	123.34
54	2w	54	5MU	C5-C6-N1	-3.47	119.77	123.34
54	2y	32	PSU	O2-C2-N1	-3.47	118.97	122.79
32	2a	1518	MA6	C4-C5-N7	-3.47	105.78	109.40
55	1x	32	5MC	C5-C6-N1	-3.47	119.77	123.34
1	2A	1915	5MU	C5-C6-N1	-3.47	119.77	123.34
54	2w	37	MIA	C12-N6-C6	-3.46	119.89	122.87
32	2a	1404	5MC	C5-C6-N1	-3.44	119.80	123.34
32	2a	1518	MA6	N3-C2-N1	-3.40	123.36	128.68
32	1a	516	PSU	C4-N3-C2	-3.40	121.44	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1518	MA6	C9-N6-C6	-3.40	109.23	119.51
32	2a	967	5MC	C5-C6-N1	-3.39	119.85	123.34
32	1a	1518	MA6	N3-C2-N1	-3.38	123.40	128.68
1	2A	1962	5MC	C5-C6-N1	-3.37	119.87	123.34
32	1a	967	5MC	C5-C6-N1	-3.37	119.87	123.34
32	2a	1519	MA6	C4-C5-N7	-3.35	105.91	109.40
1	2A	1917	PSU	O2-C2-N1	-3.34	119.11	122.79
55	2x	32	5MC	C5-C6-N1	-3.32	119.92	123.34
1	1A	1915	5MU	C5-C6-N1	-3.31	119.94	123.34
32	1a	516	PSU	O2-C2-N1	-3.30	119.16	122.79
54	2w	32	PSU	O2-C2-N1	-3.28	119.18	122.79
1	1A	1911	PSU	O2-C2-N1	-3.28	119.18	122.79
32	1a	1519	MA6	N1-C6-N6	3.25	120.48	117.06
55	2x	55	PSU	O2-C2-N1	-3.24	119.22	122.79
1	2A	1911	PSU	O2-C2-N1	-3.24	119.22	122.79
54	1y	37	MIA	N3-C2-N1	-3.24	123.62	128.68
1	2A	1915	5MU	O4-C4-C5	-3.23	121.16	124.90
32	1a	1407	5MC	C5-C6-N1	-3.23	120.02	123.34
32	2a	516	PSU	O2-C2-N1	-3.21	119.25	122.79
32	1a	1518	MA6	C4-C5-N7	-3.21	106.05	109.40
32	2a	1519	MA6	C9-N6-C6	-3.21	109.79	119.51
54	1y	54	5MU	O2-C2-N1	-3.20	118.53	122.79
54	2y	37	MIA	N3-C2-N1	-3.17	123.73	128.68
55	1x	8	4SU	C1'-N1-C2	3.15	123.26	117.57
54	1w	37	MIA	C11-S10-C2	-3.14	99.92	102.27
32	2a	1407	5MC	C5-C6-N1	-3.14	120.11	123.34
32	1a	1519	MA6	C4-C5-N7	-3.12	106.15	109.40
54	1y	32	PSU	O2-C2-N1	-3.12	119.36	122.79
1	1A	2605	PSU	O2-C2-N1	-3.12	119.36	122.79
1	2A	1939	5MU	O2-C2-N1	-3.08	118.69	122.79
1	1A	1939	5MU	O2-C2-N1	-3.08	118.70	122.79
32	1a	1519	MA6	N3-C2-N1	-3.03	123.94	128.68
1	2A	2605	PSU	O2-C2-N1	-3.03	119.46	122.79
32	2a	1519	MA6	N3-C2-N1	-3.02	123.95	128.68
54	1w	8	4SU	C1'-N1-C2	3.01	123.03	117.57
32	1a	1519	MA6	C9-N6-C6	-3.01	110.40	119.51
1	1A	2552	2MU	O2-C2-N1	-2.95	118.87	122.79
32	2a	1400	5MC	C5-C4-N3	-2.89	118.55	121.67
54	1w	37	MIA	C2-N1-C6	2.87	122.33	117.19
32	2a	1400	5MC	C1'-N1-C6	-2.83	116.42	121.12
54	2y	37	MIA	C4-C5-N7	-2.82	106.46	109.40
54	1y	46	7MG	C5-C4-N9	-2.78	102.74	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	46	7MG	C5-C6-N1	2.78	115.88	110.99
55	2x	8	4SU	C1'-N1-C6	-2.77	114.79	120.84
54	1w	54	5MU	C1'-N1-C2	2.76	122.56	117.57
32	2a	1407	5MC	C5-C4-N3	-2.76	118.70	121.67
54	2w	37	MIA	C4-C5-N7	-2.76	106.53	109.40
1	1A	2552	2MU	C2'-C1'-N1	-2.71	108.96	114.22
54	1w	37	MIA	C4-C5-N7	-2.70	106.58	109.40
55	1x	54	5MU	O2-C2-N1	-2.70	119.19	122.79
1	2A	2552	2MU	C5-C4-N3	2.70	118.88	114.84
32	1a	527	7MG	C5-C6-N1	2.70	115.74	110.99
1	1A	2552	2MU	C5-C4-N3	2.68	118.86	114.84
55	2x	32	5MC	O2-C2-N3	-2.67	117.98	122.33
55	2x	54	5MU	O2-C2-N1	-2.67	119.24	122.79
1	2A	1942	5MC	C5-C4-N3	-2.67	118.79	121.67
1	2A	1962	5MC	C5-C4-N3	-2.67	118.79	121.67
54	1y	37	MIA	C4-C5-N7	-2.66	106.62	109.40
54	2y	46	7MG	C5-C4-N9	-2.65	102.90	106.35
55	1x	8	4SU	C6-C5-C4	-2.65	117.66	119.95
54	1w	54	5MU	C5-C6-N1	-2.65	120.61	123.34
1	2A	2552	2MU	O4-C4-C5	-2.63	120.54	125.16
55	1x	32	5MC	C5-C4-N3	-2.62	118.84	121.67
54	2y	55	PSU	O2-C2-N1	-2.62	119.91	122.79
32	2a	527	7MG	C5-C6-N1	2.60	115.58	110.99
55	2x	32	5MC	C5-C4-N3	-2.60	118.87	121.67
54	2w	46	7MG	C5-C4-N9	-2.59	102.99	106.35
54	2w	37	MIA	C2-N1-C6	2.59	121.82	117.19
54	2w	46	7MG	C5-C6-N1	2.57	115.52	110.99
54	1w	37	MIA	C12-N6-C6	-2.57	118.74	122.55
55	1x	8	4SU	O2-C2-N1	2.56	126.19	122.79
1	2A	2552	2MU	O2-C2-N1	-2.56	119.38	122.79
32	1a	1407	5MC	C5-C4-N3	-2.56	118.91	121.67
55	1x	8	4SU	O2-C2-N3	-2.55	116.75	121.50
55	1x	54	5MU	C5-C6-N1	-2.55	120.72	123.34
1	1A	1942	5MC	C5-C4-N3	-2.55	118.92	121.67
32	1a	1404	5MC	C5-C4-N3	-2.55	118.93	121.67
55	2x	8	4SU	C6-C5-C4	-2.54	117.75	119.95
32	2a	1404	5MC	C5-C4-N3	-2.52	118.95	121.67
54	1w	54	5MU	C1'-N1-C6	-2.52	116.93	121.12
32	2a	967	5MC	C5-C4-N3	-2.50	118.97	121.67
54	2w	37	MIA	C11-S10-C2	-2.50	100.40	102.27
53	1v	19	PSU	C4-N3-C2	-2.50	122.74	126.34
32	2a	1404	5MC	O2-C2-N3	-2.48	118.30	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2552	2MU	O4-C4-C5	-2.47	120.81	125.16
54	1y	46	7MG	C5-C6-N1	2.47	115.34	110.99
32	1a	1518	MA6	N1-C6-N6	2.44	119.62	117.06
1	2A	2251	OMG	C5-C6-N1	2.44	118.25	113.95
32	1a	1400	5MC	C5-C4-N3	-2.43	119.05	121.67
32	1a	1207	2MG	C8-N7-C5	2.43	107.61	102.99
32	1a	1402	4OC	C6-C5-C4	2.40	119.89	116.96
54	1w	46	7MG	C5-C4-N9	-2.38	103.26	106.35
32	1a	966	M2G	C5-C6-N1	2.38	118.15	113.95
32	1a	1518	MA6	C10-N6-C9	-2.38	108.47	116.12
1	1A	2503	2MA	C8-N7-C5	2.37	107.51	102.99
1	1A	2503	2MA	C5-C6-N1	2.36	118.09	114.02
32	2a	1400	5MC	C1'-N1-C2	2.35	123.67	118.42
1	1A	1962	5MC	C5-C4-N3	-2.35	119.14	121.67
32	1a	966	M2G	C8-N7-C5	2.34	107.44	102.99
1	1A	2251	OMG	C5-C6-N1	2.33	118.07	113.95
32	1a	967	5MC	C5-C4-N3	-2.32	119.17	121.67
1	1A	1915	5MU	O2-C2-N1	-2.32	119.70	122.79
32	2a	1207	2MG	C8-N7-C5	2.31	107.38	102.99
1	2A	2503	2MA	C5-C6-N1	2.30	117.99	114.02
1	2A	2503	2MA	C8-N7-C5	2.29	107.36	102.99
55	1x	54	5MU	C5M-C5-C4	2.27	121.27	118.77
54	2y	46	7MG	C5-C6-N1	2.27	114.99	110.99
32	2a	1518	MA6	C10-N6-C9	-2.27	108.81	116.12
32	2a	527	7MG	C5-C4-N9	-2.26	103.41	106.35
1	1A	1911	PSU	C5-C6-N1	-2.25	118.73	122.11
54	2y	39	PSU	O2-C2-N1	-2.24	120.33	122.79
32	2a	1400	5MC	C5-C6-N1	-2.24	121.04	123.34
1	2A	2552	2MU	C2'-C1'-N1	-2.23	109.89	114.22
1	2A	1915	5MU	O2-C2-N1	-2.23	119.83	122.79
1	1A	2251	OMG	C8-N7-C5	2.21	107.20	102.99
55	2x	8	4SU	O2-C2-N1	2.21	125.72	122.79
32	2a	966	M2G	C5-C6-N1	2.20	117.84	113.95
54	2y	8	4SU	O2-C2-N1	-2.20	119.87	122.79
54	2w	39	PSU	C6-C5-C4	-2.19	116.66	118.20
32	1a	1498	UR3	C1'-N1-C2	2.19	120.69	116.99
54	2w	37	MIA	N3-C2-N1	-2.18	122.98	126.98
32	2a	966	M2G	C8-N7-C5	2.17	107.13	102.99
43	1l	92	0TD	OD2-CG-CB	2.17	117.83	113.15
32	2a	1519	MA6	N1-C6-N6	2.16	119.33	117.06
1	2A	2251	OMG	C8-N7-C5	2.16	107.10	102.99
54	1w	54	5MU	C5M-C5-C4	2.16	121.14	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1207	2MG	C5-C6-N1	2.16	117.76	113.95
1	2A	2251	OMG	O6-C6-C5	-2.15	120.16	124.37
54	1w	46	7MG	O6-C6-C5	-2.15	122.26	127.54
1	1A	1942	5MC	O2-C2-N3	-2.15	118.84	122.33
1	1A	2605	PSU	C6-C5-C4	-2.14	116.70	118.20
1	2A	1915	5MU	C5M-C5-C4	2.14	121.13	118.77
32	1a	1518	MA6	C10-N6-C6	-2.13	113.06	119.51
54	1w	37	MIA	N3-C2-N1	-2.13	123.06	126.98
53	1v	19	PSU	O2-C2-N3	-2.13	117.81	121.82
55	2x	8	4SU	C5-C4-S4	-2.13	121.73	124.47
32	2a	1519	MA6	C10-N6-C6	-2.12	113.08	119.51
54	2w	46	7MG	O6-C6-C5	-2.11	122.37	127.54
54	2y	32	PSU	O4'-C1'-C2'	2.10	108.11	105.14
1	1A	1915	5MU	C5M-C5-C4	2.10	121.08	118.77
55	1x	55	PSU	C5-C6-N1	-2.09	118.98	122.11
1	2A	1920	4OC	O2-C2-N3	-2.08	118.95	122.33
32	1a	1207	2MG	C5-C6-N1	2.07	117.61	113.95
32	2a	967	5MC	O2-C2-N3	-2.07	118.97	122.33
54	1y	55	PSU	O4'-C1'-C2'	2.06	108.06	105.14
32	1a	1498	UR3	C3U-N3-C2	2.05	120.91	117.31
43	2l	92	0TD	OD2-CG-CB	2.04	117.57	113.15
54	1y	32	PSU	C5-C6-N1	-2.04	119.05	122.11
54	2y	8	4SU	C1'-N1-C2	2.04	121.26	117.57
54	1w	39	PSU	C5-C6-N1	-2.03	119.06	122.11
32	2a	516	PSU	O4'-C1'-C2'	2.03	108.00	105.14
1	2A	2605	PSU	C5-C6-N1	-2.03	119.07	122.11
54	2w	54	5MU	O2-C2-N1	-2.02	120.10	122.79
32	1a	527	7MG	C5-C4-N9	-2.02	103.72	106.35
55	1x	32	5MC	O2-C2-N3	-2.02	119.05	122.33
32	2a	1407	5MC	O2-C2-N3	-2.01	119.07	122.33

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	SB-CB-CG-OD2
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	2a	967	5MC	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
53	1v	19	PSU	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
54	1y	37	MIA	O4'-C4'-C5'-O5'
54	1y	37	MIA	C3'-C4'-C5'-O5'
54	2w	37	MIA	N1-C6-N6-C12
54	1y	46	7MG	C4'-C5'-O5'-P
54	2y	46	7MG	C2'-C1'-N9-C8
54	2y	55	PSU	O4'-C1'-C5-C4
54	2y	55	PSU	C2'-C1'-C5-C6
54	2y	55	PSU	O4'-C1'-C5-C6
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	2a	967	5MC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C4'-C5'-O5'
54	2w	46	7MG	C3'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
53	1v	19	PSU	C3'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	8	4SU	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
54	1y	46	7MG	C3'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
53	2v	19	PSU	O4'-C4'-C5'-O5'
54	1y	32	PSU	O4'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C9
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C9
54	1w	54	5MU	O4'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	2a	527	7MG	C4'-C5'-O5'-P
32	2a	1404	5MC	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	C4'-C5'-O5'-P
54	1y	46	7MG	C2'-C1'-N9-C8
54	2y	37	MIA	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1404	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
32	2a	1400	5MC	C4'-C5'-O5'-P
32	1a	1518	MA6	C5-C6-N6-C9
55	2x	55	PSU	O4'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	2y	8	4SU	C4'-C5'-O5'-P
54	1w	37	MIA	N6-C12-C13-C14
54	2y	46	7MG	C2'-C1'-N9-C4
32	1a	1402	4OC	O4'-C4'-C5'-O5'
54	2y	32	PSU	O4'-C1'-C5-C4
54	1y	55	PSU	O4'-C1'-C5-C4
32	2a	1400	5MC	C3'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C4'-C5'-O5'
54	2y	32	PSU	O4'-C4'-C5'-O5'
54	2y	55	PSU	C3'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C1'-N9-C8
55	2x	8	4SU	C2'-C1'-N1-C6
53	2v	19	PSU	C3'-C4'-C5'-O5'
54	1y	32	PSU	C3'-C4'-C5'-O5'
54	1w	54	5MU	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
54	2y	32	PSU	O4'-C1'-C5-C6
1	1A	1915	5MU	O4'-C4'-C5'-O5'
43	2l	92	0TD	SB-CB-CG-OD1
55	2x	8	4SU	C2'-C1'-N1-C2
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	527	7MG	C4'-C5'-O5'-P
53	1v	19	PSU	C4'-C5'-O5'-P

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 1466 ligands modelled in this entry, 1464 are monoatomic - leaving 2 for Mogul analysis.

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2860/2915 (98%)	0.51	88 (3%) 49 32	67, 83, 117, 127	0
1	2A	2789/2915 (95%)	0.33	106 (3%) 40 26	79, 94, 115, 128	0
2	1B	120/121 (99%)	0.15	0 100 100	77, 89, 99, 110	0
2	2B	120/121 (99%)	-0.20	0 100 100	96, 106, 115, 119	0
3	1D	275/276 (99%)	2.13	132 (48%) 0 0	71, 84, 93, 110	0
3	2D	275/276 (99%)	1.87	112 (40%) 0 0	78, 89, 98, 106	0
4	1E	204/206 (99%)	1.87	85 (41%) 0 0	70, 85, 96, 106	0
4	2E	204/206 (99%)	1.43	62 (30%) 0 0	82, 92, 100, 104	0
5	1F	203/210 (96%)	1.22	53 (26%) 0 0	72, 87, 101, 111	0
5	2F	203/210 (96%)	1.42	57 (28%) 0 0	82, 96, 105, 111	0
6	1G	181/182 (99%)	0.18	5 (2%) 53 36	77, 95, 104, 116	0
6	2G	181/182 (99%)	0.17	10 (5%) 25 15	97, 106, 113, 116	0
7	1H	174/180 (96%)	0.26	2 (1%) 80 65	81, 90, 98, 104	0
7	2H	174/180 (96%)	1.77	61 (35%) 0 0	95, 106, 112, 115	0
8	1I	146/148 (98%)	0.55	21 (14%) 2 1	86, 101, 107, 111	0
8	2I	146/148 (98%)	1.16	35 (23%) 0 0	92, 109, 117, 126	0
9	1N	140/140 (100%)	2.05	67 (47%) 0 0	74, 86, 97, 103	0
9	2N	140/140 (100%)	3.26	102 (72%) 0 0	82, 96, 104, 115	0
10	1O	122/122 (100%)	2.25	65 (53%) 0 0	73, 84, 92, 100	0
10	2O	122/122 (100%)	1.78	45 (36%) 0 0	82, 92, 99, 106	0
11	1P	149/150 (99%)	1.29	40 (26%) 0 0	67, 87, 100, 108	0
11	2P	149/150 (99%)	1.88	65 (43%) 0 0	81, 98, 111, 116	0
12	1Q	141/141 (100%)	1.36	35 (24%) 0 0	76, 86, 94, 105	0
12	2Q	141/141 (100%)	1.36	40 (28%) 0 0	85, 97, 105, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	1.62	46 (38%) 0 0	72, 83, 95, 97	0
13	2R	118/118 (100%)	1.44	31 (26%) 0 0	82, 90, 97, 99	0
14	1S	110/112 (98%)	0.16	1 (0%) 84 71	80, 89, 94, 102	0
14	2S	110/112 (98%)	-0.14	0 100 100	92, 99, 104, 108	0
15	1T	131/146 (89%)	1.46	46 (35%) 0 0	78, 87, 99, 107	0
15	2T	131/146 (89%)	1.19	32 (24%) 0 0	83, 93, 104, 108	0
16	1U	116/118 (98%)	1.94	56 (48%) 0 0	70, 83, 92, 104	0
16	2U	116/118 (98%)	1.84	54 (46%) 0 0	81, 95, 105, 111	0
17	1V	101/101 (100%)	1.20	23 (22%) 0 0	72, 86, 95, 99	0
17	2V	101/101 (100%)	1.38	26 (25%) 0 0	88, 99, 106, 109	0
18	1W	112/113 (99%)	1.52	33 (29%) 0 0	72, 82, 93, 111	0
18	2W	112/113 (99%)	1.90	46 (41%) 0 0	80, 90, 100, 112	0
19	1X	95/96 (98%)	1.13	17 (17%) 1 1	71, 84, 96, 108	0
19	2X	95/96 (98%)	1.24	20 (21%) 1 0	87, 97, 105, 111	0
20	1Y	107/110 (97%)	0.81	7 (6%) 18 11	79, 89, 102, 106	0
20	2Y	107/110 (97%)	1.95	46 (42%) 0 0	92, 99, 108, 114	0
21	1Z	154/206 (74%)	0.13	2 (1%) 77 61	85, 96, 110, 116	0
21	2Z	160/206 (77%)	-0.23	0 100 100	95, 105, 112, 120	0
22	10	83/85 (97%)	1.70	13 (15%) 2 1	75, 84, 101, 110	0
22	20	83/85 (97%)	2.11	25 (30%) 0 0	90, 97, 109, 113	0
23	11	97/98 (98%)	2.76	60 (61%) 0 0	75, 86, 102, 108	0
23	21	97/98 (98%)	1.66	44 (45%) 0 0	81, 92, 103, 107	0
24	12	70/72 (97%)	0.65	6 (8%) 10 6	80, 88, 97, 104	0
24	22	70/72 (97%)	0.19	4 (5%) 23 14	90, 100, 106, 110	0
25	13	59/60 (98%)	0.76	3 (5%) 28 17	75, 85, 94, 97	0
25	23	59/60 (98%)	1.53	22 (37%) 0 0	91, 97, 106, 110	0
26	14	69/71 (97%)	-0.38	0 100 100	91, 102, 113, 117	0
26	24	69/71 (97%)	-0.51	1 (1%) 75 59	98, 110, 116, 121	0
27	15	59/60 (98%)	1.76	19 (32%) 0 0	74, 82, 93, 98	0
27	25	59/60 (98%)	1.60	18 (30%) 0 0	79, 88, 99, 105	0
28	16	53/54 (98%)	0.78	6 (11%) 5 3	76, 85, 92, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.87	9 (16%)	1	1	88, 95, 102, 105	0
29	17	48/49 (97%)	2.53	24 (50%)	0	0	73, 79, 94, 102	0
29	27	48/49 (97%)	2.92	29 (60%)	0	0	80, 86, 97, 107	0
30	18	64/65 (98%)	2.01	32 (50%)	0	0	72, 82, 88, 91	0
30	28	64/65 (98%)	2.68	41 (64%)	0	0	84, 92, 99, 100	0
31	19	37/37 (100%)	1.26	12 (32%)	0	0	78, 84, 92, 94	0
31	29	37/37 (100%)	2.47	21 (56%)	0	0	93, 101, 105, 110	0
32	1a	1488/1521 (97%)	0.11	28 (1%)	66	49	80, 97, 114, 122	0
32	2a	1491/1521 (98%)	-0.01	24 (1%)	72	55	89, 105, 116, 125	0
33	1b	231/256 (90%)	0.29	15 (6%)	18	11	92, 103, 111, 120	0
33	2b	231/256 (90%)	0.30	25 (10%)	5	3	96, 109, 115, 120	0
34	1c	206/239 (86%)	1.02	47 (22%)	0	0	89, 99, 106, 109	0
34	2c	206/239 (86%)	1.44	65 (31%)	0	0	97, 107, 111, 114	0
35	1d	208/209 (99%)	0.57	24 (11%)	4	3	87, 97, 105, 115	0
35	2d	208/209 (99%)	1.79	88 (42%)	0	0	91, 102, 111, 116	0
36	1e	148/162 (91%)	1.19	38 (25%)	0	0	86, 95, 101, 106	0
36	2e	148/162 (91%)	1.28	53 (35%)	0	0	93, 103, 110, 111	0
37	1f	100/101 (99%)	0.60	13 (13%)	3	2	89, 98, 104, 108	0
37	2f	100/101 (99%)	-0.13	2 (2%)	65	48	91, 99, 105, 110	0
38	1g	155/156 (99%)	1.08	34 (21%)	0	0	91, 98, 108, 112	0
38	2g	155/156 (99%)	0.50	18 (11%)	4	2	94, 104, 111, 114	0
39	1h	137/138 (99%)	0.96	27 (19%)	1	0	88, 97, 103, 108	0
39	2h	137/138 (99%)	1.59	48 (35%)	0	0	94, 104, 109, 116	0
40	1i	127/128 (99%)	0.47	21 (16%)	1	1	88, 99, 106, 110	0
40	2i	127/128 (99%)	1.30	44 (34%)	0	0	93, 107, 113, 115	0
41	1j	97/105 (92%)	0.58	18 (18%)	1	0	86, 102, 109, 116	0
41	2j	96/105 (91%)	1.50	28 (29%)	0	0	98, 109, 114, 117	0
42	1k	114/129 (88%)	3.55	90 (78%)	0	0	89, 99, 106, 111	0
42	2k	114/129 (88%)	1.79	42 (36%)	0	0	91, 101, 107, 110	0
43	1l	121/132 (91%)	0.82	20 (16%)	1	1	83, 91, 98, 103	0
43	2l	121/132 (91%)	1.17	34 (28%)	0	0	91, 100, 106, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.52	12 (9%) 7 4	86, 99, 107, 117	0
44	2m	122/126 (96%)	0.97	23 (18%) 1 0	97, 107, 115, 120	0
45	1n	60/61 (98%)	1.56	20 (33%) 0 0	88, 95, 101, 102	0
45	2n	60/61 (98%)	3.52	41 (68%) 0 0	96, 108, 113, 115	0
46	1o	88/89 (98%)	0.71	14 (15%) 1 1	83, 96, 104, 109	0
46	2o	88/89 (98%)	0.94	19 (21%) 0 0	94, 102, 109, 111	0
47	1p	82/88 (93%)	1.37	28 (34%) 0 0	92, 100, 106, 108	0
47	2p	82/88 (93%)	1.55	28 (34%) 0 0	90, 99, 104, 109	0
48	1q	99/105 (94%)	0.52	7 (7%) 16 9	88, 97, 103, 107	0
48	2q	99/105 (94%)	2.11	51 (51%) 0 0	91, 99, 107, 111	0
49	1r	68/88 (77%)	1.20	14 (20%) 1 0	88, 97, 104, 106	0
49	2r	68/88 (77%)	0.65	10 (14%) 2 1	91, 101, 106, 111	0
50	1s	83/93 (89%)	0.03	3 (3%) 42 28	93, 99, 106, 113	0
50	2s	83/93 (89%)	0.17	6 (7%) 15 8	102, 107, 112, 114	0
51	1t	96/106 (90%)	1.08	28 (29%) 0 0	90, 100, 105, 108	0
51	2t	96/106 (90%)	1.36	26 (27%) 0 0	91, 99, 107, 111	0
52	1u	23/27 (85%)	0.89	2 (8%) 10 6	93, 98, 101, 102	0
52	2u	23/27 (85%)	1.53	6 (26%) 0 0	102, 106, 109, 112	0
53	1v	12/24 (50%)	2.46	6 (50%) 0 0	88, 98, 119, 119	0
53	2v	7/24 (29%)	0.77	2 (28%) 0 0	100, 103, 118, 118	0
54	1w	64/76 (84%)	1.63	21 (32%) 0 0	94, 117, 124, 127	0
54	1y	67/76 (88%)	1.27	18 (26%) 0 0	83, 120, 124, 126	0
54	2w	62/76 (81%)	0.53	6 (9%) 7 4	107, 122, 127, 130	0
54	2y	66/76 (86%)	0.59	9 (13%) 3 1	97, 119, 123, 126	0
55	1x	72/77 (93%)	0.24	3 (4%) 36 23	85, 97, 110, 112	0
55	2x	72/77 (93%)	-0.12	2 (2%) 53 36	95, 108, 115, 119	0
All	All	20862/21748 (95%)	0.82	3414 (16%) 1 1	67, 96, 113, 130	0

All (3414) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	18.6
22	10	6	GLY	15.7

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Mol	Chain	Res	Type	RSRZ
22	20	7	LEU	14.7
44	2m	124	PRO	14.2
44	1m	123	ALA	13.8
22	20	5	LYS	13.7
22	20	4	LYS	13.4
38	1g	85	TYR	13.4
44	2m	123	ALA	13.0
22	10	7	LEU	12.9
31	29	37	GLY	12.8
22	10	4	LYS	12.1
23	11	2	SER	11.8
44	2m	121	LYS	11.3
45	2n	34	TYR	11.2
9	2N	8	GLN	11.2
3	2D	2	ALA	11.2
45	2n	25	VAL	11.1
38	1g	84	ASN	11.1
8	2I	123	LEU	11.0
22	10	5	LYS	10.7
29	27	47	ARG	10.4
27	15	2	ALA	10.4
22	20	3	HIS	10.3
22	20	2	ALA	10.1
22	10	3	HIS	10.1
42	2k	13	GLN	9.9
45	2n	39	LEU	9.8
40	2i	125	TYR	9.6
45	2n	38	GLY	9.5
44	2m	120	LYS	9.4
8	2I	89	TYR	9.4
41	2j	47	PHE	9.3
45	2n	37	PHE	9.2
3	2D	276	LYS	9.1
9	2N	44	PRO	9.1
10	2O	1	MET	9.0
43	2l	64	TYR	9.0
11	2P	45	LEU	9.0
22	20	6	GLY	8.9
22	20	8	GLY	8.8
38	2g	82	GLY	8.7
39	2h	133	LEU	8.7
4	2E	132	HIS	8.6

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Mol	Chain	Res	Type	RSRZ
3	1D	275	LYS	8.6
5	2F	82	ILE	8.6
5	2F	89	VAL	8.6
41	2j	62	HIS	8.6
3	1D	276	LYS	8.5
3	2D	55	GLY	8.4
29	27	48	LYS	8.4
22	10	8	GLY	8.3
3	2D	215	LEU	8.3
23	11	36	GLY	8.2
4	1E	141	ILE	8.2
35	2d	108	LEU	8.1
42	1k	50	TYR	8.0
42	1k	42	TRP	8.0
42	1k	75	TYR	8.0
9	2N	45	ASN	7.9
3	2D	38	LYS	7.9
9	2N	9	VAL	7.8
23	21	2	SER	7.8
7	2H	107	VAL	7.8
44	1m	120	LYS	7.8
31	29	16	VAL	7.8
13	2R	69	ASP	7.7
43	2l	18	VAL	7.7
5	2F	83	PHE	7.7
40	1i	115	GLY	7.7
9	2N	43	THR	7.7
22	20	11	ARG	7.7
41	2j	59	SER	7.6
45	2n	35	ARG	7.6
17	1V	73	SER	7.6
29	17	46	VAL	7.6
42	2k	89	ALA	7.5
42	1k	25	TYR	7.5
5	2F	57	VAL	7.5
27	15	60	VAL	7.5
5	1F	89	VAL	7.4
34	2c	198	VAL	7.4
5	2F	56	GLU	7.4
22	10	2	ALA	7.4
29	17	1	MET	7.3
8	2I	109	ILE	7.3

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Mol	Chain	Res	Type	RSRZ
12	1Q	33	GLY	7.3
5	2F	90	PHE	7.3
27	25	2	ALA	7.2
27	25	6	VAL	7.2
52	2u	14	TRP	7.2
8	2I	85	GLU	7.1
18	2W	92	ARG	7.1
45	2n	2	ALA	7.1
23	11	21	ARG	7.0
30	28	2	PRO	7.0
17	1V	84	LYS	7.0
9	2N	73	THR	7.0
20	2Y	35	TYR	7.0
7	2H	115	VAL	6.9
5	2F	62	ARG	6.9
48	2q	37	LYS	6.9
42	1k	30	VAL	6.9
27	25	3	LYS	6.9
9	2N	83	LYS	6.9
9	2N	116	LEU	6.9
51	1t	14	LYS	6.9
8	2I	84	GLY	6.8
17	2V	74	LYS	6.8
3	2D	4	LYS	6.8
45	2n	44	LEU	6.8
7	2H	94	TYR	6.8
47	1p	7	ALA	6.8
39	2h	83	ILE	6.8
51	2t	9	ASN	6.7
34	1c	201	TYR	6.7
18	2W	85	VAL	6.7
5	2F	78	ILE	6.7
12	2Q	103	MET	6.7
38	1g	151	TYR	6.7
48	2q	38	ARG	6.7
22	20	9	SER	6.7
47	1p	1	MET	6.7
23	11	41	ARG	6.7
38	1g	156	TRP	6.6
47	2p	1	MET	6.6
41	2j	65	LEU	6.6
42	1k	123	LYS	6.6

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Mol	Chain	Res	Type	RSRZ
23	21	39	LYS	6.6
30	28	7	HIS	6.6
4	2E	141	ILE	6.6
44	2m	102	ARG	6.6
4	1E	151	TYR	6.6
29	17	48	LYS	6.6
39	2h	111	ILE	6.6
4	2E	134	ILE	6.6
51	2t	18	GLN	6.5
29	27	1	MET	6.5
13	2R	68	ARG	6.5
44	1m	122	LYS	6.5
39	2h	112	LEU	6.5
9	2N	10	GLU	6.5
20	2Y	55	TYR	6.5
53	1v	24	A	6.5
30	28	16	ILE	6.5
38	1g	153	HIS	6.5
35	2d	37	PRO	6.5
9	2N	23	LEU	6.4
4	2E	150	VAL	6.4
3	1D	15	PHE	6.4
29	27	46	VAL	6.4
54	1w	71	G	6.4
48	2q	30	PRO	6.4
5	2F	76	GLY	6.4
9	2N	51	PHE	6.4
9	2N	75	TYR	6.4
51	2t	24	LEU	6.3
20	2Y	1	MET	6.3
23	11	46	LEU	6.3
20	2Y	42	VAL	6.3
30	28	22	VAL	6.3
12	2Q	85	LYS	6.3
44	2m	122	LYS	6.3
17	2V	75	PHE	6.3
3	2D	39	LYS	6.3
42	1k	49	GLY	6.3
30	28	61	LEU	6.3
48	2q	100	LYS	6.3
41	2j	63	PHE	6.3
9	1N	54	VAL	6.3

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Mol	Chain	Res	Type	RSRZ
42	1k	18	ARG	6.3
3	2D	6	PHE	6.3
9	2N	76	SER	6.3
41	2j	58	ASP	6.2
11	2P	38	GLN	6.2
9	2N	84	LYS	6.2
23	11	23	LYS	6.2
7	2H	103	LEU	6.2
54	2w	73	A	6.2
4	2E	133	LYS	6.2
11	2P	51	PHE	6.2
27	25	7	PRO	6.2
30	18	7	HIS	6.2
18	2W	86	LEU	6.2
42	1k	83	ILE	6.2
4	2E	137	HIS	6.2
9	2N	74	ARG	6.1
41	2j	55	LYS	6.1
38	1g	86	GLN	6.1
5	2F	69	HIS	6.1
17	1V	38	LEU	6.1
23	11	47	GLN	6.1
42	1k	87	THR	6.1
43	1l	64	TYR	6.1
4	1E	143	ASN	6.1
42	1k	14	VAL	6.1
7	2H	13	LYS	6.1
35	2d	68	TYR	6.1
45	2n	42	ILE	6.1
9	1N	72	TYR	6.1
5	2F	80	ALA	6.1
51	1t	18	GLN	6.1
3	2D	5	LYS	6.0
3	2D	221	VAL	6.0
11	2P	35	HIS	6.0
3	2D	207	GLY	6.0
16	1U	4	ALA	6.0
51	2t	23	ARG	6.0
3	1D	5	LYS	5.9
3	2D	217	ARG	5.9
19	2X	33	LYS	5.9
19	2X	68	ARG	5.9

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Mol	Chain	Res	Type	RSRZ
51	2t	21	LYS	5.9
8	2I	122	GLU	5.9
11	2P	46	LYS	5.9
29	17	47	ARG	5.9
8	2I	121	LYS	5.9
34	2c	155	GLY	5.9
35	2d	146	ILE	5.9
46	2o	87	ILE	5.9
27	25	4	HIS	5.9
42	1k	77	MET	5.9
1	2A	2897	U	5.9
5	2F	81	PRO	5.8
38	2g	156	TRP	5.8
3	2D	273	ARG	5.8
9	2N	11	PRO	5.8
3	2D	202	LYS	5.8
29	17	36	GLN	5.8
43	2l	26	ALA	5.8
7	2H	159	GLU	5.8
48	2q	32	TYR	5.8
51	1t	9	ASN	5.8
23	21	61	ARG	5.8
54	1w	72	C	5.8
45	2n	53	LEU	5.8
51	1t	8	ARG	5.7
51	2t	22	ARG	5.7
29	17	45	ALA	5.7
51	1t	20	LEU	5.7
5	1F	50	SER	5.7
23	11	97	LEU	5.7
4	2E	131	ALA	5.7
3	1D	222	ARG	5.7
53	1v	13	A	5.7
3	2D	15	PHE	5.7
9	2N	104	LYS	5.7
3	2D	51	VAL	5.7
8	2I	3	VAL	5.7
9	2N	122	VAL	5.7
29	27	2	LYS	5.7
42	1k	60	ALA	5.6
5	2F	79	GLY	5.6
3	1D	204	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
47	2p	8	ARG	5.6
22	20	10	THR	5.6
3	1D	263	ARG	5.6
40	1i	113	LYS	5.6
44	2m	119	GLY	5.6
22	20	12	ASN	5.6
36	1e	24	ARG	5.6
8	2I	87	LYS	5.6
16	2U	20	LEU	5.6
44	1m	121	LYS	5.6
29	27	18	PHE	5.6
45	2n	61	TRP	5.6
13	2R	70	LEU	5.6
45	2n	23	ARG	5.5
40	2i	127	LYS	5.5
11	2P	95	VAL	5.5
36	2e	22	GLY	5.5
38	1g	79	ARG	5.5
42	1k	13	GLN	5.5
39	2h	91	ARG	5.5
4	1E	123	ALA	5.5
39	2h	131	GLY	5.5
51	2t	13	LEU	5.5
42	1k	16	SER	5.5
42	1k	126	ARG	5.5
11	2P	125	VAL	5.5
18	2W	94	ASP	5.5
42	1k	92	GLU	5.5
4	1E	140	SER	5.5
9	2N	82	LEU	5.5
5	2F	64	ILE	5.5
36	2e	31	LEU	5.4
27	15	3	LYS	5.4
42	1k	28	THR	5.4
4	2E	157	ALA	5.4
12	2Q	12	GLN	5.4
30	28	64	TYR	5.4
40	1i	125	TYR	5.4
5	2F	72	ARG	5.4
8	1I	27	ARG	5.4
16	2U	47	TYR	5.4
3	1D	202	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
27	15	7	PRO	5.4
39	2h	2	LEU	5.4
11	2P	42	SER	5.4
48	2q	7	THR	5.4
11	2P	21	ARG	5.4
11	2P	47	ASP	5.4
12	2Q	34	LEU	5.4
23	11	49	VAL	5.4
4	2E	151	TYR	5.4
41	1j	60	ARG	5.4
54	1w	10	G	5.4
3	1D	39	LYS	5.4
36	2e	88	LYS	5.4
13	2R	21	TYR	5.4
34	2c	14	ILE	5.3
8	2I	111	PRO	5.3
5	1F	92	PRO	5.3
43	2l	5	PRO	5.3
9	2N	120	LEU	5.3
11	2P	30	THR	5.3
35	2d	165	MET	5.3
4	2E	130	GLY	5.3
11	2P	20	GLY	5.3
30	28	10	ALA	5.3
49	1r	78	LEU	5.3
39	1h	61	VAL	5.3
42	1k	47	VAL	5.3
5	1F	52	LYS	5.3
9	2N	119	ARG	5.3
39	2h	92	ARG	5.3
18	1W	95	ILE	5.3
3	2D	203	ASN	5.2
35	2d	167	GLY	5.2
16	1U	40	PHE	5.2
34	1c	179	ARG	5.2
43	1l	18	VAL	5.2
16	1U	5	LYS	5.2
42	2k	59	TYR	5.2
4	2E	149	ARG	5.2
17	2V	83	ARG	5.2
17	1V	74	LYS	5.2
33	2b	165	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
3	2D	257	LEU	5.2
9	1N	48	MET	5.2
10	2O	41	ALA	5.2
40	1i	126	SER	5.2
35	2d	168	ARG	5.2
38	2g	81	GLY	5.2
3	2D	59	LYS	5.2
10	2O	19	ILE	5.2
11	1P	15	ARG	5.2
16	2U	8	VAL	5.2
18	2W	90	ARG	5.2
4	1E	149	ARG	5.1
42	1k	73	MET	5.1
30	28	62	LEU	5.1
47	2p	74	LEU	5.1
38	2g	83	ALA	5.1
42	1k	15	ALA	5.1
48	2q	87	LYS	5.1
43	2l	7	ILE	5.1
41	2j	67	THR	5.1
34	2c	201	TYR	5.1
20	1Y	1	MET	5.1
3	1D	203	ASN	5.1
49	1r	87	ARG	5.1
4	2E	129	HIS	5.1
34	2c	60	ALA	5.1
3	1D	182	LEU	5.1
36	2e	84	PHE	5.1
42	1k	100	ALA	5.1
3	1D	273	ARG	5.1
15	1T	46	GLU	5.1
11	2P	37	GLY	5.1
19	2X	92	LEU	5.1
38	1g	154	TYR	5.1
3	2D	206	LEU	5.0
20	2Y	29	GLU	5.0
41	2j	61	GLU	5.0
1	2A	2132	U	5.0
34	2c	160	ALA	5.0
38	1g	77	SER	5.0
30	28	63	PRO	5.0
5	2F	172	TRP	5.0

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Mol	Chain	Res	Type	RSRZ
23	11	7	ILE	5.0
42	1k	120	ARG	5.0
3	1D	227	ASN	5.0
48	2q	29	HIS	5.0
7	2H	48	GLY	5.0
4	1E	154	LYS	5.0
42	1k	70	LYS	5.0
10	1O	1	MET	5.0
38	2g	154	TYR	5.0
29	17	2	LYS	5.0
35	2d	35	ARG	5.0
9	2N	140	VAL	5.0
9	2N	70	LYS	5.0
10	1O	79	PHE	5.0
42	1k	57	THR	5.0
38	1g	80	VAL	5.0
5	1F	69	HIS	5.0
34	1c	12	LEU	5.0
52	1u	14	TRP	5.0
3	1D	11	PRO	5.0
5	1F	90	PHE	5.0
34	2c	154	SER	5.0
16	2U	13	LYS	5.0
35	2d	20	TYR	4.9
5	2F	41	LEU	4.9
3	1D	219	PRO	4.9
23	11	26	ARG	4.9
42	1k	89	ALA	4.9
39	2h	134	ILE	4.9
35	2d	160	GLN	4.9
38	2g	153	HIS	4.9
44	2m	101	GLN	4.9
9	1N	107	LEU	4.9
51	2t	20	LEU	4.9
39	2h	85	ARG	4.9
5	1F	88	VAL	4.9
8	2I	19	VAL	4.9
16	2U	43	GLY	4.9
35	2d	107	ARG	4.9
11	1P	40	SER	4.9
42	1k	81	ASP	4.9
10	2O	2	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
4	1E	122	PHE	4.9
36	2e	45	PHE	4.9
3	1D	176	ARG	4.9
4	2E	127	ASP	4.9
16	2U	36	ARG	4.9
34	2c	2	GLY	4.9
36	1e	23	GLY	4.9
9	2N	117	PHE	4.9
11	1P	45	LEU	4.9
3	2D	16	MET	4.9
11	2P	149	GLU	4.9
40	2i	4	TYR	4.9
48	2q	42	TYR	4.9
48	2q	11	VAL	4.8
33	2b	187	LEU	4.8
36	2e	13	ILE	4.8
48	2q	31	LEU	4.8
10	1O	82	ASN	4.8
23	11	70	VAL	4.8
27	25	9	LYS	4.8
4	1E	132	HIS	4.8
9	2N	26	LEU	4.8
3	2D	216	GLY	4.8
12	2Q	15	GLY	4.8
15	2T	69	GLY	4.8
42	1k	29	ILE	4.8
15	1T	72	VAL	4.8
38	1g	82	GLY	4.8
5	1F	48	THR	4.8
48	2q	22	LEU	4.8
12	2Q	87	LYS	4.8
23	11	67	ILE	4.8
42	1k	80	VAL	4.8
45	2n	33	VAL	4.8
18	2W	82	LEU	4.8
36	1e	89	ILE	4.8
42	2k	108	ILE	4.8
47	2p	17	TYR	4.8
9	2N	77	GLY	4.8
35	2d	184	LYS	4.8
42	2k	32	ILE	4.8
9	1N	109	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
10	1O	97	ARG	4.8
30	28	21	LYS	4.8
19	2X	69	TYR	4.8
4	1E	1	MET	4.7
42	1k	56	GLY	4.7
23	11	60	PHE	4.7
41	2j	11	PHE	4.7
5	1F	93	LYS	4.7
28	26	54	ILE	4.7
51	2t	14	LYS	4.7
11	1P	49	ARG	4.7
11	2P	54	GLY	4.7
54	1w	73	A	4.7
47	2p	59	TRP	4.7
35	2d	104	VAL	4.7
35	2d	185	PHE	4.7
17	2V	73	SER	4.7
39	2h	119	LEU	4.7
7	2H	148	ILE	4.7
48	2q	90	ILE	4.7
45	1n	23	ARG	4.7
4	1E	158	GLY	4.7
27	25	10	LYS	4.7
45	1n	50	LYS	4.7
18	2W	93	ALA	4.7
41	2j	98	ILE	4.7
31	29	15	LYS	4.7
54	1y	1	G	4.7
5	2F	65	TRP	4.7
9	2N	13	TRP	4.7
42	1k	63	LEU	4.7
45	2n	26	ARG	4.7
51	2t	25	ARG	4.7
23	21	38	SER	4.7
3	2D	9	TYR	4.7
3	1D	221	VAL	4.7
3	2D	54	ARG	4.7
35	1d	118	ARG	4.7
35	2d	64	LEU	4.7
3	2D	8	PRO	4.7
12	2Q	73	PRO	4.7
13	2R	10	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
18	1W	69	LEU	4.7
42	1k	98	LEU	4.7
5	2F	77	ASP	4.7
31	29	17	ILE	4.7
42	1k	108	ILE	4.7
3	1D	243	GLY	4.7
4	1E	124	GLY	4.7
47	1p	25	ARG	4.7
3	2D	84	TYR	4.7
10	1O	7	TYR	4.7
9	2N	99	LEU	4.7
6	2G	137	GLU	4.7
35	2d	162	LEU	4.7
3	2D	204	ILE	4.7
9	1N	85	ILE	4.7
39	2h	100	ILE	4.7
9	1N	119	ARG	4.7
7	2H	123	PHE	4.6
35	2d	140	VAL	4.6
9	1N	116	LEU	4.6
11	1P	3	LEU	4.6
40	2i	115	GLY	4.6
47	1p	36	ILE	4.6
36	1e	88	LYS	4.6
42	1k	82	VAL	4.6
38	1g	78	ARG	4.6
4	2E	128	SER	4.6
7	2H	105	LEU	4.6
20	2Y	50	ARG	4.6
4	2E	126	PRO	4.6
3	1D	233	HIS	4.6
54	1w	70	G	4.6
4	1E	195	LEU	4.6
11	2P	62	LEU	4.6
19	2X	70	LEU	4.6
30	28	25	MET	4.6
3	2D	208	LYS	4.6
11	2P	39	LYS	4.6
42	1k	122	LYS	4.6
3	1D	206	LEU	4.6
23	11	24	ALA	4.6
10	1O	122	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
15	1T	28	VAL	4.6
7	2H	90	LYS	4.6
29	17	14	LYS	4.6
30	28	59	LYS	4.6
3	1D	268	ARG	4.6
41	2j	60	ARG	4.6
4	2E	10	GLY	4.6
33	1b	77	ALA	4.6
42	1k	20	TYR	4.6
29	27	14	LYS	4.6
3	1D	205	VAL	4.5
4	2E	142	GLY	4.6
11	2P	123	LEU	4.5
34	2c	52	LEU	4.5
41	2j	66	ARG	4.5
20	2Y	48	ALA	4.5
34	2c	184	TYR	4.5
1	2A	2896	C	4.5
41	2j	54	PHE	4.5
49	2r	84	LYS	4.5
23	11	62	VAL	4.5
12	1Q	41	TRP	4.5
42	2k	126	ARG	4.5
36	2e	90	VAL	4.5
49	1r	40	LEU	4.5
8	1I	1	MET	4.5
11	2P	18	ARG	4.5
20	2Y	45	VAL	4.5
49	2r	85	LEU	4.5
11	2P	29	LYS	4.5
31	29	1	MET	4.5
41	2j	50	ILE	4.5
34	1c	164	ARG	4.5
35	2d	122	ARG	4.5
42	1k	78	GLN	4.5
1	1A	2145	C	4.5
4	1E	147	PRO	4.5
12	2Q	80	GLU	4.5
4	1E	125	GLY	4.5
9	1N	75	TYR	4.5
45	2n	47	LEU	4.5
34	2c	8	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
9	2N	109	LYS	4.5
11	2P	36	LYS	4.5
16	1U	32	PHE	4.5
35	1d	110	PHE	4.5
5	2F	87	GLY	4.5
4	1E	129	HIS	4.5
9	2N	72	TYR	4.5
19	2X	13	LEU	4.5
41	2j	56	HIS	4.5
1	1A	529	A	4.5
40	2i	65	VAL	4.5
9	2N	12	ARG	4.5
11	2P	33	ARG	4.5
15	1T	64	ARG	4.5
3	2D	219	PRO	4.5
3	1D	16	MET	4.5
5	2F	49	ALA	4.5
19	1X	29	TRP	4.5
16	2U	40	PHE	4.5
4	1E	139	GLY	4.5
9	2N	61	ARG	4.5
47	2p	4	ILE	4.5
27	15	5	PRO	4.5
36	1e	22	GLY	4.5
27	25	19	ARG	4.5
10	1O	10	VAL	4.5
16	2U	33	ARG	4.4
7	2H	114	VAL	4.4
48	2q	23	VAL	4.4
10	1O	5	GLN	4.4
11	2P	59	LEU	4.4
47	2p	6	LEU	4.4
10	2O	7	TYR	4.4
19	2X	18	TYR	4.4
3	2D	14	ARG	4.4
11	1P	108	LYS	4.4
22	20	13	GLY	4.4
13	1R	10	LEU	4.4
13	1R	42	LYS	4.4
45	2n	7	ILE	4.4
5	1F	83	PHE	4.4
13	1R	20	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
54	1w	1	G	4.4
12	1Q	85	LYS	4.4
45	1n	25	VAL	4.4
3	2D	52	ARG	4.4
16	1U	25	TRP	4.4
5	2F	75	HIS	4.4
11	1P	48	PRO	4.4
45	2n	41	ARG	4.4
23	11	34	THR	4.4
23	11	42	GLN	4.4
48	2q	27	PHE	4.4
36	1e	81	GLU	4.4
28	26	7	ILE	4.4
15	1T	45	PHE	4.4
20	1Y	4	LYS	4.4
9	2N	60	ILE	4.4
30	28	12	LYS	4.4
47	2p	9	PHE	4.4
18	2W	81	ALA	4.4
27	25	11	THR	4.4
42	1k	43	SER	4.4
15	2T	99	LEU	4.4
3	2D	236	GLY	4.4
20	2Y	4	LYS	4.4
30	28	5	LYS	4.4
16	1U	28	ARG	4.3
7	2H	133	VAL	4.3
36	1e	82	VAL	4.3
5	2F	73	ALA	4.3
18	1W	90	ARG	4.3
28	26	2	ALA	4.3
45	2n	29	ARG	4.3
7	2H	116	GLU	4.3
54	2w	72	C	4.3
37	1f	48	LEU	4.3
11	1P	11	GLY	4.3
32	1a	1511	G	4.3
32	2a	78	G	4.3
10	1O	44	LYS	4.3
23	11	98	LEU	4.3
48	2q	21	VAL	4.3
3	1D	53	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
12	1Q	76	LYS	4.3
5	2F	61	GLY	4.3
45	2n	22	THR	4.3
16	1U	37	GLU	4.3
27	25	8	LYS	4.3
45	2n	36	PHE	4.3
42	2k	119	CYS	4.3
30	18	50	LEU	4.3
41	2j	10	GLY	4.3
3	1D	254	THR	4.3
7	2H	145	ALA	4.3
12	1Q	82	ARG	4.3
16	2U	39	LEU	4.3
7	2H	35	VAL	4.3
23	11	4	VAL	4.3
34	1c	87	LEU	4.3
17	1V	81	TYR	4.3
5	2F	50	SER	4.3
3	1D	257	LEU	4.3
34	2c	13	GLY	4.3
34	2c	196	LEU	4.3
9	2N	48	MET	4.3
45	2n	49	HIS	4.3
10	1O	63	VAL	4.3
30	28	15	LYS	4.3
12	2Q	38	GLU	4.2
3	1D	226	MET	4.2
40	1i	114	TYR	4.2
23	11	50	ARG	4.2
3	2D	223	GLY	4.2
11	2P	50	ARG	4.2
12	2Q	11	LYS	4.2
43	2l	32	PHE	4.2
45	2n	56	VAL	4.2
18	2W	103	ILE	4.2
39	2h	94	TYR	4.2
29	27	15	THR	4.2
30	18	5	LYS	4.2
33	2b	37	ASN	4.2
4	1E	156	MET	4.2
9	2N	5	VAL	4.2
9	2N	108	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
9	2N	111	PRO	4.2
3	1D	225	ALA	4.2
18	1W	112	GLY	4.2
54	1y	2	C	4.2
40	2i	64	THR	4.2
3	2D	18	VAL	4.2
5	2F	88	VAL	4.2
47	2p	19	ILE	4.2
35	2d	164	ALA	4.2
42	1k	74	ALA	4.2
6	2G	133	LEU	4.2
9	1N	82	LEU	4.2
9	1N	120	LEU	4.2
16	1U	27	LEU	4.2
46	2o	67	LEU	4.2
23	21	14	VAL	4.2
38	1g	87	VAL	4.2
7	2H	89	ILE	4.2
39	2h	136	GLU	4.2
42	1k	96	ARG	4.2
45	2n	30	ALA	4.2
35	2d	19	LEU	4.2
1	1A	2146	C	4.2
3	2D	17	THR	4.2
39	2h	86	ILE	4.2
42	1k	54	ARG	4.2
42	2k	25	TYR	4.2
11	1P	39	LYS	4.2
17	2V	72	VAL	4.2
20	2Y	7	VAL	4.2
18	2W	99	ARG	4.2
42	1k	91	ARG	4.2
4	1E	142	GLY	4.2
46	1o	56	LEU	4.2
17	1V	75	PHE	4.2
54	1y	24	G	4.2
34	2c	40	ARG	4.2
5	1F	51	THR	4.2
10	1O	65	THR	4.2
30	28	3	LYS	4.2
12	2Q	79	LEU	4.1
34	2c	204	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
45	2n	52	GLN	4.1
7	2H	152	ARG	4.1
12	2Q	81	VAL	4.1
48	2q	39	SER	4.1
7	2H	151	ILE	4.1
51	2t	26	ASN	4.1
9	2N	7	LYS	4.1
7	2H	88	LEU	4.1
34	1c	196	LEU	4.1
3	2D	13	ARG	4.1
3	2D	211	ARG	4.1
10	1O	81	ASP	4.1
40	2i	109	VAL	4.1
16	2U	88	ILE	4.1
8	1I	23	PRO	4.1
34	1c	193	TYR	4.1
36	2e	12	LEU	4.1
4	1E	155	LYS	4.1
9	2N	54	VAL	4.1
15	2T	48	ILE	4.1
35	2d	67	ILE	4.1
54	2w	71	G	4.1
3	2D	53	PHE	4.1
11	1P	38	GLN	4.1
15	1T	89	VAL	4.1
30	18	23	VAL	4.1
34	2c	207	VAL	4.1
23	11	11	ARG	4.1
3	2D	7	LYS	4.1
18	2W	89	ALA	4.1
4	2E	135	HIS	4.1
16	1U	117	GLN	4.1
40	2i	114	TYR	4.1
9	1N	122	VAL	4.1
17	2V	5	VAL	4.1
11	2P	52	GLU	4.1
12	2Q	41	TRP	4.1
51	1t	11	SER	4.1
10	1O	46	ALA	4.1
13	1R	100	LEU	4.1
36	1e	21	ALA	4.1
45	2n	6	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
4	1E	3	GLY	4.1
4	1E	116	VAL	4.1
39	2h	90	GLY	4.1
39	2h	93	VAL	4.1
36	2e	89	ILE	4.1
17	2V	71	LEU	4.1
54	1y	56	C	4.1
1	2A	586	A	4.1
54	2w	31	A	4.1
3	1D	37	LEU	4.1
27	25	13	LYS	4.1
34	2c	199	LYS	4.1
34	2c	197	GLY	4.1
34	1c	33	LEU	4.1
44	2m	90	LEU	4.1
11	2P	15	ARG	4.0
18	1W	97	LYS	4.1
3	1D	9	TYR	4.0
9	2N	46	VAL	4.0
11	2P	64	LYS	4.0
17	1V	78	LYS	4.0
17	2V	1	MET	4.0
41	2j	51	ARG	4.0
23	11	63	ALA	4.0
42	1k	17	GLY	4.0
10	2O	47	ILE	4.0
13	1R	21	TYR	4.0
23	11	95	LEU	4.0
10	1O	114	ILE	4.0
9	2N	34	LEU	4.0
43	2l	10	LEU	4.0
30	28	4	MET	4.0
12	1Q	81	VAL	4.0
41	2j	46	ARG	4.0
47	2p	5	ARG	4.0
1	2A	2801(A)	A	4.0
3	1D	166	GLN	4.0
30	28	60	LEU	4.0
11	1P	51	PHE	4.0
1	1A	614(B)	G	4.0
38	1g	81	GLY	4.0
30	28	14	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
51	2t	70	SER	4.0
9	2N	85	ILE	4.0
42	2k	71	LYS	4.0
43	2l	28	LYS	4.0
12	2Q	104	PHE	4.0
38	1g	145	ALA	4.0
43	2l	15	ARG	4.0
54	1w	3	C	4.0
10	1O	85	VAL	4.0
42	1k	26	ASN	4.0
20	2Y	63	LYS	4.0
51	1t	21	LYS	4.0
36	2e	10	MET	4.0
4	1E	145	LYS	4.0
9	2N	50	ASP	4.0
11	2P	124	LYS	4.0
12	1Q	68	ILE	4.0
18	2W	95	ILE	4.0
20	2Y	61	ILE	4.0
5	1F	72	ARG	4.0
40	2i	36	TYR	4.0
9	1N	53	VAL	3.9
16	1U	2	PRO	3.9
9	1N	30	ILE	3.9
31	29	36	GLN	3.9
54	2y	53	G	3.9
20	2Y	25	GLY	3.9
31	29	24	TYR	3.9
9	2N	90	MET	3.9
39	2h	9	MET	3.9
51	2t	29	LYS	3.9
20	2Y	32	PRO	3.9
35	2d	70	ILE	3.9
3	1D	155	LEU	3.9
16	2U	18	LEU	3.9
19	2X	66	LEU	3.9
34	2c	10	PHE	3.9
48	2q	4	LYS	3.9
3	2D	226	MET	3.9
54	1y	33	U	3.9
47	1p	21	VAL	3.9
47	2p	20	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
10	2O	18	LYS	3.9
1	1A	2506	U	3.9
54	1y	34	G	3.9
9	2N	52	VAL	3.9
16	2U	63	VAL	3.9
11	1P	44	GLY	3.9
17	2V	94	LEU	3.9
37	1f	61	LEU	3.9
42	1k	66	LEU	3.9
42	1k	86	GLY	3.9
39	2h	87	SER	3.9
42	1k	44	SER	3.9
17	2V	78	LYS	3.9
5	2F	66	PRO	3.9
40	2i	110	GLU	3.9
42	1k	31	THR	3.9
1	2A	229	A	3.9
19	1X	68	ARG	3.9
43	1l	22	SER	3.9
3	2D	270	ILE	3.9
11	1P	19	VAL	3.9
28	16	54	ILE	3.9
33	2b	108	ILE	3.9
35	2d	98	GLU	3.9
39	2h	6	ILE	3.9
42	2k	14	VAL	3.9
39	2h	10	LEU	3.9
41	2j	48	THR	3.9
42	2k	91	ARG	3.9
9	1N	47	ALA	3.9
4	1E	134	ILE	3.9
9	1N	52	VAL	3.9
10	1O	86	ILE	3.9
15	1T	57	PHE	3.9
9	1N	84	LYS	3.9
17	2V	20	LEU	3.9
23	11	44	PRO	3.9
45	2n	45	ARG	3.9
11	1P	35	HIS	3.9
23	11	37	ILE	3.9
23	21	37	ILE	3.9
13	2R	17	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
25	23	26	LEU	3.9
29	27	9	ARG	3.9
51	2t	28	ALA	3.9
4	2E	140	SER	3.9
7	2H	41	MET	3.9
7	2H	85	LYS	3.8
17	2V	76	LYS	3.8
32	2a	84	U	3.8
11	2P	65	ARG	3.8
13	1R	17	ARG	3.8
36	1e	28	PHE	3.8
47	2p	73	LEU	3.8
42	1k	51	LYS	3.8
9	1N	61	ARG	3.8
4	2E	115	GLY	3.8
11	2P	43	GLY	3.8
3	1D	175	LEU	3.8
10	2O	8	LEU	3.8
34	2c	178	LEU	3.8
3	2D	184	LYS	3.8
42	1k	61	ALA	3.8
44	2m	103	THR	3.8
3	2D	201	HIS	3.8
34	1c	170	GLN	3.8
9	2N	16	ILE	3.8
10	1O	22	ILE	3.8
16	2U	17	ILE	3.8
38	2g	80	VAL	3.8
39	2h	13	ILE	3.8
3	2D	61	LEU	3.8
5	2F	181	LEU	3.8
15	1T	105	LEU	3.8
16	1U	20	LEU	3.8
35	1d	157	LEU	3.8
23	21	15	ALA	3.8
29	27	33	ARG	3.8
3	2D	250	TRP	3.8
37	1f	57	GLN	3.8
9	1N	71	ILE	3.8
22	10	9	SER	3.8
36	2e	129	ILE	3.8
4	1E	152	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
43	2l	27	LEU	3.8
45	2n	50	LYS	3.8
17	1V	83	ARG	3.8
23	11	20	ARG	3.8
36	1e	18	ARG	3.8
39	2h	84	ARG	3.8
8	1I	120	ILE	3.8
18	2W	46	PHE	3.8
23	21	13	ILE	3.8
39	2h	132	GLU	3.8
3	1D	244	ARG	3.8
4	2E	138	PRO	3.8
3	1D	253	GLN	3.8
9	1N	45	ASN	3.8
20	2Y	3	VAL	3.8
25	23	9	VAL	3.8
54	1y	36	A	3.8
16	1U	17	ILE	3.8
20	2Y	64	GLU	3.8
30	18	8	LYS	3.8
40	1i	119	ALA	3.8
43	2l	29	GLY	3.8
1	1A	2141	G	3.8
3	1D	271	ILE	3.8
7	2H	169	VAL	3.8
20	2Y	43	ASN	3.8
41	1j	58	ASP	3.8
51	2t	8	ARG	3.8
3	1D	248	SER	3.8
3	1D	261	LYS	3.8
4	1E	153	GLY	3.8
9	2N	69	GLN	3.8
44	2m	95	GLY	3.8
39	2h	99	GLU	3.8
9	2N	103	VAL	3.8
42	1k	40	ILE	3.8
9	2N	112	LEU	3.8
13	2R	29	LEU	3.8
15	1T	114	LEU	3.8
22	10	12	ASN	3.8
3	2D	275	LYS	3.8
16	1U	24	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
32	2a	1202	G	3.8
53	1v	12	A	3.8
53	1v	15	A	3.8
3	2D	11	PRO	3.8
3	2D	232	PRO	3.8
5	1F	80	ALA	3.8
13	1R	12	ARG	3.8
18	1W	93	ALA	3.8
29	27	23	ARG	3.8
3	1D	49	ILE	3.8
10	1O	98	VAL	3.8
33	2b	201	ILE	3.8
35	2d	112	VAL	3.8
3	1D	4	LYS	3.7
10	1O	18	LYS	3.7
27	15	9	LYS	3.7
3	2D	220	HIS	3.7
4	1E	137	HIS	3.7
8	1I	28	ASN	3.7
35	2d	4	TYR	3.7
5	2F	74	ARG	3.7
36	1e	14	ARG	3.7
47	1p	59	TRP	3.7
51	2t	12	ALA	3.7
20	2Y	24	VAL	3.7
38	1g	141	VAL	3.7
1	1A	1026	U	3.7
19	1X	92	LEU	3.7
35	2d	188	LEU	3.7
34	1c	155	GLY	3.7
8	2I	100	ALA	3.7
12	2Q	77	LYS	3.7
34	1c	167	TRP	3.7
4	2E	122	PHE	3.7
8	2I	35	LEU	3.7
10	1O	19	ILE	3.7
10	1O	40	VAL	3.7
40	2i	26	VAL	3.7
29	27	42	LEU	3.7
36	1e	19	MET	3.7
5	1F	95	ARG	3.7
12	2Q	82	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
16	2U	14	HIS	3.7
51	2t	17	ARG	3.7
44	2m	6	GLY	3.7
42	2k	35	PRO	3.7
3	1D	252	TRP	3.7
9	1N	51	PHE	3.7
6	2G	34	LEU	3.7
17	2V	82	ARG	3.7
29	27	35	ARG	3.7
9	1N	105	GLY	3.7
3	1D	232	PRO	3.7
10	1O	52	VAL	3.7
22	20	14	ARG	3.7
7	2H	138	LYS	3.7
16	1U	21	ALA	3.7
47	2p	39	TYR	3.7
3	1D	133	LEU	3.7
39	2h	95	VAL	3.7
49	1r	76	LEU	3.7
4	1E	131	ALA	3.7
34	2c	65	ALA	3.7
33	2b	32	ILE	3.7
12	1Q	83	MET	3.7
9	1N	49	GLY	3.7
23	11	33	LYS	3.7
23	11	39	LYS	3.7
35	2d	166	LYS	3.7
42	1k	71	LYS	3.7
43	1l	28	LYS	3.7
43	2l	19	ARG	3.7
3	1D	144	ALA	3.7
5	1F	49	ALA	3.7
23	11	71	TYR	3.7
4	1E	150	VAL	3.7
12	1Q	37	LEU	3.7
34	1c	153	VAL	3.7
35	2d	133	VAL	3.7
36	2e	109	ILE	3.7
42	1k	103	LEU	3.7
31	29	12	ASP	3.7
44	2m	110	ARG	3.7
30	18	2	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
42	2k	75	TYR	3.7
43	1l	98	TYR	3.7
42	1k	67	ASP	3.6
50	2s	38	SER	3.7
7	2H	108	GLY	3.6
45	1n	59	ALA	3.6
10	1O	58	VAL	3.6
42	1k	59	TYR	3.6
30	28	29	LYS	3.6
3	1D	251	GLY	3.6
9	2N	93	THR	3.6
12	2Q	10	ARG	3.6
39	2h	135	CYS	3.6
17	2V	80	GLN	3.6
40	2i	124	GLN	3.6
12	2Q	40	ALA	3.6
11	1P	17	LYS	3.6
23	11	48	LYS	3.6
40	1i	127	LYS	3.6
4	2E	189	PRO	3.6
7	2H	45	VAL	3.6
9	2N	14	VAL	3.6
9	2N	30	ILE	3.6
9	2N	98	VAL	3.6
10	1O	2	ILE	3.6
16	1U	47	TYR	3.6
34	2c	39	ILE	3.6
48	2q	98	LEU	3.6
51	1t	24	LEU	3.6
5	2F	51	THR	3.6
3	1D	38	LYS	3.6
18	2W	98	LYS	3.6
7	2H	24	VAL	3.6
13	1R	48	VAL	3.6
18	2W	6	ILE	3.6
39	1h	109	ILE	3.6
4	1E	117	MET	3.6
39	2h	22	GLU	3.6
4	1E	113	PHE	3.6
10	2O	17	ARG	3.6
33	2b	188	ALA	3.6
45	2n	57	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
54	1w	2	C	3.6
3	2D	271	ILE	3.6
33	1b	215	LEU	3.6
36	1e	13	ILE	3.6
39	1h	133	LEU	3.6
42	1k	21	ILE	3.6
3	1D	223	GLY	3.6
52	2u	17	THR	3.6
5	1F	62	ARG	3.6
3	1D	111	LEU	3.6
4	2E	116	VAL	3.6
41	2j	6	ILE	3.6
9	1N	70	LYS	3.6
4	1E	128	SER	3.6
11	2P	58	THR	3.6
5	2F	63	LYS	3.6
20	2Y	67	LEU	3.6
23	21	27	GLU	3.6
42	2k	90	GLY	3.6
32	1a	1508	G	3.6
38	1g	155	ARG	3.6
52	2u	22	ARG	3.6
23	11	38	SER	3.6
4	2E	155	LYS	3.6
54	1y	35	A	3.6
8	2I	79	ILE	3.6
12	2Q	91	GLU	3.6
15	2T	110	ILE	3.6
42	1k	95	ILE	3.6
9	2N	114	ARG	3.6
45	1n	37	PHE	3.6
34	1c	199	LYS	3.6
18	1W	86	LEU	3.6
9	2N	97	ARG	3.6
11	2P	49	ARG	3.6
10	1O	33	ALA	3.5
12	2Q	121	ALA	3.5
29	17	24	THR	3.5
35	1d	108	LEU	3.5
35	2d	130	GLY	3.5
47	2p	24	ALA	3.5
48	2q	8	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
3	1D	17	THR	3.5
48	2q	36	ILE	3.5
3	2D	233	HIS	3.5
9	1N	108	PRO	3.5
10	1O	4	PRO	3.5
17	1V	76	LYS	3.5
35	2d	134	ASP	3.5
10	2O	79	PHE	3.5
20	2Y	5	MET	3.5
35	2d	163	GLU	3.5
35	2d	23	GLY	3.5
45	2n	31	ARG	3.5
16	2U	16	LYS	3.5
18	2W	97	LYS	3.5
33	2b	133	LYS	3.5
9	1N	79	PRO	3.5
43	1l	94	PRO	3.5
43	2l	98	TYR	3.5
23	21	26	ARG	3.5
7	2H	30	LYS	3.5
10	2O	33	ALA	3.5
33	1b	118	LEU	3.5
16	2U	90	VAL	3.5
18	2W	96	ILE	3.5
35	1d	148	VAL	3.5
22	20	45	PHE	3.5
18	2W	38	TYR	3.5
43	1l	19	ARG	3.5
9	2N	15	LEU	3.5
13	1R	51	LEU	3.5
5	1F	56	GLU	3.5
7	2H	10	PRO	3.5
12	2Q	14	ARG	3.5
40	1i	111	ARG	3.5
30	28	50	LEU	3.5
23	11	18	ILE	3.5
16	2U	25	TRP	3.5
11	1P	36	LYS	3.5
3	1D	8	PRO	3.5
34	2c	15	THR	3.5
40	2i	27	THR	3.5
3	1D	247	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
31	29	23	VAL	3.5
3	1D	213	ARG	3.5
3	1D	214	TRP	3.5
3	1D	250	TRP	3.5
15	1T	87	ASP	3.5
41	1j	59	SER	3.5
8	2I	86	THR	3.5
29	27	7	PRO	3.5
4	2E	114	ALA	3.5
13	1R	41	ALA	3.5
16	1U	42	ALA	3.5
20	2Y	106	LEU	3.5
39	1h	2	LEU	3.5
3	2D	253	GLN	3.5
5	1F	78	ILE	3.5
4	2E	136	ARG	3.5
11	2P	19	VAL	3.5
12	2Q	94	VAL	3.5
18	2W	105	VAL	3.5
35	2d	114	ARG	3.5
46	2o	60	VAL	3.5
11	2P	97	PRO	3.5
34	2c	158	GLY	3.5
35	2d	183	GLY	3.5
3	2D	58	HIS	3.5
9	1N	73	THR	3.5
49	1r	82	THR	3.5
23	11	32	LYS	3.5
34	2c	101	LEU	3.5
40	2i	92	TYR	3.5
36	1e	25	ARG	3.5
1	1A	2578	G	3.5
5	2F	68	LYS	3.4
27	25	5	PRO	3.4
8	2I	1	MET	3.4
20	2Y	2	ARG	3.4
24	12	69	ARG	3.4
5	1F	67	GLN	3.4
10	1O	38	VAL	3.4
12	2Q	96	VAL	3.4
3	1D	200	ASP	3.4
3	1D	255	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
44	1m	119	GLY	3.4
9	2N	38	HIS	3.4
9	1N	60	ILE	3.4
25	23	21	ALA	3.4
15	2T	72	VAL	3.4
42	1k	55	LYS	3.4
54	1w	4	C	3.4
1	2A	2585	U	3.4
4	1E	163	GLU	3.4
18	1W	92	ARG	3.4
23	11	17	SER	3.4
43	2l	22	SER	3.4
19	1X	13	LEU	3.4
25	23	8	LEU	3.4
41	1j	65	LEU	3.4
9	2N	57	ALA	3.4
3	1D	18	VAL	3.4
23	11	16	ASN	3.4
35	1d	5	ILE	3.4
5	1F	44	ARG	3.4
35	2d	115	ARG	3.4
36	1e	139	LEU	3.4
38	1g	88	PRO	3.4
7	2H	96	ALA	3.4
10	2O	114	ILE	3.4
23	21	10	LYS	3.4
39	1h	86	ILE	3.4
46	2o	48	LYS	3.4
20	2Y	51	VAL	3.4
33	2b	197	VAL	3.4
3	1D	42	GLY	3.4
11	2P	44	GLY	3.4
23	21	28	GLY	3.4
42	1k	125	PHE	3.4
43	1l	89	ARG	3.4
49	2r	87	ARG	3.4
11	2P	72	PRO	3.4
12	2Q	17	LEU	3.4
27	15	8	LYS	3.4
30	28	11	LYS	3.4
34	2c	4	LYS	3.4
48	2q	40	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
34	2c	37	GLN	3.4
15	2T	102	ILE	3.4
38	1g	73	MET	3.4
7	2H	113	VAL	3.4
15	2T	70	VAL	3.4
31	29	25	VAL	3.4
9	1N	74	ARG	3.4
11	1P	30	THR	3.4
30	18	46	ARG	3.4
44	1m	103	THR	3.4
48	2q	95	TYR	3.4
28	26	8	LYS	3.4
39	2h	88	LYS	3.4
3	2D	37	LEU	3.4
9	2N	107	LEU	3.4
41	1j	8	LEU	3.4
15	2T	1	MET	3.4
16	2U	10	ARG	3.4
29	27	22	MET	3.4
9	2N	78	TYR	3.4
54	1w	23	A	3.4
4	2E	2	LYS	3.4
3	2D	182	LEU	3.4
12	2Q	37	LEU	3.4
20	2Y	105	ALA	3.4
4	1E	133	LYS	3.4
16	1U	34	LYS	3.4
35	2d	169	LYS	3.4
47	2p	35	LYS	3.4
25	23	30	ARG	3.4
20	2Y	47	LYS	3.4
5	1F	75	HIS	3.4
9	2N	113	GLY	3.4
23	21	41	ARG	3.3
35	2d	118	ARG	3.3
23	21	33	LYS	3.3
30	18	61	LEU	3.3
3	2D	224	ALA	3.3
4	1E	4	ILE	3.3
4	2E	156	MET	3.3
23	11	64	ALA	3.3
34	2c	200	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
36	1e	86	ALA	3.3
29	17	10	ARG	3.3
44	2m	104	ARG	3.3
5	2F	70	THR	3.3
27	15	10	LYS	3.3
4	1E	120	TRP	3.3
5	2F	84	VAL	3.3
9	1N	140	VAL	3.3
10	1O	16	ALA	3.3
12	1Q	66	ILE	3.3
30	28	58	ILE	3.3
30	18	14	VAL	3.3
37	1f	88	VAL	3.3
42	1k	65	ALA	3.3
40	2i	9	ARG	3.3
9	2N	65	LYS	3.3
30	18	59	LYS	3.3
11	1P	32	THR	3.3
3	2D	49	ILE	3.3
7	2H	121	ILE	3.3
4	2E	167	VAL	3.3
9	2N	79	PRO	3.3
16	1U	35	ALA	3.3
28	26	5	VAL	3.3
32	1a	1531	A	3.3
42	1k	68	ALA	3.3
11	2P	60	MET	3.3
39	1h	9	MET	3.3
3	2D	89	SER	3.3
29	27	37	LYS	3.3
11	2P	94	GLU	3.3
5	1F	79	GLY	3.3
3	2D	145	VAL	3.3
5	2F	52	LYS	3.3
10	2O	99	PHE	3.3
11	2P	78	PRO	3.3
17	2V	14	VAL	3.3
20	2Y	65	ALA	3.3
42	2k	96	ARG	3.3
43	2l	31	PRO	3.3
10	1O	8	LEU	3.3
47	1p	6	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
3	1D	184	LYS	3.3
10	1O	17	ARG	3.3
3	1D	2	ALA	3.3
3	2D	40	THR	3.3
10	1O	47	ILE	3.3
16	2U	28	ARG	3.3
22	20	41	ARG	3.3
29	27	4	THR	3.3
30	18	11	LYS	3.3
19	2X	28	PHE	3.3
5	1F	81	PRO	3.3
7	2H	36	PRO	3.3
10	2O	81	ASP	3.3
13	1R	98	LEU	3.3
15	2T	114	LEU	3.3
17	2V	81	TYR	3.3
7	2H	95	ARG	3.3
18	2W	11	ARG	3.3
23	21	18	ILE	3.3
42	1k	23	ALA	3.3
42	2k	95	ILE	3.3
3	1D	10	THR	3.3
36	2e	55	VAL	3.3
1	2A	2155	G	3.3
3	2D	181	GLU	3.3
15	1T	65	LYS	3.3
19	2X	63	LYS	3.3
32	1a	1503	A	3.3
32	2a	60	A	3.3
42	1k	90	GLY	3.3
23	11	13	ILE	3.3
11	2P	126	VAL	3.3
28	26	4	GLU	3.3
40	2i	112	LYS	3.3
23	11	73	LEU	3.3
3	1D	51	VAL	3.3
3	1D	272	ALA	3.3
7	2H	144	VAL	3.3
13	1R	97	VAL	3.3
23	21	62	VAL	3.3
5	2F	53	THR	3.3
9	2N	40	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
38	2g	78	ARG	3.3
5	1F	87	GLY	3.3
18	1W	43	GLY	3.3
3	1D	270	ILE	3.2
20	2Y	60	PHE	3.2
30	18	64	TYR	3.2
9	1N	118	LYS	3.2
16	1U	22	LYS	3.2
33	2b	41	ILE	3.2
41	1j	55	LYS	3.2
46	2o	47	LYS	3.2
16	2U	11	ARG	3.2
47	1p	28	ARG	3.2
42	2k	31	THR	3.2
4	1E	182	LEU	3.2
13	2R	4	LEU	3.2
19	1X	66	LEU	3.2
27	25	30	LEU	3.2
38	1g	103	TRP	3.2
48	1q	98	LEU	3.2
11	2P	75	ILE	3.2
18	2W	76	VAL	3.2
51	1t	83	ARG	3.2
3	1D	178	PRO	3.2
5	2F	93	LYS	3.2
3	2D	239	ARG	3.2
16	2U	44	ASN	3.2
18	1W	99	ARG	3.2
42	1k	64	ALA	3.2
3	1D	246	PRO	3.2
9	1N	44	PRO	3.2
9	2N	1	MET	3.2
11	2P	23	PRO	3.2
31	29	33	LYS	3.2
3	2D	56	GLY	3.2
3	2D	210	GLY	3.2
3	2D	235	GLY	3.2
3	1D	231	HIS	3.2
29	17	23	ARG	3.2
5	1F	64	ILE	3.2
3	2D	158	ALA	3.2
10	2O	43	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
16	2U	9	VAL	3.2
17	1V	14	VAL	3.2
42	1k	72	ALA	3.2
42	2k	20	TYR	3.2
45	1n	30	ALA	3.2
4	1E	202	LYS	3.2
1	1A	2505	G	3.2
42	1k	58	PRO	3.2
42	1k	121	PRO	3.2
16	2U	98	LEU	3.2
23	21	76	ARG	3.2
41	1j	45	ARG	3.2
7	2H	162	ILE	3.2
34	2c	202	ILE	3.2
44	2m	78	ILE	3.2
51	1t	16	HIS	3.2
4	2E	154	LYS	3.2
5	1F	97	TYR	3.2
10	1O	42	SER	3.2
30	18	52	LYS	3.2
34	1c	4	LYS	3.2
40	1i	109	VAL	3.2
47	1p	39	TYR	3.2
34	2c	205	GLY	3.2
40	2i	90	PRO	3.2
11	2P	55	ARG	3.2
16	1U	33	ARG	3.2
49	1r	43	PHE	3.2
35	2d	126	ILE	3.2
10	1O	84	ALA	3.2
10	2O	42	SER	3.2
10	2O	5	GLN	3.2
10	2O	21	CYS	3.2
11	1P	50	ARG	3.2
31	29	9	ARG	3.2
3	2D	177	LEU	3.2
11	1P	59	LEU	3.2
23	11	12	PRO	3.2
23	21	68	PRO	3.2
33	2b	44	LEU	3.2
35	2d	157	LEU	3.2
44	2m	66	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
13	2R	9	LYS	3.2
1	2A	1783	A	3.2
3	2D	161	THR	3.2
16	2U	72	HIS	3.2
35	2d	34	GLU	3.2
35	2d	111	ALA	3.2
12	2Q	13	GLN	3.2
36	2e	133	TYR	3.2
20	2Y	41	GLY	3.2
3	2D	249	PRO	3.2
18	2W	14	PRO	3.2
34	1c	101	LEU	3.2
47	1p	35	LYS	3.2
5	2F	186	ILE	3.2
30	18	16	ILE	3.2
31	29	26	ILE	3.2
1	2A	2506	U	3.2
10	1O	83	ALA	3.2
10	2O	58	VAL	3.2
13	2R	50	HIS	3.2
17	1V	79	VAL	3.2
27	15	20	ARG	3.2
41	1j	62	HIS	3.2
7	2H	14	GLY	3.2
13	1R	40	LYS	3.2
18	2W	13	SER	3.2
42	1k	27	ASN	3.2
42	1k	117	ASN	3.2
12	1Q	34	LEU	3.2
30	18	53	PRO	3.2
40	2i	123	PRO	3.2
15	2T	50	ILE	3.1
10	1O	26	LYS	3.1
20	2Y	36	ALA	3.1
1	2A	2505	G	3.1
3	1D	147	LEU	3.1
5	1F	33	LEU	3.1
16	2U	31	SER	3.1
34	2c	23	TYR	3.1
23	11	82	LEU	3.1
33	2b	101	MET	3.1
3	1D	7	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
4	1E	26	ILE	3.1
34	2c	21	ARG	3.1
20	2Y	46	LYS	3.1
51	2t	41	ILE	3.1
7	2H	131	VAL	3.1
30	18	22	VAL	3.1
4	1E	78	LEU	3.1
13	2R	51	LEU	3.1
15	2T	104	ASN	3.1
19	2X	95	LEU	3.1
36	1e	119	LEU	3.1
53	1v	14	A	3.1
5	1F	66	PRO	3.1
35	2d	73	ARG	3.1
45	1n	17	LYS	3.1
34	2c	77	ILE	3.1
3	1D	3	VAL	3.1
34	2c	64	VAL	3.1
41	2j	49	VAL	3.1
4	1E	148	GLY	3.1
30	28	9	GLY	3.1
42	1k	19	ALA	3.1
47	2p	22	THR	3.1
4	2E	195	LEU	3.1
5	1F	41	LEU	3.1
3	1D	52	ARG	3.1
3	2D	274	ARG	3.1
9	1N	78	TYR	3.1
10	1O	108	GLU	3.1
11	2P	41	ARG	3.1
9	2N	58	ASP	3.1
36	1e	26	PHE	3.1
42	2k	70	LYS	3.1
9	2N	95	PRO	3.1
8	1I	79	ILE	3.1
30	28	23	VAL	3.1
23	11	19	GLN	3.1
25	23	19	GLN	3.1
3	2D	147	LEU	3.1
4	2E	146	THR	3.1
7	2H	33	LEU	3.1
7	2H	122	THR	3.1

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Mol	Chain	Res	Type	RSRZ
9	1N	26	LEU	3.1
9	2N	22	THR	3.1
9	2N	39	ARG	3.1
12	1Q	10	ARG	3.1
36	2e	27	ARG	3.1
35	2d	106	TYR	3.1
23	11	65	SER	3.1
16	1U	80	ILE	3.1
4	1E	130	GLY	3.1
1	1A	2576	G	3.1
15	1T	90	GLN	3.1
29	27	45	ALA	3.1
36	2e	29	GLY	3.1
42	2k	65	ALA	3.1
47	2p	48	TRP	3.1
48	2q	26	GLN	3.1
9	2N	59	LYS	3.1
1	1A	1983	C	3.1
15	1T	29	ARG	3.1
16	2U	37	GLU	3.1
48	2q	91	ARG	3.1
5	1F	123	LEU	3.1
36	2e	43	LEU	3.1
45	2n	13	THR	3.1
47	1p	73	LEU	3.1
7	2H	163	TYR	3.1
36	2e	26	PHE	3.1
18	1W	94	ASP	3.1
39	2h	89	PRO	3.1
42	1k	24	SER	3.1
1	1A	2062	A	3.1
3	1D	229	VAL	3.1
9	1N	77	GLY	3.1
13	1R	114	VAL	3.1
42	1k	88	GLY	3.1
47	1p	24	ALA	3.1
55	1x	76	A	3.1
8	2I	27	ARG	3.1
3	2D	111	LEU	3.1
13	2R	20	LEU	3.1
54	1w	25	C	3.1
54	1y	3	C	3.1

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Mol	Chain	Res	Type	RSRZ
12	1Q	47	ILE	3.1
34	2c	157	ILE	3.1
42	1k	101	SER	3.1
48	1q	36	ILE	3.1
20	2Y	59	GLY	3.1
5	1F	40	GLN	3.1
23	11	61	ARG	3.1
27	25	45	VAL	3.1
1	1A	781	A	3.1
35	1d	78	LEU	3.1
40	2i	85	LEU	3.1
11	2P	27	HIS	3.1
3	1D	190	TYR	3.1
41	1j	57	LYS	3.1
47	2p	3	LYS	3.1
3	1D	14	ARG	3.1
3	1D	245	PRO	3.1
11	2P	109	GLY	3.1
34	1c	134	ILE	3.1
38	2g	4	ARG	3.1
45	1n	29	ARG	3.1
45	2n	32	SER	3.1
46	2o	68	ARG	3.1
35	2d	110	PHE	3.1
48	2q	6	LEU	3.1
10	1O	64	ARG	3.1
38	2g	79	ARG	3.1
3	2D	246	PRO	3.1
4	2E	124	GLY	3.1
23	11	45	ASN	3.1
27	15	11	THR	3.1
5	2F	67	GLN	3.1
25	23	47	VAL	3.0
47	1p	65	GLN	3.1
42	1k	97	ALA	3.0
23	11	69	LYS	3.0
3	1D	269	PHE	3.0
6	2G	152	LEU	3.0
16	2U	12	ARG	3.0
54	2y	23	A	3.0
40	1i	110	GLU	3.0
8	1I	109	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
16	1U	45	TYR	3.0
44	1m	87	TYR	3.0
9	2N	55	VAL	3.0
11	1P	31	ALA	3.0
16	2U	22	LYS	3.0
23	11	10	LYS	3.0
54	2y	18	G	3.0
4	1E	19	ARG	3.0
18	1W	23	LEU	3.0
43	2l	33	ARG	3.0
37	2f	89	MET	3.0
30	18	3	LYS	3.0
40	2i	63	ILE	3.0
5	2F	92	PRO	3.0
20	1Y	7	VAL	3.0
25	23	54	VAL	3.0
36	2e	32	VAL	3.0
3	2D	247	ALA	3.0
7	2H	165	ALA	3.0
30	18	55	ALA	3.0
19	2X	60	ARG	3.0
32	1a	1529	G	3.0
3	2D	237	GLU	3.0
3	1D	258	LYS	3.0
4	1E	127	ASP	3.0
11	1P	46	LYS	3.0
17	2V	84	LYS	3.0
29	17	11	LYS	3.0
35	2d	33	MET	3.0
42	1k	99	GLN	3.0
1	1A	2142	C	3.0
1	2A	756	C	3.0
16	2U	2	PRO	3.0
35	2d	170	VAL	3.0
35	2d	189	PRO	3.0
36	2e	82	VAL	3.0
42	1k	109	VAL	3.0
13	2R	101	ALA	3.0
44	2m	5	ALA	3.0
28	26	11	LEU	3.0
35	2d	94	LEU	3.0
4	2E	145	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
9	2N	89	LYS	3.0
40	1i	112	LYS	3.0
15	2T	71	GLY	3.0
18	1W	111	HIS	3.0
4	2E	160	TYR	3.0
9	2N	35	ARG	3.0
9	2N	86	PRO	3.0
15	2T	100	TYR	3.0
27	25	20	ARG	3.0
48	2q	35	VAL	3.0
1	2A	6	A	3.0
3	1D	208	LYS	3.0
9	1N	76	SER	3.0
13	1R	44	LEU	3.0
16	1U	15	LYS	3.0
16	2U	32	PHE	3.0
41	1j	47	PHE	3.0
4	2E	158	GLY	3.0
38	1g	106	GLN	3.0
11	2P	102	ARG	3.0
52	2u	13	ILE	3.0
15	1T	34	VAL	3.0
30	28	52	LYS	3.0
31	29	2	LYS	3.0
33	2b	33	TYR	3.0
36	1e	51	VAL	3.0
38	2g	84	ASN	3.0
43	2l	16	GLU	3.0
43	2l	21	LYS	3.0
51	2t	30	LYS	3.0
4	1E	183	LEU	3.0
34	2c	12	LEU	3.0
35	2d	120	LEU	3.0
47	2p	49	LEU	3.0
4	2E	153	GLY	3.0
19	1X	76	ARG	3.0
4	2E	159	HIS	3.0
9	2N	130	HIS	3.0
17	1V	72	VAL	3.0
3	1D	265	PRO	3.0
3	2D	62	TYR	3.0
11	1P	12	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
23	11	15	ALA	3.0
28	16	2	ALA	3.0
18	1W	19	LEU	3.0
1	2A	2591	C	3.0
1	2A	1128	A	3.0
1	2A	2051	A	3.0
7	2H	93	GLY	3.0
32	2a	815	A	3.0
42	1k	62	GLN	3.0
46	1o	36	ILE	3.0
51	1t	55	ILE	3.0
37	1f	60	PHE	3.0
47	1p	32	TYR	3.0
1	1A	444	C	3.0
23	21	11	ARG	3.0
34	2c	59	ARG	3.0
34	2c	81	GLY	3.0
7	2H	106	THR	3.0
34	1c	135	LYS	3.0
3	1D	106	ILE	3.0
10	2O	63	VAL	3.0
15	2T	63	VAL	3.0
17	2V	79	VAL	3.0
4	1E	144	ARG	2.9
8	2I	68	LEU	2.9
19	2X	73	ARG	2.9
47	1p	31	LYS	2.9
49	1r	71	LYS	2.9
3	2D	254	THR	2.9
32	1a	800	G	2.9
3	1D	92	ILE	2.9
10	1O	68	GLU	2.9
1	1A	764	A	2.9
1	2A	2577	A	2.9
32	2a	1357	A	2.9
9	1N	14	VAL	2.9
25	23	51	ALA	2.9
13	2R	54	LEU	2.9
16	1U	18	LEU	2.9
16	1U	43	GLY	2.9
34	1c	39	ILE	2.9
1	1A	1248	G	2.9

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Mol	Chain	Res	Type	RSRZ
1	2A	2509	G	2.9
9	1N	83	LYS	2.9
13	2R	5	LYS	2.9
18	2W	17	VAL	2.9
27	25	15	ARG	2.9
4	1E	15	PHE	2.9
5	2F	55	GLY	2.9
9	2N	33	LEU	2.9
17	2V	38	LEU	2.9
24	12	53	LEU	2.9
25	23	4	LEU	2.9
30	18	60	LEU	2.9
35	1d	101	LEU	2.9
17	1V	80	GLN	2.9
36	1e	20	GLN	2.9
1	2A	2610	C	2.9
36	1e	129	ILE	2.9
47	1p	4	ILE	2.9
12	2Q	76	LYS	2.9
23	21	21	ARG	2.9
9	1N	55	VAL	2.9
9	1N	62	VAL	2.9
41	2j	44	VAL	2.9
20	2Y	6	HIS	2.9
34	2c	33	LEU	2.9
35	2d	155	LEU	2.9
35	2d	176	LEU	2.9
18	2W	87	PRO	2.9
55	1x	73	A	2.9
27	15	59	GLU	2.9
4	2E	118	LYS	2.9
11	1P	33	ARG	2.9
13	2R	105	ARG	2.9
7	2H	17	VAL	2.9
42	2k	87	THR	2.9
35	2d	75	PHE	2.9
12	2Q	125	LEU	2.9
20	2Y	58	GLY	2.9
23	21	22	GLY	2.9
34	2c	115	LEU	2.9
4	1E	138	PRO	2.9
9	2N	101	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
25	23	20	LYS	2.9
32	1a	1507	A	2.9
33	2b	132	LYS	2.9
3	1D	218	ARG	2.9
4	1E	136	ARG	2.9
11	1P	71	VAL	2.9
36	2e	119	LEU	2.9
47	1p	60	LEU	2.9
50	2s	71	LEU	2.9
30	28	8	LYS	2.9
38	1g	148	ASN	2.9
16	1U	9	VAL	2.9
34	1c	198	VAL	2.9
3	2D	57	GLY	2.9
10	2O	20	MET	2.9
1	1A	2896	C	2.9
11	2P	17	LYS	2.9
12	2Q	2	LEU	2.9
13	1R	79	LEU	2.9
23	21	64	ALA	2.9
38	2g	152	ALA	2.9
1	1A	1130	U	2.9
9	1N	115	ARG	2.9
35	1d	168	ARG	2.9
36	1e	15	ARG	2.9
41	2j	53	PRO	2.9
49	2r	34	TYR	2.9
1	2A	804	A	2.9
34	2c	124	ILE	2.9
5	1F	55	GLY	2.9
12	2Q	90	VAL	2.9
13	1R	9	LYS	2.9
40	2i	113	LYS	2.9
54	2y	22	G	2.9
47	2p	2	VAL	2.9
9	2N	115	ARG	2.9
16	2U	60	LEU	2.9
40	2i	19	LEU	2.9
45	1n	44	LEU	2.9
1	1A	34	C	2.9
16	1U	6	THR	2.9
33	1b	95	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
10	2O	22	ILE	2.9
46	1o	87	ILE	2.9
4	2E	51	PHE	2.9
15	2T	22	PHE	2.9
1	2A	1763	G	2.9
11	2P	77	ARG	2.9
16	2U	7	GLY	2.9
32	1a	162	A	2.9
35	2d	198	VAL	2.9
4	1E	114	ALA	2.9
9	1N	15	LEU	2.9
9	1N	57	ALA	2.9
23	21	98	LEU	2.9
27	25	25	LEU	2.9
29	17	31	LEU	2.9
40	2i	79	LEU	2.9
43	1l	26	ALA	2.9
48	2q	43	LEU	2.9
36	2e	87	SER	2.8
46	1o	48	LYS	2.8
3	1D	105	ILE	2.8
20	2Y	38	ILE	2.8
35	2d	144	ASP	2.8
3	1D	177	LEU	2.8
9	1N	91	LEU	2.8
30	18	4	MET	2.8
32	1a	1513	A	2.8
53	1v	23	A	2.8
9	1N	104	LYS	2.8
11	1P	29	LYS	2.8
23	21	65	SER	2.8
1	2A	2055	C	2.8
42	2k	39	PRO	2.8
5	1F	54	ARG	2.8
5	1F	82	ILE	2.8
9	1N	114	ARG	2.8
10	1O	77	ILE	2.8
9	2N	127	ASP	2.8
12	1Q	32	TYR	2.8
15	1T	115	ARG	2.8
35	2d	49	ARG	2.8
20	2Y	15	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
40	2i	108	VAL	2.8
16	1U	109	LEU	2.8
13	2R	39	PRO	2.8
9	1N	12	ARG	2.8
15	1T	62	THR	2.8
34	2c	35	GLU	2.8
36	1e	27	ARG	2.8
42	1k	41	THR	2.8
15	2T	61	PHE	2.8
18	2W	10	VAL	2.8
3	2D	133	LEU	2.8
3	2D	155	LEU	2.8
5	2F	176	LEU	2.8
20	1Y	67	LEU	2.8
38	1g	144	MET	2.8
48	2q	24	GLU	2.8
19	2X	76	ARG	2.8
35	1d	47	ARG	2.8
46	2o	38	ARG	2.8
3	1D	220	HIS	2.8
34	1c	165	THR	2.8
36	1e	11	ILE	2.8
42	1k	32	ILE	2.8
1	2A	2578	G	2.8
24	12	37	PHE	2.8
3	2D	205	VAL	2.8
27	15	6	VAL	2.8
46	1o	60	VAL	2.8
8	2I	72	LEU	2.8
27	15	58	LEU	2.8
34	2c	28	GLN	2.8
32	2a	1257	U	2.8
3	1D	228	PRO	2.8
4	2E	147	PRO	2.8
42	2k	123	LYS	2.8
49	2r	61	LYS	2.8
1	2A	687	C	2.8
33	2b	163	PHE	2.8
37	1f	55	ASP	2.8
4	1E	188	VAL	2.8
13	1R	66	VAL	2.8
4	1E	79	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
5	1F	38	ARG	2.8
23	11	40	ARG	2.8
29	17	12	ARG	2.8
50	1s	81	ARG	2.8
9	1N	66	LYS	2.8
15	1T	33	LYS	2.8
35	2d	158	ILE	2.8
39	2h	80	ILE	2.8
40	2i	81	ILE	2.8
42	1k	115	PRO	2.8
15	2T	40	THR	2.8
1	1A	2551	C	2.8
9	2N	68	GLU	2.8
9	2N	87	LEU	2.8
13	1R	29	LEU	2.8
23	21	46	LEU	2.8
28	16	34	LEU	2.8
35	2d	121	VAL	2.8
36	1e	123	LEU	2.8
29	17	20	ALA	2.8
42	2k	51	LYS	2.8
45	2n	59	ALA	2.8
9	2N	106	MET	2.8
32	2a	79	G	2.8
54	1w	24	G	2.8
4	1E	126	PRO	2.8
4	2E	139	GLY	2.8
9	2N	126	PRO	2.8
3	1D	173	VAL	2.8
4	2E	107	THR	2.8
10	2O	38	VAL	2.8
10	2O	97	ARG	2.8
34	2c	6	HIS	2.8
36	2e	33	VAL	2.8
18	1W	16	LYS	2.8
29	27	29	LYS	2.8
48	2q	88	TYR	2.8
9	2N	18	ALA	2.8
54	1w	13	C	2.8
7	2H	101	ARG	2.8
16	1U	79	PHE	2.8
8	1I	20	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
22	20	68	GLU	2.8
38	1g	32	ARG	2.8
44	1m	94	ARG	2.8
48	2q	58	GLU	2.8
9	1N	138	LEU	2.8
10	2O	25	LEU	2.8
18	1W	29	LEU	2.8
36	2e	123	LEU	2.8
51	2t	71	THR	2.8
16	1U	68	ALA	2.8
1	2A	1129	A	2.7
1	2A	2059	A	2.7
29	17	22	MET	2.7
42	2k	38	ASN	2.7
54	1y	73	A	2.7
5	1F	47	GLY	2.7
11	1P	41	ARG	2.7
31	29	19	ARG	2.7
34	1c	152	ILE	2.7
42	2k	125	PHE	2.7
45	2n	58	LYS	2.7
1	1A	2509	G	2.7
11	2P	63	PRO	2.7
25	23	16	PRO	2.7
11	1P	47	ASP	2.7
3	1D	145	VAL	2.7
3	2D	12	SER	2.7
39	2h	4	ASP	2.7
4	1E	104	VAL	2.7
4	2E	196	VAL	2.7
29	27	31	LEU	2.7
48	2q	9	VAL	2.7
12	1Q	36	ALA	2.7
12	2Q	93	TYR	2.7
16	2U	41	ALA	2.7
23	21	71	TYR	2.7
1	1A	2579	C	2.7
15	1T	108	ARG	2.7
29	27	10	ARG	2.7
45	2n	55	GLY	2.7
51	1t	29	LYS	2.7
33	1b	122	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
39	1h	45	ILE	2.7
3	2D	231	HIS	2.7
13	1R	18	LEU	2.7
31	19	25	VAL	2.7
48	2q	10	VAL	2.7
29	27	6	GLN	2.7
4	1E	157	ALA	2.7
11	2P	31	ALA	2.7
13	1R	109	ALA	2.7
36	2e	30	ALA	2.7
5	1F	63	LYS	2.7
13	1R	95	THR	2.7
31	29	18	ARG	2.7
1	1A	1761	C	2.7
16	1U	44	ASN	2.7
23	21	60	PHE	2.7
32	1a	815	A	2.7
33	2b	152	PHE	2.7
41	1j	63	PHE	2.7
24	22	60	LEU	2.7
31	19	3	VAL	2.7
35	2d	96	LEU	2.7
51	1t	13	LEU	2.7
13	2R	40	LYS	2.7
12	1Q	51	ARG	2.7
32	2a	1030(A)	G	2.7
39	2h	58	TYR	2.7
4	2E	117	MET	2.7
39	2h	128	GLY	2.7
46	2o	89	GLY	2.7
4	1E	96	PHE	2.7
19	1X	28	PHE	2.7
19	2X	80	ILE	2.7
1	2A	196	A	2.7
1	2A	2058	A	2.7
5	2F	196	LEU	2.7
8	1I	38	LEU	2.7
18	2W	4	LYS	2.7
27	15	45	VAL	2.7
48	2q	84	LEU	2.7
40	1i	117	HIS	2.7
42	1k	46	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	1252	G	2.7
20	1Y	61	ILE	2.7
31	19	17	ILE	2.7
34	1c	182	ILE	2.7
35	2d	204	ILE	2.7
3	1D	59	LYS	2.7
8	2I	12	LEU	2.7
9	1N	99	LEU	2.7
10	2O	4	PRO	2.7
10	2O	85	VAL	2.7
13	2R	44	LEU	2.7
13	2R	65	LEU	2.7
16	1U	39	LEU	2.7
36	2e	24	ARG	2.7
17	2V	77	ALA	2.7
11	1P	13	ASN	2.7
12	1Q	120	ILE	2.7
34	1c	202	ILE	2.7
1	1A	2603	G	2.7
33	1b	98	LEU	2.7
36	2e	100	VAL	2.7
1	2A	2057	A	2.7
29	27	5	TRP	2.7
29	27	32	LYS	2.7
45	1n	32	SER	2.7
13	1R	47	PHE	2.7
19	1X	1	MET	2.7
36	1e	133	TYR	2.7
48	2q	71	PHE	2.7
10	2O	78	ARG	2.7
11	1P	18	ARG	2.7
19	1X	8	ILE	2.7
29	17	21	ARG	2.7
41	1j	48	THR	2.7
47	1p	19	ILE	2.7
1	2A	1656	C	2.7
3	2D	196	VAL	2.7
17	1V	71	LEU	2.7
9	2N	135	PRO	2.7
11	2P	71	VAL	2.7
22	20	79	VAL	2.7
23	11	30	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
30	18	40	GLU	2.7
37	1f	9	VAL	2.7
39	1h	4	ASP	2.7
45	2n	54	PRO	2.7
9	2N	47	ALA	2.7
15	1T	71	GLY	2.7
40	2i	119	ALA	2.7
15	1T	22	PHE	2.7
29	27	34	ARG	2.7
42	1k	48	ILE	2.7
3	1D	230	ASP	2.7
4	1E	184	VAL	2.7
18	2W	36	LEU	2.7
19	1X	70	LEU	2.7
35	2d	179	GLU	2.7
36	1e	135	THR	2.7
46	2o	37	ASN	2.7
25	23	24	LYS	2.7
30	18	21	LYS	2.7
43	2l	20	LYS	2.7
51	1t	34	LYS	2.7
5	2F	47	GLY	2.7
36	2e	59	GLY	2.7
16	2U	21	ALA	2.7
3	1D	48	ARG	2.7
13	2R	22	ARG	2.7
7	2H	134	SER	2.6
12	1Q	103	MET	2.6
9	1N	16	ILE	2.6
15	1T	52	ILE	2.6
15	1T	100	TYR	2.6
35	1d	126	ILE	2.6
13	1R	99	LYS	2.6
18	1W	98	LYS	2.6
34	2c	188	LEU	2.6
35	1d	11	LEU	2.6
14	1S	28	VAL	2.6
23	21	70	VAL	2.6
43	2l	8	ASN	2.6
5	2F	86	GLY	2.6
50	2s	84	GLY	2.6
3	1D	93	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
38	1g	83	ALA	2.6
45	1n	2	ALA	2.6
54	1w	68	C	2.6
4	2E	119	ARG	2.6
30	28	30	ARG	2.6
45	1n	41	ARG	2.6
20	2Y	68	HIS	2.6
1	2A	1125	G	2.6
4	2E	11	MET	2.6
10	2O	44	LYS	2.6
16	2U	34	LYS	2.6
18	2W	78	GLU	2.6
20	2Y	26	LYS	2.6
32	2a	104	G	2.6
43	2l	85	ILE	2.6
54	1w	69	G	2.6
20	2Y	57	GLN	2.6
32	1a	768	A	2.6
45	1n	21	TYR	2.6
17	1V	95	LEU	2.6
33	2b	118	LEU	2.6
3	1D	185	VAL	2.6
4	1E	173	VAL	2.6
7	1H	19	VAL	2.6
9	2N	62	VAL	2.6
10	1O	121	VAL	2.6
20	2Y	49	VAL	2.6
42	2k	84	VAL	2.6
48	2q	73	VAL	2.6
18	2W	91	GLY	2.6
3	2D	60	ARG	2.6
5	1F	94	PRO	2.6
37	1f	46	ARG	2.6
1	1A	806	C	2.6
32	1a	1501	C	2.6
38	2g	150	ALA	2.6
20	1Y	34	LYS	2.6
28	16	53	LYS	2.6
7	2H	72	ILE	2.6
9	1N	90	MET	2.6
1	2A	1264	G	2.6
15	1T	68	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
53	2v	22	U	2.6
32	1a	769	G	2.6
46	1o	57	LEU	2.6
51	2t	10	LEU	2.6
54	1w	6	G	2.6
4	2E	148	GLY	2.6
12	2Q	86	GLY	2.6
15	1T	49	VAL	2.6
30	28	49	VAL	2.6
33	2b	164	VAL	2.6
34	1c	207	VAL	2.6
47	1p	2	VAL	2.6
51	1t	25	ARG	2.6
54	1y	23	A	2.6
4	1E	146	THR	2.6
4	1E	191	PRO	2.6
12	2Q	39	PRO	2.6
16	1U	38	THR	2.6
33	1b	188	ALA	2.6
36	2e	17	ALA	2.6
7	2H	104	GLU	2.6
43	1l	16	GLU	2.6
17	2V	4	ILE	2.6
4	1E	181	LEU	2.6
48	1q	97	SER	2.6
48	2q	68	ARG	2.6
3	1D	56	GLY	2.6
31	19	16	VAL	2.6
34	1c	55	VAL	2.6
48	2q	41	LYS	2.6
49	1r	84	LYS	2.6
51	1t	68	LYS	2.6
19	1X	11	PRO	2.6
34	1c	206	GLU	2.6
1	2A	2146	C	2.6
18	2W	106	ILE	2.6
8	1I	72	LEU	2.6
12	1Q	79	LEU	2.6
47	2p	60	LEU	2.6
10	2O	61	VAL	2.6
18	1W	76	VAL	2.6
40	2i	5	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
51	1t	38	LYS	2.6
7	2H	32	GLU	2.6
16	2U	4	ALA	2.6
31	29	5	ALA	2.6
34	1c	10	PHE	2.6
42	2k	33	THR	2.6
54	2y	35	A	2.6
1	1A	2511	U	2.6
3	1D	236	GLY	2.6
8	2I	77	LEU	2.6
9	1N	112	LEU	2.6
11	1P	62	LEU	2.6
16	1U	16	LYS	2.6
16	1U	104	GLN	2.6
30	28	41	ILE	2.6
8	2I	81	VAL	2.6
33	1b	81	VAL	2.6
39	1h	62	TYR	2.6
28	26	24	GLU	2.6
44	2m	73	GLU	2.6
3	1D	6	PHE	2.6
12	1Q	104	PHE	2.6
15	1T	104	ASN	2.6
33	2b	232	PRO	2.6
40	2i	106	ALA	2.6
3	1D	161	THR	2.6
46	1o	65	ARG	2.6
46	1o	88	ARG	2.6
46	2o	54	ARG	2.6
1	1A	1770	G	2.6
3	1D	46	GLN	2.6
52	1u	13	ILE	2.6
1	1A	435	C	2.6
8	2I	6	LEU	2.6
10	1O	95	GLY	2.6
23	11	9	GLY	2.6
34	2c	185	GLY	2.6
39	1h	59	LEU	2.6
7	2H	164	TYR	2.6
10	1O	57	VAL	2.6
13	1R	69	ASP	2.6
31	19	7	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
48	2q	85	VAL	2.6
16	1U	57	PHE	2.6
10	1O	31	LYS	2.6
11	1P	8	PRO	2.6
11	2P	16	ARG	2.6
30	28	24	ALA	2.6
31	29	35	ARG	2.6
49	2r	43	PHE	2.6
15	1T	110	ILE	2.6
18	1W	96	ILE	2.6
20	2Y	12	THR	2.6
1	2A	1253	A	2.6
8	1I	9	LEU	2.6
8	1I	35	LEU	2.6
10	2O	122	LEU	2.6
34	2c	159	GLY	2.6
35	2d	11	LEU	2.6
48	2q	33	GLY	2.6
1	1A	1176	G	2.6
1	1A	2498	C	2.6
4	1E	87	GLU	2.6
32	2a	108	G	2.6
23	11	51	VAL	2.6
39	2h	129	VAL	2.6
5	1F	68	LYS	2.6
30	18	47	LYS	2.6
36	2e	15	ARG	2.6
51	2t	15	ARG	2.6
34	2c	189	ALA	2.6
3	2D	252	TRP	2.6
33	1b	94	ASN	2.6
12	1Q	13	GLN	2.5
3	2D	50	THR	2.5
42	2k	40	ILE	2.5
13	1R	115	GLU	2.5
35	2d	97	LEU	2.5
3	2D	3	VAL	2.5
3	2D	230	ASP	2.5
31	29	22	ARG	2.5
40	2i	66	ARG	2.5
43	1l	91	LYS	2.5
54	2w	40	C	2.5

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Mol	Chain	Res	Type	RSRZ
1	2A	2802	G	2.5
12	1Q	44	ALA	2.5
15	2T	45	PHE	2.5
42	1k	107	SER	2.5
4	2E	143	ASN	2.5
9	2N	42	TRP	2.5
3	1D	65	ILE	2.5
13	1R	34	ILE	2.5
43	1l	85	ILE	2.5
50	2s	49	ILE	2.5
8	2I	128	LEU	2.5
3	1D	217	ARG	2.5
3	2D	255	LYS	2.5
10	1O	109	LYS	2.5
11	1P	57	THR	2.5
12	2Q	75	THR	2.5
35	2d	202	LEU	2.5
11	1P	21	ARG	2.5
16	1U	59	ARG	2.5
32	1a	1196	U	2.5
32	2a	1532	U	2.5
34	2c	142	MET	2.5
40	1i	121	ARG	2.5
43	2l	23	LYS	2.5
16	1U	90	VAL	2.5
31	19	23	VAL	2.5
46	2o	63	ARG	2.5
48	2q	92	ARG	2.5
32	1a	1527	C	2.5
54	1w	49	C	2.5
34	1c	154	SER	2.5
54	1w	5	G	2.5
3	1D	174	ILE	2.5
3	2D	256	GLY	2.5
12	1Q	91	GLU	2.5
34	2c	206	GLU	2.5
11	1P	14	LYS	2.5
39	1h	6	ILE	2.5
3	2D	213	ARG	2.5
16	2U	64	ARG	2.5
38	2g	16	LEU	2.5
39	2h	12	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
46	2o	34	LEU	2.5
52	2u	10	ARG	2.5
4	1E	105	THR	2.5
32	1a	1528	U	2.5
43	1l	67	THR	2.5
13	1R	13	HIS	2.5
13	1R	49	ASP	2.5
1	1A	2575	C	2.5
10	1O	111	PHE	2.5
1	2A	1847	A	2.5
10	1O	60	ALA	2.5
23	1l	43	TYR	2.5
15	1T	73	GLU	2.5
30	28	44	LYS	2.5
36	2e	83	GLU	2.5
39	1h	72	PRO	2.5
1	2A	743	G	2.5
1	2A	2052	G	2.5
3	1D	64	ILE	2.5
3	2D	222	ARG	2.5
13	1R	33	ARG	2.5
18	2W	37	ARG	2.5
39	2h	55	GLY	2.5
47	1p	33	ILE	2.5
47	2p	33	ILE	2.5
4	2E	120	TRP	2.5
15	1T	10	VAL	2.5
16	1U	8	VAL	2.5
19	1X	30	VAL	2.5
39	2h	82	HIS	2.5
51	1t	71	THR	2.5
5	2F	129	PHE	2.5
15	2T	76	PHE	2.5
1	1A	436	C	2.5
3	1D	199	ALA	2.5
8	1I	121	LYS	2.5
16	2U	35	ALA	2.5
27	15	56	LYS	2.5
38	1g	146	GLU	2.5
1	1A	1932	A	2.5
1	2A	1254	A	2.5
1	2A	1379	A	2.5

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Mol	Chain	Res	Type	RSRZ
3	2D	218	ARG	2.5
5	2F	54	ARG	2.5
9	2N	91	LEU	2.5
12	1Q	2	LEU	2.5
27	15	30	LEU	2.5
35	1d	120	LEU	2.5
46	2o	57	LEU	2.5
1	1A	2513	G	2.5
10	1O	43	VAL	2.5
34	2c	153	VAL	2.5
39	1h	118	VAL	2.5
8	2I	108	THR	2.5
10	1O	96	THR	2.5
16	2U	15	LYS	2.5
23	21	69	LYS	2.5
10	1O	94	ARG	2.5
22	10	25	ARG	2.5
4	1E	6	GLY	2.5
10	2O	15	GLY	2.5
45	2n	60	SER	2.5
48	1q	33	GLY	2.5
1	2A	1785	A	2.5
10	1O	39	ILE	2.5
15	1T	75	ILE	2.5
17	2V	96	ILE	2.5
6	1G	82	LEU	2.5
1	2A	810	U	2.5
12	2Q	97	VAL	2.5
23	21	23	LYS	2.5
36	2e	115	VAL	2.5
20	2Y	62	GLU	2.5
22	20	69	PHE	2.5
13	1R	45	ARG	2.5
41	2j	45	ARG	2.5
47	2p	25	ARG	2.5
9	2N	80	GLY	2.5
34	1c	184	TYR	2.5
8	2I	5	LEU	2.5
16	2U	62	ILE	2.5
46	2o	56	LEU	2.5
51	2t	33	ILE	2.5
16	2U	19	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
51	1t	74	LYS	2.5
55	2x	76	A	2.5
3	1D	142	VAL	2.5
18	2W	20	VAL	2.5
25	23	29	ARG	2.5
1	2A	748	G	2.5
1	2A	799	G	2.5
3	1D	256	GLY	2.5
11	2P	68	GLN	2.5
13	1R	36	THR	2.5
32	1a	1520	G	2.5
34	2c	53	ALA	2.5
38	1g	150	ALA	2.5
40	2i	69	GLY	2.5
8	1I	25	TYR	2.5
15	2T	52	ILE	2.5
34	1c	124	ILE	2.5
36	1e	121	LYS	2.5
42	2k	29	ILE	2.5
5	1F	154	VAL	2.5
5	2F	46	ARG	2.5
7	2H	43	VAL	2.5
19	2X	59	VAL	2.5
24	22	1	MET	2.5
41	1j	66	ARG	2.5
13	1R	5	LYS	2.5
22	10	24	LYS	2.5
1	2A	1835	G	2.5
5	1F	101	LEU	2.5
17	1V	40	LEU	2.5
33	1b	33	TYR	2.5
35	1d	54	TYR	2.5
48	2q	89	LEU	2.5
51	2t	63	ILE	2.5
54	1y	75	C	2.4
1	2A	1026	U	2.4
16	1U	106	PHE	2.4
40	2i	17	VAL	2.4
43	2l	11	VAL	2.4
46	2o	59	MET	2.4
47	2p	80	PHE	2.4
1	2A	1780	A	2.4

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Mol	Chain	Res	Type	RSRZ
1	2A	2713	A	2.4
18	2W	83	LYS	2.4
11	2P	57	THR	2.4
18	1W	24	ILE	2.4
18	1W	100	THR	2.4
18	2W	12	ILE	2.4
34	1c	14	ILE	2.4
37	1f	98	LEU	2.4
39	1h	80	ILE	2.4
39	1h	83	ILE	2.4
52	2u	6	ARG	2.4
17	1V	36	PRO	2.4
10	2O	102	VAL	2.4
18	1W	17	VAL	2.4
15	1T	1	MET	2.4
30	28	26	LYS	2.4
36	2e	130	ASN	2.4
4	1E	187	ALA	2.4
9	1N	18	ALA	2.4
10	2O	16	ALA	2.4
27	25	14	ALA	2.4
1	2A	1787	A	2.4
12	1Q	112	GLU	2.4
35	1d	122	ARG	2.4
36	2e	107	ARG	2.4
39	1h	18	ARG	2.4
25	13	53	LEU	2.4
5	2F	59	TYR	2.4
4	2E	152	LYS	2.4
16	1U	13	LYS	2.4
16	2U	30	LYS	2.4
29	17	25	PRO	2.4
33	1b	202	PRO	2.4
42	2k	82	VAL	2.4
48	1q	11	VAL	2.4
48	2q	99	SER	2.4
32	1a	1526	G	2.4
11	1P	68	GLN	2.4
10	1O	49	ARG	2.4
16	1U	41	ALA	2.4
40	1i	106	ALA	2.4
45	2n	10	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
13	1R	43	GLU	2.4
4	1E	197	ILE	2.4
24	12	24	LEU	2.4
54	2y	21	A	2.4
3	1D	36	PRO	2.4
16	2U	24	TYR	2.4
34	2c	29	TYR	2.4
15	1T	70	VAL	2.4
18	1W	10	VAL	2.4
26	24	56	VAL	2.4
4	1E	121	ASN	2.4
50	2s	82	GLY	2.4
16	2U	50	ARG	2.4
23	11	52	ARG	2.4
32	1a	811	C	2.4
32	1a	1523	G	2.4
32	2a	80	G	2.4
54	1y	53	G	2.4
6	2G	75	LYS	2.4
40	1i	116	LYS	2.4
24	22	35	LEU	2.4
35	2d	123	HIS	2.4
36	1e	91	LEU	2.4
36	2e	110	LEU	2.4
41	2j	68	HIS	2.4
42	2k	63	LEU	2.4
46	1o	34	LEU	2.4
1	2A	2587	A	2.4
15	2T	77	PRO	2.4
20	2Y	27	VAL	2.4
39	1h	138	TRP	2.4
43	2l	39	VAL	2.4
3	2D	42	GLY	2.4
9	1N	80	GLY	2.4
10	2O	64	ARG	2.4
17	1V	101	GLY	2.4
33	2b	205	ASP	2.4
34	1c	172	ARG	2.4
35	2d	139	ARG	2.4
46	2o	64	ARG	2.4
12	1Q	77	LYS	2.4
36	2e	47	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
43	2l	91	LYS	2.4
16	1U	115	ALA	2.4
18	2W	48	ALA	2.4
1	1A	442	G	2.4
1	1A	530	G	2.4
1	2A	2602	A	2.4
4	1E	167	VAL	2.4
22	10	38	VAL	2.4
39	2h	97	VAL	2.4
44	2m	105	THR	2.4
51	1t	23	ARG	2.4
19	2X	2	LYS	2.4
19	2X	77	LYS	2.4
3	2D	212	SER	2.4
10	1O	20	MET	2.4
3	1D	224	ALA	2.4
9	2N	124	ALA	2.4
1	2A	1657	C	2.4
1	2A	1675	C	2.4
20	2Y	44	ILE	2.4
34	1c	43	LEU	2.4
35	1d	97	LEU	2.4
1	2A	1764	G	2.4
19	1X	43	VAL	2.4
23	11	27	GLU	2.4
34	1c	2	GLY	2.4
35	1d	198	VAL	2.4
42	2k	86	GLY	2.4
43	2l	25	PRO	2.4
48	2q	28	PRO	2.4
8	2I	93	THR	2.4
9	2N	32	THR	2.4
32	1a	1257	U	2.4
1	1A	2614	A	2.4
1	2A	1784	A	2.4
34	2c	56	ASP	2.4
3	2D	19	ALA	2.4
3	2D	225	ALA	2.4
1	2A	758	C	2.4
6	1G	133	LEU	2.4
10	1O	91	LEU	2.4
28	16	10	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
35	1d	204	ILE	2.4
41	2j	8	LEU	2.4
49	2r	66	LEU	2.4
30	28	13	ARG	2.4
35	2d	132	ARG	2.4
36	2e	14	ARG	2.4
4	2E	163	GLU	2.4
15	1T	63	VAL	2.4
16	1U	63	VAL	2.4
36	1e	49	PRO	2.4
38	2g	85	TYR	2.4
1	1A	2052	G	2.4
9	1N	22	THR	2.4
10	1O	6	THR	2.4
30	18	6	THR	2.4
54	2y	63	G	2.4
1	1A	590	A	2.4
1	1A	2602	A	2.4
16	2U	109	LEU	2.4
22	20	72	ARG	2.4
23	21	7	ILE	2.4
23	21	25	LYS	2.4
29	17	32	LYS	2.4
30	28	57	ARG	2.4
35	2d	14	ARG	2.4
36	2e	11	ILE	2.4
36	2e	121	LYS	2.4
38	2g	149	ARG	2.4
40	2i	16	ARG	2.4
51	1t	22	ARG	2.4
1	2A	790	C	2.4
11	2P	93	GLY	2.3
30	28	65	GLU	2.3
33	1b	152	PHE	2.3
18	1W	47	VAL	2.3
41	1j	93	GLY	2.3
31	19	36	GLN	2.3
35	1d	38	TYR	2.3
5	1F	43	LYS	2.3
16	1U	78	THR	2.3
5	1F	34	TRP	2.3
11	2P	40	SER	2.3

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Mol	Chain	Res	Type	RSRZ
19	1X	65	ARG	2.3
31	19	22	ARG	2.3
40	2i	83	ARG	2.3
54	2y	34	G	2.3
1	1A	2014	A	2.3
13	1R	113	LEU	2.3
35	2d	28	SER	2.3
35	2d	78	LEU	2.3
36	1e	12	LEU	2.3
37	1f	21	LEU	2.3
39	1h	134	ILE	2.3
54	1y	64	A	2.3
36	2e	81	GLU	2.3
1	1A	671	C	2.3
1	1A	1827	C	2.3
1	2A	208	C	2.3
10	1O	55	GLY	2.3
11	2P	34	GLY	2.3
32	1a	336	C	2.3
8	2I	18	VAL	2.3
43	2l	55	VAL	2.3
5	1F	59	TYR	2.3
28	16	8	LYS	2.3
30	18	26	LYS	2.3
3	1D	239	ARG	2.3
51	2t	80	ARG	2.3
7	1H	105	LEU	2.3
1	2A	832	G	2.3
10	2O	69	ILE	2.3
15	2T	88	ILE	2.3
17	1V	70	ILE	2.3
25	13	8	LEU	2.3
34	2c	91	LEU	2.3
35	1d	64	LEU	2.3
39	2h	36	LEU	2.3
34	2c	22	TRP	2.3
43	2l	62	SER	2.3
1	2A	207	A	2.3
1	2A	1132	A	2.3
1	2A	2015	A	2.3
1	2A	2712(A)	A	2.3
3	1D	55	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
15	1T	92	GLY	2.3
29	27	27	GLY	2.3
41	1j	11	PHE	2.3
43	1l	29	GLY	2.3
1	1A	2055	C	2.3
13	2R	48	VAL	2.3
40	2i	117	HIS	2.3
44	2m	74	VAL	2.3
32	1a	793	U	2.3
38	2g	155	ARG	2.3
40	1i	128	ARG	2.3
40	2i	111	ARG	2.3
4	2E	123	ALA	2.3
10	2O	30	ALA	2.3
18	1W	44	ALA	2.3
8	1I	30	LEU	2.3
10	2O	65	THR	2.3
18	1W	39	THR	2.3
22	20	21	LEU	2.3
36	1e	118	ILE	2.3
39	1h	136	GLU	2.3
42	2k	98	LEU	2.3
3	2D	22	SER	2.3
9	2N	118	LYS	2.3
30	28	34	TRP	2.3
1	1A	575	A	2.3
1	1A	2572	A	2.3
1	2A	1266	G	2.3
1	2A	2062	A	2.3
1	2A	2581	G	2.3
22	20	40	GLN	2.3
23	21	4	VAL	2.3
31	29	3	VAL	2.3
54	1y	74	C	2.3
35	2d	138	TYR	2.3
23	11	6	GLU	2.3
23	11	72	GLU	2.3
34	1c	200	ALA	2.3
4	2E	52	LEU	2.3
18	2W	29	LEU	2.3
36	1e	76	ILE	2.3
37	1f	10	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
49	1r	85	LEU	2.3
10	1O	14	THR	2.3
17	2V	69	LYS	2.3
11	1P	34	GLY	2.3
42	2k	26	ASN	2.3
5	1F	45	ARG	2.3
3	1D	118	VAL	2.3
10	1O	61	VAL	2.3
10	2O	62	VAL	2.3
22	20	38	VAL	2.3
23	21	49	VAL	2.3
1	1A	443	A	2.3
1	1A	1669	A	2.3
16	1U	49	HIS	2.3
32	2a	900	A	2.3
46	2o	50	HIS	2.3
54	2y	36	A	2.3
4	1E	189	PRO	2.3
7	2H	83	TYR	2.3
12	2Q	74	TYR	2.3
8	1I	12	LEU	2.3
17	1V	6	LYS	2.3
38	1g	108	ALA	2.3
44	2m	65	LYS	2.3
47	1p	17	TYR	2.3
9	2N	71	ILE	2.3
18	1W	6	ILE	2.3
37	1f	79	LEU	2.3
3	1D	157	ARG	2.3
29	27	39	ARG	2.3
35	2d	109	GLY	2.3
45	2n	51	GLY	2.3
47	1p	18	ARG	2.3
16	1U	29	SER	2.3
15	2T	90	GLN	2.3
35	2d	128	VAL	2.3
37	2f	6	VAL	2.3
23	21	66	HIS	2.3
45	2n	46	GLU	2.3
1	2A	669	G	2.3
32	2a	780	A	2.3
3	1D	131	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
7	2H	171	LEU	2.3
8	1I	24	GLY	2.3
8	2I	4	ILE	2.3
23	21	67	ILE	2.3
39	2h	107	LEU	2.3
35	2d	13	ARG	2.3
46	1o	68	ARG	2.3
5	2F	139	PHE	2.3
7	2H	109	PHE	2.3
47	1p	9	PHE	2.3
40	1i	124	GLN	2.3
16	2U	105	VAL	2.3
13	1R	102	GLU	2.3
40	1i	118	LYS	2.3
45	2n	11	LYS	2.3
48	2q	3	LYS	2.3
1	2A	2586	C	2.3
1	1A	1132	A	2.3
1	1A	2577	A	2.3
1	2A	2014	A	2.3
6	2G	135	LEU	2.3
8	1I	89	TYR	2.3
10	1O	32	TYR	2.3
10	1O	104	ARG	2.3
16	1U	52	ARG	2.3
18	2W	51	LEU	2.3
25	23	28	LEU	2.3
39	1h	112	LEU	2.3
45	1n	20	ALA	2.3
32	2a	706	A	2.3
45	1n	39	LEU	2.3
46	1o	64	ARG	2.3
46	1o	66	LEU	2.3
48	1q	31	LEU	2.3
50	1s	78	ARG	2.3
15	1T	102	ILE	2.3
54	1y	21	A	2.3
1	1A	1826	G	2.3
40	2i	33	PHE	2.3
45	1n	16	PHE	2.3
9	2N	66	LYS	2.3
47	1p	27	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
48	2q	34	LYS	2.3
9	1N	103	VAL	2.3
43	1l	43	VAL	2.3
48	2q	94	ASN	2.3
13	1R	14	SER	2.3
5	2F	44	ARG	2.3
17	1V	82	ARG	2.3
47	1p	68	ASP	2.3
1	1A	1675	C	2.3
9	1N	81	GLY	2.3
9	1N	87	LEU	2.3
12	1Q	17	LEU	2.3
12	1Q	20	ALA	2.3
17	2V	40	LEU	2.3
18	1W	36	LEU	2.3
49	2r	58	LEU	2.3
36	2e	80	ILE	2.3
40	2i	77	ILE	2.3
1	2A	782	A	2.3
1	2A	1829	A	2.3
15	1T	113	LYS	2.3
18	2W	16	LYS	2.3
35	2d	63	LYS	2.3
1	2A	242	G	2.3
1	2A	2607	G	2.3
19	2X	81	VAL	2.2
39	2h	79	VAL	2.2
15	2T	39	ARG	2.2
35	2d	125	HIS	2.2
42	1k	22	HIS	2.2
48	1q	29	HIS	2.2
36	2e	46	GLY	2.2
41	1j	20	ALA	2.2
15	1T	50	ILE	2.2
36	2e	60	TYR	2.2
39	1h	31	PHE	2.2
42	2k	21	ILE	2.2
6	1G	48	GLU	2.2
11	2P	74	GLU	2.2
1	2A	2176	A	2.2
30	18	57	ARG	2.2
31	19	35	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
35	2d	105	VAL	2.2
42	2k	109	VAL	2.2
3	2D	10	THR	2.2
30	18	12	LYS	2.2
7	2H	71	LEU	2.2
8	1I	5	LEU	2.2
16	2U	48	ALA	2.2
6	1G	88	ILE	2.2
3	1D	172	TYR	2.2
4	1E	160	TYR	2.2
9	1N	42	TRP	2.2
38	1g	26	PHE	2.2
4	1E	9	VAL	2.2
4	1E	198	VAL	2.2
38	1g	149	ARG	2.2
50	2s	78	ARG	2.2
1	2A	1655	A	2.2
1	2A	1762	A	2.2
7	2H	140	LYS	2.2
25	23	7	LYS	2.2
33	1b	27	LYS	2.2
44	1m	111	LYS	2.2
1	1A	2553	G	2.2
5	2F	94	PRO	2.2
13	1R	111	LEU	2.2
32	2a	793	U	2.2
41	1j	10	GLY	2.2
54	1y	47	U	2.2
22	10	36	ILE	2.2
33	1b	123	ALA	2.2
40	1i	122	ALA	2.2
46	1o	53	HIS	2.2
51	2t	16	HIS	2.2
6	2G	39	ILE	2.2
49	1r	29	PHE	2.2
15	2T	68	TYR	2.2
33	2b	36	ARG	2.2
1	1A	1774	C	2.2
1	2A	786	C	2.2
15	2T	28	VAL	2.2
39	2h	26	VAL	2.2
1	1A	1789	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	2A	764	A	2.2
1	2A	1969	A	2.2
1	1A	1693	U	2.2
1	1A	2554	U	2.2
9	1N	110	GLY	2.2
3	1D	237	GLU	2.2
5	1F	181	LEU	2.2
5	2F	175	THR	2.2
7	2H	124	GLU	2.2
10	1O	25	LEU	2.2
36	2e	23	GLY	2.2
16	2U	89	GLU	2.2
40	2i	47	LEU	2.2
27	15	28	PRO	2.2
34	2c	182	ILE	2.2
35	1d	158	ILE	2.2
36	2e	28	PHE	2.2
42	2k	77	MET	2.2
46	2o	36	ILE	2.2
1	1A	956	G	2.2
3	2D	258	LYS	2.2
4	1E	185	LYS	2.2
10	2O	53	LYS	2.2
12	1Q	132	VAL	2.2
13	1R	107	ASP	2.2
1	2A	783	A	2.2
13	2R	67	LEU	2.2
16	1U	56	ASP	2.2
33	1b	128	GLU	2.2
46	1o	89	GLY	2.2
10	2O	51	ALA	2.2
13	1R	8	ARG	2.2
13	1R	96	ARG	2.2
19	1X	27	THR	2.2
42	1k	33	THR	2.2
51	1t	84	LEU	2.2
4	1E	109	LYS	2.2
12	2Q	83	MET	2.2
15	2T	79	HIS	2.2
35	2d	29	PRO	2.2
42	1k	39	PRO	2.2
16	2U	104	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
44	1m	117	VAL	2.2
1	1A	2501	C	2.2
3	1D	235	GLY	2.2
11	2P	53	GLY	2.2
30	18	20	GLY	2.2
32	1a	796	C	2.2
36	1e	29	GLY	2.2
36	1e	122	GLU	2.2
47	1p	30	GLY	2.2
54	1y	13	C	2.2
15	1T	74	ARG	2.2
15	2T	64	ARG	2.2
16	1U	3	ARG	2.2
16	1U	30	LYS	2.2
23	21	40	ARG	2.2
38	1g	3	ARG	2.2
40	2i	70	LYS	2.2
3	1D	50	THR	2.2
12	1Q	43	THR	2.2
1	2A	2054	A	2.2
3	2D	178	PRO	2.2
5	1F	70	THR	2.2
36	2e	125	SER	2.2
25	23	2	PRO	2.2
39	2h	109	ILE	2.2
8	2I	25	TYR	2.2
1	1A	832	G	2.2
1	2A	2116	G	2.2
1	2A	2608	G	2.2
3	1D	150	LYS	2.2
3	2D	180	GLY	2.2
11	1P	20	GLY	2.2
11	2P	108	LYS	2.2
15	2T	108	ARG	2.2
17	1V	85	LYS	2.2
23	21	20	ARG	2.2
29	17	35	ARG	2.2
34	1c	156	ARG	2.2
39	2h	125	ARG	2.2
42	2k	42	TRP	2.2
43	1l	13	LYS	2.2
51	1t	15	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
9	1N	23	LEU	2.2
34	2c	111	LEU	2.2
5	2F	194	MET	2.2
8	2I	78	THR	2.2
13	2R	110	PRO	2.2
35	2d	91	SER	2.2
36	1e	106	PRO	2.2
42	2k	16	SER	2.2
45	1n	22	THR	2.2
5	2F	163	VAL	2.2
30	18	56	GLU	2.2
34	2c	55	VAL	2.2
36	2e	122	GLU	2.2
39	2h	98	LYS	2.2
42	2k	30	VAL	2.2
11	1P	37	GLY	2.2
16	1U	11	ARG	2.2
30	28	20	GLY	2.2
34	1c	131	ARG	2.2
36	2e	126	ARG	2.2
1	1A	564	C	2.2
18	2W	77	ASP	2.2
22	20	75	LEU	2.2
35	2d	21	LEU	2.2
45	1n	61	TRP	2.2
35	2d	161	ASN	2.2
54	1w	11	C	2.2
10	2O	86	ILE	2.2
44	1m	107	ALA	2.2
45	2n	48	ALA	2.2
10	1O	112	MET	2.2
30	28	19	SER	2.2
47	1p	22	THR	2.2
4	1E	172	VAL	2.2
4	2E	79	ARG	2.2
29	27	11	LYS	2.2
1	1A	2590	A	2.2
5	1F	57	VAL	2.2
12	1Q	35	VAL	2.2
13	1R	117	VAL	2.2
32	2a	901	A	2.2
34	1c	205	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
35	1d	68	TYR	2.2
45	1n	18	VAL	2.2
43	2l	14	GLY	2.1
15	2T	101	PHE	2.1
22	20	57	PHE	2.1
25	23	37	LEU	2.1
34	2c	186	PHE	2.1
38	1g	104	LEU	2.1
49	2r	31	LEU	2.1
51	1t	72	LEU	2.1
1	1A	2612	C	2.1
1	2A	2507	C	2.1
8	1I	26	ALA	2.1
10	1O	76	ALA	2.1
12	1Q	45	GLN	2.1
16	2U	96	ALA	2.1
17	2V	70	ILE	2.1
1	1A	778	G	2.1
1	1A	792	G	2.1
1	2A	2131	G	2.1
3	1D	12	SER	2.1
9	1N	40	PRO	2.1
35	2d	18	LYS	2.1
43	1l	21	LYS	2.1
54	1w	27	G	2.1
7	2H	158	HIS	2.1
29	17	41	ARG	2.1
31	19	18	ARG	2.1
31	29	20	HIS	2.1
42	1k	79	SER	2.1
13	2R	95	THR	2.1
51	1t	80	ARG	2.1
3	2D	234	GLY	2.1
9	2N	53	VAL	2.1
15	1T	30	VAL	2.1
23	11	31	GLY	2.1
23	21	29	GLY	2.1
25	23	6	VAL	2.1
42	1k	84	VAL	2.1
9	2N	123	TYR	2.1
1	1A	1829	A	2.1
18	2W	69	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	1D	159	ALA	2.1
4	1E	203	LYS	2.1
15	1T	86	ILE	2.1
24	22	41	ILE	2.1
27	15	14	ALA	2.1
30	18	10	ALA	2.1
34	2c	146	ALA	2.1
1	1A	2143	C	2.1
3	1D	69	ARG	2.1
7	2H	46	GLU	2.1
11	2P	61	ARG	2.1
18	1W	84	ARG	2.1
29	17	28	ARG	2.1
32	1a	1515	C	2.1
32	2a	812	C	2.1
47	2p	41	PRO	2.1
1	1A	2446	G	2.1
1	2A	745	G	2.1
12	1Q	129	THR	2.1
13	1R	108	GLY	2.1
23	11	74	VAL	2.1
30	28	6	THR	2.1
34	1c	159	GLY	2.1
39	2h	61	VAL	2.1
3	1D	95	LEU	2.1
4	2E	182	LEU	2.1
10	1O	66	LYS	2.1
1	2A	750	A	2.1
15	1T	76	PHE	2.1
33	2b	28	PHE	2.1
39	1h	39	LEU	2.1
40	2i	37	PHE	2.1
43	1l	23	LYS	2.1
43	2l	84	LEU	2.1
1	2A	614(A)	U	2.1
1	2A	757	U	2.1
3	2D	166	GLN	2.1
36	2e	20	GLN	2.1
53	2v	23	A	2.1
47	2p	7	ALA	2.1
3	1D	128	GLY	2.1
4	2E	125	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
4	2E	165	VAL	2.1
9	2N	128	HIS	2.1
16	1U	31	SER	2.1
23	21	17	SER	2.1
1	2A	742	G	2.1
23	21	32	LYS	2.1
4	1E	170	LEU	2.1
9	2N	134	ARG	2.1
13	2R	8	ARG	2.1
15	1T	103	ARG	2.1
16	2U	106	PHE	2.1
20	2Y	31	LEU	2.1
35	1d	138	TYR	2.1
25	23	35	ARG	2.1
35	1d	66	ARG	2.1
35	2d	206	PHE	2.1
40	1i	37	PHE	2.1
47	1p	49	LEU	2.1
49	1r	31	LEU	2.1
1	2A	747	U	2.1
15	1T	48	ILE	2.1
16	1U	89	GLU	2.1
44	2m	94	ARG	2.1
1	1A	2439	A	2.1
1	2A	677	A	2.1
1	2A	2614	A	2.1
3	1D	191	ALA	2.1
3	2D	240	ALA	2.1
4	2E	77	ILE	2.1
33	2b	29	ALA	2.1
43	1l	7	ILE	2.1
43	2l	100	ILE	2.1
48	2q	60	ILE	2.1
11	1P	54	GLY	2.1
32	2a	63	C	2.1
35	2d	173	TRP	2.1
34	1c	64	VAL	2.1
34	1c	173	VAL	2.1
39	1h	93	VAL	2.1
39	1h	137	VAL	2.1
15	2T	62	THR	2.1
4	1E	51	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
11	2P	91	PHE	2.1
13	2R	111	LEU	2.1
19	1X	47	PHE	2.1
29	17	19	ARG	2.1
31	19	24	TYR	2.1
35	2d	153	ARG	2.1
41	2j	64	GLU	2.1
48	2q	74	LEU	2.1
32	2a	324	G	2.1
3	1D	82	ILE	2.1
18	1W	103	ILE	2.1
32	1a	1532	U	2.1
38	1g	120	ILE	2.1
51	1t	63	ILE	2.1
1	1A	746	A	2.1
1	1A	1762	A	2.1
1	2A	1977	A	2.1
12	1Q	87	LYS	2.1
19	1X	78	LYS	2.1
40	2i	116	LYS	2.1
4	1E	23	VAL	2.1
23	21	51	VAL	2.1
37	1f	90	VAL	2.1
38	1g	105	VAL	2.1
3	1D	212	SER	2.1
3	2D	183	ARG	2.1
23	11	66	HIS	2.1
11	2P	32	THR	2.1
29	17	18	PHE	2.1
47	2p	34	GLU	2.1
4	1E	18	ASP	2.1
18	2W	9	TYR	2.1
1	1A	2449	U	2.1
3	1D	107	ALA	2.1
16	2U	42	ALA	2.1
18	1W	89	ALA	2.1
18	2W	24	ILE	2.1
34	2c	71	ALA	2.1
39	1h	16	ALA	2.1
1	1A	2447	G	2.1
1	2A	189	G	2.1
3	1D	207	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	2A	567	A	2.1
1	2A	746	A	2.1
4	1E	111	ARG	2.1
4	1E	196	VAL	2.1
7	2H	97	ARG	2.1
8	1I	103	ARG	2.1
47	2p	51	VAL	2.1
55	1x	38	A	2.1
9	1N	100	GLU	2.1
16	2U	49	HIS	2.1
34	1c	18	TRP	2.1
4	1E	27	LEU	2.1
40	2i	126	SER	2.1
43	1l	60	LEU	2.1
17	2V	85	LYS	2.1
35	2d	27	TYR	2.1
4	1E	28	ALA	2.1
5	1F	42	ALA	2.1
36	2e	86	ALA	2.1
43	2l	56	ALA	2.1
5	2F	85	GLY	2.1
39	1h	47	GLY	2.1
42	1k	52	GLY	2.1
1	1A	36	G	2.1
1	1A	2147	G	2.1
36	2e	25	ARG	2.1
22	20	23	VAL	2.1
33	2b	26	PRO	2.1
41	1j	44	VAL	2.1
45	1n	56	VAL	2.1
1	1A	196	A	2.1
1	1A	2050	C	2.1
1	2A	575	A	2.1
9	1N	34	LEU	2.1
9	1N	121	LYS	2.1
13	1R	28	LEU	2.1
13	2R	79	LEU	2.1
15	2T	19	LEU	2.1
34	1c	128	PHE	2.1
15	1T	84	GLN	2.1
48	2q	97	SER	2.1
6	2G	146	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
30	28	55	ALA	2.1
34	1c	15	THR	2.1
34	2c	57	ILE	2.1
49	2r	50	ILE	2.1
1	1A	2144	U	2.1
1	2A	1778	U	2.1
54	1w	59	U	2.1
15	1T	47	GLY	2.1
23	21	36	GLY	2.1
30	18	13	ARG	2.1
35	2d	65	ARG	2.1
3	2D	241	PRO	2.1
20	1Y	39	VAL	2.1
34	1c	151	VAL	2.1
1	2A	944	G	2.1
32	2a	378	G	2.1
13	2R	18	LEU	2.0
16	1U	60	LEU	2.0
16	2U	27	LEU	2.0
24	12	10	LEU	2.0
30	18	48	PHE	2.1
33	2b	70	PHE	2.1
1	1A	1952	A	2.0
1	1A	2021	C	2.0
32	1a	694	A	2.0
35	2d	119	GLN	2.0
3	1D	136	ILE	2.0
6	2G	136	ARG	2.0
9	2N	27	ALA	2.0
15	1T	51	ARG	2.0
18	2W	7	ALA	2.0
27	15	19	ARG	2.0
40	2i	7	THR	2.0
48	2q	25	ARG	2.0
12	2Q	92	GLY	2.0
51	1t	69	GLY	2.0
3	2D	35	LYS	2.0
4	2E	188	VAL	2.0
8	2I	119	PRO	2.0
10	2O	10	VAL	2.0
18	2W	50	VAL	2.0
31	19	1	MET	2.0

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Mol	Chain	Res	Type	RSRZ
10	2O	29	ASN	2.0
40	1i	123	PRO	2.0
3	1D	94	LEU	2.0
4	2E	113	PHE	2.0
5	2F	148	LEU	2.0
25	23	53	LEU	2.0
35	2d	101	LEU	2.0
49	1r	44	LEU	2.0
49	1r	79	LEU	2.0
1	1A	765	G	2.0
1	2A	558	G	2.0
1	2A	738	G	2.0
10	1O	23	ARG	2.0
32	2a	1034	G	2.0
1	1A	38	A	2.0
4	1E	77	ILE	2.0
5	1F	65	TRP	2.0
18	1W	12	ILE	2.0
19	2X	89	ILE	2.0
24	12	50	ILE	2.0
32	1a	1434	A	2.0
36	1e	80	ILE	2.0
38	2g	10	ARG	2.0
1	2A	787	U	2.0
1	2A	811	U	2.0
3	1D	154	LYS	2.0
5	1F	76	GLY	2.0
10	1O	9	GLU	2.0
16	1U	19	LYS	2.0
54	2w	47	U	2.0
5	1F	36	VAL	2.0
21	1Z	126	VAL	2.0
42	1k	119	CYS	2.0
44	2m	7	VAL	2.0
46	2o	45	VAL	2.0
3	2D	36	PRO	2.0
5	1F	192	LEU	2.0
17	1V	94	LEU	2.0
23	21	16	ASN	2.0
25	13	19	GLN	2.0
28	26	9	LEU	2.0
34	1c	34	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
50	1s	71	LEU	2.0
18	2W	88	ARG	2.0
34	2c	164	ARG	2.0
12	1Q	64	ILE	2.0
15	1T	107	ASP	2.0
13	1R	19	ALA	2.0
13	1R	101	ALA	2.0
1	1A	669	G	2.0
1	1A	2499	C	2.0
1	2A	2050	C	2.0
42	2k	101	SER	2.0
51	1t	12	ALA	2.0
9	2N	4	TYR	2.0
32	2a	1220	G	2.0
55	2x	70	G	2.0
6	2G	160	VAL	2.0
8	2I	21	VAL	2.0
49	1r	39	VAL	2.0
3	2D	48	ARG	2.0
13	2R	47	PHE	2.0
9	2N	56	ASN	2.0
11	2P	48	PRO	2.0
21	1Z	44	PHE	2.0
13	2R	24	GLN	2.0
29	27	28	ARG	2.0
34	1c	178	LEU	2.0
39	1h	63	LEU	2.0
12	2Q	47	ILE	2.0
3	1D	163	ALA	2.0
3	1D	234	GLY	2.0
3	2D	238	GLY	2.0
36	1e	101	ILE	2.0
36	2e	8	GLU	2.0
36	2e	131	ILE	2.0
10	2O	46	ALA	2.0
43	2l	68	ALA	2.0
1	1A	981	A	2.0
1	1A	1268	A	2.0
1	1A	1825	A	2.0
9	1N	5	VAL	2.0
18	1W	85	VAL	2.0
20	2Y	72	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
40	2i	28	VAL	2.0
12	2Q	1	MET	2.0
6	1G	152	LEU	2.0
8	2I	38	LEU	2.0
20	2Y	56	PRO	2.0
25	23	12	PRO	2.0
34	2c	7	PRO	2.0
39	2h	39	LEU	2.0
43	2l	71	PRO	2.0
8	2I	28	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	5MU	2y	54	21/22	0.66	0.34	101,120,137,154	0
54	PSU	2w	55	20/21	0.68	0.16	105,120,127,131	0
54	PSU	2w	39	20/21	0.72	0.40	115,123,126,127	0
54	4SU	2w	8	20/21	0.75	0.16	122,126,137,146	0
54	PSU	1y	55	20/21	0.76	0.35	119,126,131,138	0
54	PSU	2y	55	20/21	0.76	0.39	114,121,139,154	0
54	4SU	2y	8	20/21	0.77	0.13	115,120,129,132	0
54	4SU	1y	8	20/21	0.77	0.15	115,120,127,132	0
54	PSU	1w	55	20/21	0.80	0.21	102,112,115,117	0
54	7MG	2y	46	24/25	0.81	0.36	114,121,128,137	0
54	4SU	1w	8	20/21	0.82	0.22	112,119,134,134	0
54	PSU	2y	39	20/21	0.82	0.33	110,119,130,143	0
54	PSU	2y	32	20/21	0.82	0.37	109,122,134,138	0
54	PSU	1y	39	20/21	0.82	0.36	107,116,137,143	0
54	MIA	2y	37	22/30	0.84	0.29	107,116,130,143	0
54	MIA	2w	37	25/30	0.85	0.19	91,115,118,133	0
54	7MG	2w	46	24/25	0.85	0.15	113,122,129,141	0
53	PSU	2v	19	20/21	0.86	0.18	105,112,119,120	0
54	7MG	1w	46	24/25	0.86	0.17	105,115,124,133	0
32	5MC	2a	1400	21/22	0.86	0.33	87,108,118,120	0
54	5MU	2w	54	21/22	0.88	0.13	103,113,118,121	0
55	PSU	2x	55	20/21	0.89	0.11	106,112,122,123	0
54	7MG	1y	46	24/25	0.89	0.26	109,119,125,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	5MU	1y	54	21/22	0.89	0.25	114,120,132,137	0
54	PSU	1w	32	20/21	0.90	0.24	90,101,108,117	0
54	PSU	1y	32	20/21	0.90	0.29	105,113,128,129	0
32	PSU	2a	516	20/21	0.90	0.16	92,103,111,114	0
54	MIA	1w	37	29/30	0.90	0.26	78,99,107,108	0
32	2MG	2a	1207	24/25	0.90	0.16	100,107,116,125	0
54	MIA	1y	37	22/30	0.91	0.24	108,117,123,134	0
55	4SU	2x	8	20/21	0.91	0.11	97,110,116,120	0
54	PSU	2w	32	20/21	0.91	0.29	108,114,123,126	0
54	PSU	1w	39	20/21	0.91	0.29	97,105,119,120	0
32	5MC	2a	967	21/22	0.91	0.16	99,102,110,118	0
32	5MC	2a	1404	21/22	0.91	0.17	84,99,105,110	0
1	5MU	1A	1915	21/22	0.93	0.17	82,100,104,110	0
32	4OC	2a	1402	22/23	0.93	0.17	97,104,109,114	0
1	PSU	1A	2605	20/21	0.93	0.28	66,79,85,86	0
53	PSU	1v	19	20/21	0.93	0.14	79,95,102,102	0
43	0TD	1l	92	10/11	0.93	0.22	88,91,97,113	0
32	7MG	2a	527	24/25	0.93	0.18	89,95,101,112	0
55	5MC	2x	32	21/22	0.93	0.22	99,105,110,112	0
55	4SU	1x	8	20/21	0.93	0.15	93,100,106,110	0
1	PSU	2A	1911	20/21	0.94	0.14	86,98,105,106	0
55	5MU	2x	54	21/22	0.94	0.13	103,111,114,124	0
1	5MU	2A	1915	21/22	0.94	0.13	101,107,111,116	0
1	PSU	2A	1917	20/21	0.94	0.13	86,103,108,111	0
32	4OC	1a	1402	22/23	0.94	0.26	82,92,98,100	0
1	4OC	2A	1920	21/23	0.94	0.15	89,98,103,108	0
54	5MU	1w	54	21/22	0.94	0.25	104,108,117,119	0
1	5MC	2A	1962	21/22	0.94	0.17	77,89,95,99	0
32	5MC	1a	1407	21/22	0.94	0.23	76,88,93,97	0
32	UR3	2a	1498	21/22	0.94	0.24	88,98,102,106	0
32	MA6	2a	1519	24/25	0.94	0.30	86,99,103,105	0
43	0TD	2l	92	10/11	0.94	0.15	95,101,103,110	0
32	PSU	1a	516	20/21	0.94	0.17	84,92,98,104	0
1	PSU	1A	1911	20/21	0.94	0.18	70,90,95,100	0
1	OMG	2A	2251	24/25	0.95	0.33	74,88,94,96	0
1	2MA	2A	2503	23/24	0.95	0.27	70,81,88,92	0
1	PSU	1A	1917	20/21	0.95	0.18	83,90,95,96	0
32	5MC	1a	1404	21/22	0.95	0.28	74,83,96,97	0
1	PSU	2A	2605	20/21	0.95	0.25	79,88,93,96	0
55	5MC	1x	32	21/22	0.95	0.23	84,95,100,102	0
32	5MC	2a	1407	21/22	0.95	0.16	93,98,101,106	0
55	5MU	1x	54	21/22	0.95	0.14	86,97,101,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MC	2A	1942	21/22	0.95	0.17	88,94,99,106	0
32	M2G	2a	966	25/26	0.95	0.19	93,99,106,113	0
1	5MC	1A	1962	21/22	0.95	0.22	72,83,91,94	0
32	2MG	1a	1207	24/25	0.95	0.17	77,95,102,105	0
55	PSU	1x	55	20/21	0.95	0.12	94,100,107,116	0
32	7MG	1a	527	24/25	0.96	0.20	78,89,96,98	0
1	2MU	1A	2552	21/23	0.96	0.31	58,78,84,92	0
32	M2G	1a	966	25/26	0.96	0.26	81,87,96,98	0
1	5MU	1A	1939	21/22	0.96	0.26	66,78,86,90	0
32	5MC	1a	967	21/22	0.96	0.23	77,88,95,101	0
1	5MU	2A	1939	21/22	0.96	0.23	75,86,91,95	0
1	5MC	1A	1942	21/22	0.96	0.20	65,81,86,88	0
1	4OC	1A	1920	21/23	0.96	0.21	76,89,95,96	0
32	MA6	2a	1518	24/25	0.96	0.22	90,97,101,102	0
32	5MC	1a	1400	21/22	0.96	0.26	81,91,96,104	0
32	UR3	1a	1498	21/22	0.97	0.28	78,85,89,93	0
1	2MU	2A	2552	21/23	0.97	0.17	74,84,89,91	0
32	MA6	1a	1518	24/25	0.97	0.24	58,85,89,93	0
1	OMG	1A	2251	24/25	0.97	0.25	66,80,85,86	0
32	MA6	1a	1519	24/25	0.97	0.34	82,87,92,99	0
1	2MA	1A	2503	23/24	0.97	0.32	58,74,81,83	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3317	1/1	0.32	0.65	92,92,92,92	0
56	MG	2A	3201	1/1	0.34	0.22	102,102,102,102	0
56	MG	1A	3190	1/1	0.34	0.48	118,118,118,118	0
56	MG	1A	3242	1/1	0.37	0.33	78,78,78,78	0
56	MG	2a	3060	1/1	0.37	0.43	101,101,101,101	0
56	MG	2a	3082	1/1	0.37	0.31	109,109,109,109	0
56	MG	2a	3154	1/1	0.38	0.16	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3557	1/1	0.40	0.36	89,89,89,89	0
56	MG	2A	3315	1/1	0.40	0.84	103,103,103,103	0
56	MG	1a	3094	1/1	0.44	1.77	96,96,96,96	0
56	MG	1a	3214	1/1	0.45	0.26	103,103,103,103	0
56	MG	2A	3031	1/1	0.45	0.20	100,100,100,100	0
56	MG	1A	3104	1/1	0.46	0.98	90,90,90,90	0
56	MG	1A	3497	1/1	0.46	0.22	96,96,96,96	0
56	MG	2A	3017	1/1	0.48	0.30	98,98,98,98	0
56	MG	1A	3377	1/1	0.48	0.45	102,102,102,102	0
56	MG	1A	3429	1/1	0.50	0.25	87,87,87,87	0
56	MG	1a	3111	1/1	0.51	0.42	103,103,103,103	0
56	MG	1A	3194	1/1	0.53	0.26	72,72,72,72	0
56	MG	1A	3240	1/1	0.53	0.37	101,101,101,101	0
56	MG	1A	3157	1/1	0.54	0.13	92,92,92,92	0
56	MG	1A	3036	1/1	0.54	0.80	99,99,99,99	0
56	MG	1A	3099	1/1	0.55	0.40	77,77,77,77	0
56	MG	1A	3133	1/1	0.55	0.36	76,76,76,76	0
56	MG	1A	3359	1/1	0.56	0.77	89,89,89,89	0
56	MG	1A	3433	1/1	0.56	1.77	97,97,97,97	0
56	MG	2a	3080	1/1	0.56	0.28	85,85,85,85	0
56	MG	1A	3041	1/1	0.56	0.23	105,105,105,105	0
56	MG	1A	3534	1/1	0.56	0.30	86,86,86,86	0
56	MG	2A	3205	1/1	0.57	0.32	111,111,111,111	0
56	MG	2a	3059	1/1	0.57	0.46	79,79,79,79	0
56	MG	1A	3441	1/1	0.57	0.38	103,103,103,103	0
56	MG	1a	3077	1/1	0.58	0.22	84,84,84,84	0
56	MG	1A	3367	1/1	0.58	0.25	104,104,104,104	0
56	MG	1A	3148	1/1	0.58	0.42	79,79,79,79	0
56	MG	2a	3034	1/1	0.59	0.23	79,79,79,79	0
56	MG	1a	3005	1/1	0.60	0.21	80,80,80,80	0
56	MG	2A	3146	1/1	0.60	0.23	79,79,79,79	0
56	MG	2a	3107	1/1	0.60	0.10	106,106,106,106	0
56	MG	1A	3615	1/1	0.60	0.22	95,95,95,95	0
56	MG	2A	3074	1/1	0.61	0.30	102,102,102,102	0
56	MG	2A	3111	1/1	0.61	0.67	81,81,81,81	0
56	MG	1A	3527	1/1	0.61	0.24	74,74,74,74	0
56	MG	1A	3651	1/1	0.61	0.19	90,90,90,90	0
56	MG	1a	3211	1/1	0.61	0.30	77,77,77,77	0
56	MG	2a	3102	1/1	0.61	0.23	90,90,90,90	0
56	MG	2A	3034	1/1	0.61	0.17	71,71,71,71	0
56	MG	2A	3057	1/1	0.61	0.71	89,89,89,89	0
56	MG	2A	3316	1/1	0.62	0.48	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3302	1/1	0.63	0.14	82,82,82,82	0
56	MG	1A	3142	1/1	0.64	0.53	73,73,73,73	0
56	MG	2a	3087	1/1	0.64	0.46	94,94,94,94	0
56	MG	1A	3105	1/1	0.64	0.25	74,74,74,74	0
56	MG	1a	3043	1/1	0.64	0.41	95,95,95,95	0
56	MG	2a	3007	1/1	0.64	0.54	99,99,99,99	0
56	MG	1a	3167	1/1	0.65	0.48	109,109,109,109	0
56	MG	2a	3015	1/1	0.65	0.15	98,98,98,98	0
56	MG	2A	3158	1/1	0.65	0.67	78,78,78,78	0
56	MG	2a	3058	1/1	0.65	0.61	93,93,93,93	0
56	MG	1A	3569	1/1	0.65	0.11	95,95,95,95	0
56	MG	1a	3122	1/1	0.65	1.05	93,93,93,93	0
56	MG	2a	3017	1/1	0.66	2.14	89,89,89,89	0
56	MG	1A	3364	1/1	0.66	0.30	96,96,96,96	0
56	MG	2a	3051	1/1	0.66	0.31	79,79,79,79	0
56	MG	2A	3323	1/1	0.66	0.15	104,104,104,104	0
56	MG	1A	3145	1/1	0.67	0.27	93,93,93,93	0
56	MG	1A	3191	1/1	0.67	0.26	90,90,90,90	0
56	MG	1A	3098	1/1	0.67	1.35	80,80,80,80	0
56	MG	1A	3123	1/1	0.67	0.47	93,93,93,93	0
56	MG	2A	3160	1/1	0.67	0.13	88,88,88,88	0
56	MG	2A	3184	1/1	0.67	0.28	82,82,82,82	0
56	MG	1a	3116	1/1	0.67	0.47	90,90,90,90	0
56	MG	2a	3106	1/1	0.67	0.22	124,124,124,124	0
56	MG	1a	3008	1/1	0.67	0.15	66,66,66,66	0
56	MG	1a	3149	1/1	0.67	0.21	110,110,110,110	0
57	ZN	14	501	1/1	0.67	0.04	162,162,162,162	0
56	MG	2A	3287	1/1	0.68	0.16	83,83,83,83	0
56	MG	1a	3085	1/1	0.68	0.34	89,89,89,89	0
56	MG	2a	3049	1/1	0.68	0.18	79,79,79,79	0
56	MG	2a	3138	1/1	0.68	0.28	95,95,95,95	0
56	MG	1A	3408	1/1	0.68	0.20	96,96,96,96	0
56	MG	1A	3524	1/1	0.68	0.36	84,84,84,84	0
56	MG	2A	3162	1/1	0.69	0.23	77,77,77,77	0
56	MG	1A	3565	1/1	0.69	0.28	83,83,83,83	0
56	MG	1A	3034	1/1	0.69	0.10	79,79,79,79	0
56	MG	2a	3158	1/1	0.69	0.22	116,116,116,116	0
56	MG	1A	3573	1/1	0.69	0.21	88,88,88,88	0
56	MG	1A	3128	1/1	0.70	0.22	75,75,75,75	0
56	MG	2A	3094	1/1	0.71	0.22	85,85,85,85	0
56	MG	1a	3173	1/1	0.71	0.25	75,75,75,75	0
56	MG	1A	3585	1/1	0.71	0.19	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3070	1/1	0.71	0.21	87,87,87,87	0
56	MG	1A	3303	1/1	0.71	0.27	78,78,78,78	0
56	MG	1A	3160	1/1	0.71	0.26	76,76,76,76	0
56	MG	1A	3506	1/1	0.71	0.52	118,118,118,118	0
56	MG	2a	3100	1/1	0.71	0.26	94,94,94,94	0
56	MG	2A	3166	1/1	0.71	0.27	79,79,79,79	0
56	MG	1A	3151	1/1	0.71	0.27	64,64,64,64	0
56	MG	2A	3196	1/1	0.71	0.33	81,81,81,81	0
56	MG	1A	3572	1/1	0.71	0.18	85,85,85,85	0
56	MG	1A	3277	1/1	0.71	0.21	73,73,73,73	0
56	MG	2A	3278	1/1	0.71	0.16	89,89,89,89	0
56	MG	2a	3053	1/1	0.71	0.82	90,90,90,90	0
56	MG	1a	3082	1/1	0.72	0.80	75,75,75,75	0
56	MG	1a	3028	1/1	0.72	0.20	76,76,76,76	0
56	MG	2A	3290	1/1	0.72	0.14	94,94,94,94	0
56	MG	1A	3533	1/1	0.72	0.37	114,114,114,114	0
56	MG	1a	3162	1/1	0.72	0.31	93,93,93,93	0
56	MG	2A	3099	1/1	0.72	0.62	89,89,89,89	0
56	MG	2A	3022	1/1	0.72	0.16	96,96,96,96	0
56	MG	2A	3119	1/1	0.72	0.15	90,90,90,90	0
56	MG	2a	3006	1/1	0.72	0.31	104,104,104,104	0
56	MG	1A	3239	1/1	0.72	0.25	93,93,93,93	0
56	MG	2a	3077	1/1	0.72	0.17	95,95,95,95	0
56	MG	1A	3612	1/1	0.73	0.24	95,95,95,95	0
56	MG	2a	3054	1/1	0.73	0.18	90,90,90,90	0
56	MG	1A	3505	1/1	0.73	0.15	70,70,70,70	0
56	MG	2A	3019	1/1	0.73	0.21	101,101,101,101	0
56	MG	2A	3092	1/1	0.73	0.48	99,99,99,99	0
56	MG	2a	3130	1/1	0.73	0.09	74,74,74,74	0
56	MG	1A	3636	1/1	0.73	0.34	73,73,73,73	0
56	MG	2a	3037	1/1	0.73	0.21	106,106,106,106	0
56	MG	2A	3245	1/1	0.73	0.41	94,94,94,94	0
56	MG	2a	3179	1/1	0.73	0.12	106,106,106,106	0
56	MG	1A	3513	1/1	0.73	0.63	88,88,88,88	0
56	MG	2a	3031	1/1	0.74	0.88	109,109,109,109	0
56	MG	2A	3244	1/1	0.74	0.11	90,90,90,90	0
56	MG	2A	3070	1/1	0.74	0.35	74,74,74,74	0
56	MG	2A	3192	1/1	0.74	0.12	77,77,77,77	0
56	MG	2A	3193	1/1	0.74	0.35	86,86,86,86	0
56	MG	1A	3583	1/1	0.74	0.15	88,88,88,88	0
56	MG	1A	3390	1/1	0.74	0.27	87,87,87,87	0
56	MG	2a	3088	1/1	0.74	0.32	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	3105	1/1	0.74	0.25	86,86,86,86	0
56	MG	2A	3197	1/1	0.75	0.20	78,78,78,78	0
56	MG	1a	3163	1/1	0.75	0.41	66,66,66,66	0
56	MG	1a	3092	1/1	0.75	0.71	85,85,85,85	0
56	MG	1A	3368	1/1	0.75	0.78	99,99,99,99	0
56	MG	2A	3087	1/1	0.75	0.28	88,88,88,88	0
56	MG	2a	3097	1/1	0.75	0.31	89,89,89,89	0
56	MG	1A	3352	1/1	0.75	0.26	95,95,95,95	0
56	MG	1A	3268	1/1	0.75	0.21	68,68,68,68	0
56	MG	1A	3423	1/1	0.76	0.38	78,78,78,78	0
56	MG	1A	3257	1/1	0.76	0.27	80,80,80,80	0
56	MG	1a	3182	1/1	0.76	0.21	102,102,102,102	0
56	MG	1A	3149	1/1	0.76	0.53	76,76,76,76	0
56	MG	2A	3058	1/1	0.76	0.32	78,78,78,78	0
56	MG	2A	3123	1/1	0.76	0.18	81,81,81,81	0
56	MG	1a	3016	1/1	0.76	0.92	87,87,87,87	0
56	MG	2A	3156	1/1	0.76	0.17	69,69,69,69	0
56	MG	2a	3166	1/1	0.76	0.14	115,115,115,115	0
56	MG	1A	3014	1/1	0.76	0.39	93,93,93,93	0
56	MG	1A	3555	1/1	0.76	0.23	80,80,80,80	0
56	MG	1a	3027	1/1	0.77	0.18	76,76,76,76	0
56	MG	1A	3304	1/1	0.77	0.21	76,76,76,76	0
56	MG	2A	3198	1/1	0.77	0.17	83,83,83,83	0
56	MG	1A	3415	1/1	0.77	0.21	78,78,78,78	0
56	MG	2A	3138	1/1	0.77	0.20	102,102,102,102	0
56	MG	2A	3243	1/1	0.77	0.13	88,88,88,88	0
56	MG	1a	3067	1/1	0.77	0.18	80,80,80,80	0
56	MG	2A	3148	1/1	0.77	0.16	96,96,96,96	0
56	MG	1A	3045	1/1	0.77	0.23	94,94,94,94	0
56	MG	1A	3629	1/1	0.77	0.28	106,106,106,106	0
56	MG	1A	3280	1/1	0.77	0.20	77,77,77,77	0
56	MG	1A	3518	1/1	0.77	0.27	97,97,97,97	0
56	MG	1A	3244	1/1	0.77	0.23	81,81,81,81	0
56	MG	1A	3394	1/1	0.77	0.46	91,91,91,91	0
56	MG	2A	3003	1/1	0.77	0.23	84,84,84,84	0
56	MG	1A	3442	1/1	0.77	0.15	77,77,77,77	0
56	MG	1A	3549	1/1	0.78	0.26	83,83,83,83	0
56	MG	1A	3121	1/1	0.78	0.42	76,76,76,76	0
56	MG	1A	3176	1/1	0.78	0.23	95,95,95,95	0
56	MG	2A	3318	1/1	0.78	0.21	87,87,87,87	0
56	MG	2A	3142	1/1	0.78	0.61	81,81,81,81	0
56	MG	2A	3331	1/1	0.78	0.28	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3198	1/1	0.78	0.11	83,83,83,83	0
56	MG	2a	3090	1/1	0.78	0.22	91,91,91,91	0
56	MG	1A	3252	1/1	0.78	0.20	73,73,73,73	0
56	MG	2A	3206	1/1	0.78	0.35	73,73,73,73	0
56	MG	1A	3428	1/1	0.78	0.26	79,79,79,79	0
56	MG	1A	3125	1/1	0.78	0.30	77,77,77,77	0
56	MG	1A	3376	1/1	0.78	0.19	92,92,92,92	0
56	MG	2A	3249	1/1	0.78	0.11	81,81,81,81	0
56	MG	1A	3318	1/1	0.78	0.46	99,99,99,99	0
56	MG	1A	3320	1/1	0.78	0.23	65,65,65,65	0
56	MG	2A	3110	1/1	0.78	0.15	79,79,79,79	0
56	MG	2A	3294	1/1	0.78	0.38	104,104,104,104	0
56	MG	2A	3297	1/1	0.78	0.19	93,93,93,93	0
56	MG	1a	3051	1/1	0.78	0.33	99,99,99,99	0
56	MG	1A	3199	1/1	0.79	0.23	70,70,70,70	0
56	MG	1a	3152	1/1	0.79	0.18	102,102,102,102	0
56	MG	1A	3479	1/1	0.79	0.14	86,86,86,86	0
56	MG	1A	3571	1/1	0.79	0.05	98,98,98,98	0
56	MG	1a	3037	1/1	0.79	0.42	82,82,82,82	0
56	MG	2A	3143	1/1	0.79	0.24	93,93,93,93	0
56	MG	1A	3486	1/1	0.79	0.23	68,68,68,68	0
56	MG	2a	3092	1/1	0.79	0.19	88,88,88,88	0
56	MG	1a	3106	1/1	0.79	0.07	98,98,98,98	0
56	MG	2a	3028	1/1	0.79	0.14	85,85,85,85	0
56	MG	2A	3071	1/1	0.79	0.20	75,75,75,75	0
56	MG	1a	3189	1/1	0.79	0.23	85,85,85,85	0
56	MG	2A	3078	1/1	0.79	0.23	75,75,75,75	0
56	MG	1A	3554	1/1	0.79	0.14	109,109,109,109	0
56	MG	1A	3161	1/1	0.79	0.17	90,90,90,90	0
56	MG	2a	3141	1/1	0.79	0.10	82,82,82,82	0
56	MG	1a	3238	1/1	0.79	0.15	99,99,99,99	0
56	MG	1A	3114	1/1	0.79	0.42	93,93,93,93	0
56	MG	2A	3310	1/1	0.79	0.06	91,91,91,91	0
56	MG	2a	3169	1/1	0.79	0.25	78,78,78,78	0
56	MG	2A	3101	1/1	0.79	0.46	83,83,83,83	0
56	MG	1a	3134	1/1	0.79	0.39	77,77,77,77	0
56	MG	1A	3420	1/1	0.80	0.36	76,76,76,76	0
56	MG	1a	3053	1/1	0.80	1.62	79,79,79,79	0
56	MG	1a	3222	1/1	0.80	0.11	91,91,91,91	0
56	MG	2a	3063	1/1	0.80	0.25	83,83,83,83	0
56	MG	1a	3230	1/1	0.80	0.23	84,84,84,84	0
56	MG	1a	3117	1/1	0.80	0.14	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3661	1/1	0.80	0.35	87,87,87,87	0
56	MG	1a	3068	1/1	0.80	0.15	95,95,95,95	0
56	MG	1a	3072	1/1	0.80	0.20	94,94,94,94	0
56	MG	2A	3112	1/1	0.80	0.31	89,89,89,89	0
56	MG	2A	3114	1/1	0.80	0.37	79,79,79,79	0
56	MG	1A	3579	1/1	0.80	0.51	118,118,118,118	0
56	MG	1A	3159	1/1	0.80	0.11	69,69,69,69	0
56	MG	2A	3227	1/1	0.80	0.11	81,81,81,81	0
56	MG	2A	3234	1/1	0.80	0.72	84,84,84,84	0
56	MG	2A	3237	1/1	0.80	0.18	92,92,92,92	0
56	MG	1A	3258	1/1	0.80	0.29	95,95,95,95	0
56	MG	2A	3051	1/1	0.80	0.29	80,80,80,80	0
56	MG	2a	3036	1/1	0.80	0.10	95,95,95,95	0
56	MG	1A	3181	1/1	0.80	1.48	78,78,78,78	0
56	MG	2a	3144	1/1	0.80	0.24	101,101,101,101	0
56	MG	2a	3048	1/1	0.80	0.33	94,94,94,94	0
56	MG	1A	3056	1/1	0.80	0.27	80,80,80,80	0
56	MG	2a	3050	1/1	0.80	0.29	105,105,105,105	0
56	MG	1a	3179	1/1	0.80	0.13	90,90,90,90	0
56	MG	1A	3058	1/1	0.80	0.15	80,80,80,80	0
56	MG	1A	3511	1/1	0.80	0.17	62,62,62,62	0
56	MG	1A	3400	1/1	0.81	0.25	90,90,90,90	0
56	MG	2A	3055	1/1	0.81	0.13	92,92,92,92	0
56	MG	1A	3447	1/1	0.81	0.30	91,91,91,91	0
56	MG	1a	3069	1/1	0.81	0.18	81,81,81,81	0
56	MG	1a	3004	1/1	0.81	0.19	101,101,101,101	0
56	MG	1A	3168	1/1	0.81	0.19	78,78,78,78	0
56	MG	1A	3291	1/1	0.81	0.18	79,79,79,79	0
56	MG	1A	3580	1/1	0.81	0.15	74,74,74,74	0
56	MG	1a	3019	1/1	0.81	0.53	96,96,96,96	0
56	MG	1a	3201	1/1	0.81	0.50	93,93,93,93	0
56	MG	1a	3203	1/1	0.81	0.34	105,105,105,105	0
56	MG	1A	3295	1/1	0.81	0.34	66,66,66,66	0
56	MG	1A	3174	1/1	0.81	0.39	77,77,77,77	0
56	MG	2A	3332	1/1	0.81	0.48	116,116,116,116	0
56	MG	2A	3336	1/1	0.81	0.21	77,77,77,77	0
56	MG	2A	3337	1/1	0.81	0.14	78,78,78,78	0
56	MG	2a	3099	1/1	0.81	0.20	93,93,93,93	0
56	MG	2A	3351	1/1	0.81	0.15	84,84,84,84	0
56	MG	2a	3004	1/1	0.81	0.29	98,98,98,98	0
56	MG	1a	3030	1/1	0.81	0.47	105,105,105,105	0
56	MG	1a	3110	1/1	0.81	0.10	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3116	1/1	0.81	0.20	82,82,82,82	0
56	MG	1a	3033	1/1	0.81	0.28	87,87,87,87	0
56	MG	2A	3216	1/1	0.81	0.75	87,87,87,87	0
56	MG	1A	3016	1/1	0.81	0.28	66,66,66,66	0
56	MG	1a	3039	1/1	0.81	0.21	80,80,80,80	0
56	MG	1A	3002	1/1	0.81	0.17	72,72,72,72	0
56	MG	2A	3134	1/1	0.81	0.42	91,91,91,91	0
56	MG	1A	3053	1/1	0.81	0.38	95,95,95,95	0
56	MG	2a	3167	1/1	0.81	0.30	101,101,101,101	0
56	MG	1a	3136	1/1	0.81	0.23	84,84,84,84	0
56	MG	1A	3015	1/1	0.81	0.13	86,86,86,86	0
56	MG	2A	3258	1/1	0.81	0.34	103,103,103,103	0
56	MG	1A	3192	1/1	0.82	0.14	74,74,74,74	0
56	MG	2a	3085	1/1	0.82	0.16	83,83,83,83	0
56	MG	1A	3647	1/1	0.82	0.15	93,93,93,93	0
56	MG	1a	3220	1/1	0.82	0.35	80,80,80,80	0
56	MG	1A	3385	1/1	0.82	0.30	74,74,74,74	0
56	MG	1A	3657	1/1	0.82	0.43	79,79,79,79	0
56	MG	1a	3233	1/1	0.82	0.19	76,76,76,76	0
56	MG	1A	3567	1/1	0.82	0.13	87,87,87,87	0
56	MG	2A	3298	1/1	0.82	0.56	76,76,76,76	0
56	MG	1A	3180	1/1	0.82	0.77	93,93,93,93	0
56	MG	1A	3196	1/1	0.82	0.23	81,81,81,81	0
56	MG	2A	3090	1/1	0.82	0.22	98,98,98,98	0
56	MG	1A	3293	1/1	0.82	0.13	78,78,78,78	0
56	MG	2A	3217	1/1	0.82	0.52	82,82,82,82	0
56	MG	2A	3222	1/1	0.82	0.23	89,89,89,89	0
56	MG	1a	3133	1/1	0.82	0.15	90,90,90,90	0
56	MG	2A	3097	1/1	0.82	0.41	91,91,91,91	0
56	MG	2A	3098	1/1	0.82	0.57	79,79,79,79	0
56	MG	1a	3090	1/1	0.82	0.53	87,87,87,87	0
56	MG	2a	3061	1/1	0.82	0.07	92,92,92,92	0
56	MG	1A	3249	1/1	0.82	0.34	77,77,77,77	0
56	MG	2A	3344	1/1	0.82	0.10	106,106,106,106	0
56	MG	2a	3177	1/1	0.82	0.16	86,86,86,86	0
56	MG	2A	3165	1/1	0.82	0.14	77,77,77,77	0
56	MG	2A	3247	1/1	0.82	0.16	101,101,101,101	0
56	MG	2a	3047	1/1	0.83	0.14	83,83,83,83	0
56	MG	1a	3126	1/1	0.83	0.15	100,100,100,100	0
56	MG	2A	3011	1/1	0.83	0.21	87,87,87,87	0
56	MG	2A	3131	1/1	0.83	0.41	95,95,95,95	0
56	MG	1a	3063	1/1	0.83	0.27	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3203	1/1	0.83	0.29	74,74,74,74	0
56	MG	2A	3277	1/1	0.83	0.40	93,93,93,93	0
56	MG	1A	3208	1/1	0.83	0.22	74,74,74,74	0
56	MG	2A	3283	1/1	0.83	0.20	84,84,84,84	0
56	MG	1a	3143	1/1	0.83	0.27	91,91,91,91	0
56	MG	2A	3033	1/1	0.83	0.33	81,81,81,81	0
56	MG	1A	3234	1/1	0.83	0.36	96,96,96,96	0
56	MG	2A	3151	1/1	0.83	0.13	78,78,78,78	0
56	MG	2A	3153	1/1	0.83	0.35	81,81,81,81	0
56	MG	1A	3265	1/1	0.83	0.26	65,65,65,65	0
56	MG	1A	3319	1/1	0.83	0.54	100,100,100,100	0
56	MG	2A	3313	1/1	0.83	0.15	96,96,96,96	0
56	MG	1A	3391	1/1	0.83	0.27	80,80,80,80	0
56	MG	1a	3165	1/1	0.83	0.49	87,87,87,87	0
56	MG	2a	3089	1/1	0.83	0.14	86,86,86,86	0
56	MG	2A	3060	1/1	0.83	0.17	79,79,79,79	0
56	MG	1a	3083	1/1	0.83	0.30	93,93,93,93	0
56	MG	1a	3169	1/1	0.83	0.16	80,80,80,80	0
56	MG	2A	3186	1/1	0.83	0.20	79,79,79,79	0
56	MG	1A	3444	1/1	0.83	0.23	83,83,83,83	0
56	MG	1a	3089	1/1	0.83	0.16	78,78,78,78	0
56	MG	1A	3147	1/1	0.83	0.15	86,86,86,86	0
56	MG	1a	3187	1/1	0.83	0.27	78,78,78,78	0
56	MG	1A	3459	1/1	0.83	0.11	62,62,62,62	0
56	MG	1A	3620	1/1	0.83	0.51	91,91,91,91	0
56	MG	1a	3097	1/1	0.83	0.88	95,95,95,95	0
56	MG	1A	3087	1/1	0.83	0.14	79,79,79,79	0
56	MG	2a	3009	1/1	0.83	0.32	84,84,84,84	0
56	MG	2a	3010	1/1	0.83	0.08	86,86,86,86	0
56	MG	1A	3197	1/1	0.83	0.25	72,72,72,72	0
56	MG	2a	3161	1/1	0.83	0.14	104,104,104,104	0
56	MG	1A	3144	1/1	0.83	0.18	85,85,85,85	0
56	MG	2A	3104	1/1	0.83	0.16	98,98,98,98	0
56	MG	1a	3049	1/1	0.83	0.21	87,87,87,87	0
56	MG	1A	3419	1/1	0.83	0.16	87,87,87,87	0
56	MG	1A	3113	1/1	0.83	0.14	75,75,75,75	0
56	MG	1a	3062	1/1	0.83	0.27	71,71,71,71	0
57	ZN	24	501	1/1	0.83	0.06	168,168,168,168	0
56	MG	2A	3266	1/1	0.84	0.10	88,88,88,88	0
56	MG	2A	3026	1/1	0.84	0.19	92,92,92,92	0
56	MG	1A	3030	1/1	0.84	0.50	69,69,69,69	0
56	MG	1A	3299	1/1	0.84	0.20	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	3007	1/1	0.84	0.19	67,67,67,67	0
56	MG	1A	3453	1/1	0.84	0.19	84,84,84,84	0
56	MG	1A	3457	1/1	0.84	0.18	77,77,77,77	0
56	MG	1A	3548	1/1	0.84	0.62	91,91,91,91	0
56	MG	1A	3601	1/1	0.84	0.91	102,102,102,102	0
56	MG	1a	3174	1/1	0.84	0.15	87,87,87,87	0
56	MG	2A	3061	1/1	0.84	0.18	76,76,76,76	0
56	MG	2a	3078	1/1	0.84	0.15	85,85,85,85	0
56	MG	1A	3012	1/1	0.84	0.13	78,78,78,78	0
56	MG	1A	3001	1/1	0.84	0.10	70,70,70,70	0
56	MG	1A	3617	1/1	0.84	0.14	69,69,69,69	0
56	MG	1A	3371	1/1	0.84	0.29	52,52,52,52	0
56	MG	1a	3191	1/1	0.84	0.12	93,93,93,93	0
56	MG	1A	3622	1/1	0.84	0.19	91,91,91,91	0
56	MG	2A	3328	1/1	0.84	0.12	90,90,90,90	0
56	MG	2A	3194	1/1	0.84	0.16	85,85,85,85	0
56	MG	1a	3107	1/1	0.84	0.17	84,84,84,84	0
56	MG	1a	3205	1/1	0.84	0.11	102,102,102,102	0
56	MG	1A	3253	1/1	0.84	0.28	71,71,71,71	0
56	MG	1A	3633	1/1	0.84	0.22	75,75,75,75	0
56	MG	2A	3204	1/1	0.84	0.53	90,90,90,90	0
56	MG	1a	3115	1/1	0.84	0.12	89,89,89,89	0
56	MG	2A	3100	1/1	0.84	0.21	86,86,86,86	0
56	MG	2a	3121	1/1	0.84	0.26	114,114,114,114	0
56	MG	2A	3215	1/1	0.84	0.18	86,86,86,86	0
56	MG	1A	3287	1/1	0.84	0.13	80,80,80,80	0
56	MG	1a	3052	1/1	0.84	0.15	84,84,84,84	0
56	MG	2a	3012	1/1	0.84	0.14	79,79,79,79	0
56	MG	1A	3026	1/1	0.84	0.27	77,77,77,77	0
56	MG	1A	3339	1/1	0.84	1.46	112,112,112,112	0
56	MG	2a	3159	1/1	0.84	0.33	92,92,92,92	0
56	MG	2a	3160	1/1	0.84	0.11	104,104,104,104	0
56	MG	1A	3343	1/1	0.84	0.20	72,72,72,72	0
56	MG	1A	3658	1/1	0.84	0.23	98,98,98,98	0
56	MG	2A	3013	1/1	0.84	0.36	79,79,79,79	0
56	MG	1A	3137	1/1	0.84	0.20	82,82,82,82	0
56	MG	2A	3127	1/1	0.84	0.10	78,78,78,78	0
56	MG	2A	3018	1/1	0.84	0.20	85,85,85,85	0
56	MG	1A	3674	1/1	0.84	0.33	81,81,81,81	0
56	MG	1a	3070	1/1	0.84	0.20	85,85,85,85	0
56	MG	1A	3019	1/1	0.85	0.19	81,81,81,81	0
56	MG	1a	3060	1/1	0.85	0.17	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3062	1/1	0.85	0.32	94,94,94,94	0
56	MG	1A	3608	1/1	0.85	0.12	87,87,87,87	0
56	MG	2A	3195	1/1	0.85	0.31	84,84,84,84	0
56	MG	2a	3076	1/1	0.85	0.17	99,99,99,99	0
56	MG	1a	3108	1/1	0.85	0.24	93,93,93,93	0
56	MG	2A	3024	1/1	0.85	0.22	95,95,95,95	0
56	MG	1A	3552	1/1	0.85	0.14	100,100,100,100	0
56	MG	2A	3028	1/1	0.85	0.40	68,68,68,68	0
56	MG	2A	3203	1/1	0.85	0.43	87,87,87,87	0
56	MG	1a	3180	1/1	0.85	0.19	90,90,90,90	0
56	MG	1A	3205	1/1	0.85	0.15	78,78,78,78	0
56	MG	1A	3007	1/1	0.85	0.12	91,91,91,91	0
56	MG	2A	3207	1/1	0.85	0.46	68,68,68,68	0
56	MG	2A	3209	1/1	0.85	0.38	83,83,83,83	0
56	MG	2A	3041	1/1	0.85	0.23	69,69,69,69	0
56	MG	1A	3372	1/1	0.85	0.17	63,63,63,63	0
56	MG	1A	3417	1/1	0.85	0.19	79,79,79,79	0
56	MG	1A	3246	1/1	0.85	0.14	78,78,78,78	0
56	MG	1A	3519	1/1	0.85	0.17	88,88,88,88	0
56	MG	1a	3127	1/1	0.85	0.21	82,82,82,82	0
56	MG	1A	3521	1/1	0.85	0.15	64,64,64,64	0
56	MG	2a	3118	1/1	0.85	0.04	115,115,115,115	0
56	MG	2a	3120	1/1	0.85	0.67	103,103,103,103	0
56	MG	1a	3036	1/1	0.85	0.14	90,90,90,90	0
56	MG	1A	3455	1/1	0.85	0.15	63,63,63,63	0
56	MG	2A	3152	1/1	0.85	0.68	85,85,85,85	0
56	MG	1A	3219	1/1	0.85	0.13	84,84,84,84	0
56	MG	1a	3224	1/1	0.85	0.21	77,77,77,77	0
56	MG	2A	3253	1/1	0.85	0.17	74,74,74,74	0
56	MG	2A	3080	1/1	0.85	0.08	80,80,80,80	0
56	MG	2A	3263	1/1	0.85	0.52	86,86,86,86	0
56	MG	1A	3354	1/1	0.85	0.21	83,83,83,83	0
56	MG	1A	3153	1/1	0.85	0.37	72,72,72,72	0
56	MG	2a	3162	1/1	0.85	0.15	126,126,126,126	0
56	MG	1A	3543	1/1	0.85	0.28	86,86,86,86	0
56	MG	1A	3063	1/1	0.85	0.16	80,80,80,80	0
56	MG	2A	3181	1/1	0.85	0.69	90,90,90,90	0
56	MG	1a	3099	1/1	0.85	0.10	90,90,90,90	0
56	MG	1a	3166	1/1	0.85	0.15	100,100,100,100	0
56	MG	2A	3295	1/1	0.85	0.31	91,91,91,91	0
56	MG	2A	3190	1/1	0.85	0.11	98,98,98,98	0
56	MG	1A	3065	1/1	0.86	0.43	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3431	1/1	0.86	0.14	76,76,76,76	0
56	MG	2a	3066	1/1	0.86	0.22	106,106,106,106	0
56	MG	1a	3140	1/1	0.86	0.33	84,84,84,84	0
56	MG	1A	3330	1/1	0.86	0.26	96,96,96,96	0
56	MG	1A	3103	1/1	0.86	0.86	68,68,68,68	0
56	MG	1A	3150	1/1	0.86	0.20	91,91,91,91	0
56	MG	1A	3443	1/1	0.86	0.09	82,82,82,82	0
56	MG	1A	3139	1/1	0.86	0.21	79,79,79,79	0
56	MG	1A	3525	1/1	0.86	0.21	101,101,101,101	0
56	MG	1a	3018	1/1	0.86	0.37	74,74,74,74	0
56	MG	2A	3025	1/1	0.86	0.21	88,88,88,88	0
56	MG	2A	3333	1/1	0.86	0.12	101,101,101,101	0
56	MG	1A	3177	1/1	0.86	0.66	89,89,89,89	0
56	MG	1A	3589	1/1	0.86	0.11	86,86,86,86	0
56	MG	1A	3529	1/1	0.86	0.16	71,71,71,71	0
56	MG	1A	3452	1/1	0.86	0.16	97,97,97,97	0
56	MG	1A	3609	1/1	0.86	0.67	74,74,74,74	0
56	MG	1a	3103	1/1	0.86	0.19	79,79,79,79	0
56	MG	2A	3048	1/1	0.86	0.23	83,83,83,83	0
56	MG	1A	3122	1/1	0.86	0.24	77,77,77,77	0
56	MG	2A	3144	1/1	0.86	0.42	75,75,75,75	0
56	MG	2A	3053	1/1	0.86	0.10	77,77,77,77	0
56	MG	1A	3251	1/1	0.86	0.43	69,69,69,69	0
56	MG	1A	3154	1/1	0.86	0.18	59,59,59,59	0
56	MG	1A	3075	1/1	0.86	0.15	78,78,78,78	0
56	MG	1A	3621	1/1	0.86	0.13	69,69,69,69	0
56	MG	2A	3154	1/1	0.86	0.70	74,74,74,74	0
56	MG	2a	3142	1/1	0.86	0.24	103,103,103,103	0
56	MG	1A	3011	1/1	0.86	0.38	65,65,65,65	0
56	MG	1A	3022	1/1	0.86	0.38	83,83,83,83	0
56	MG	2a	3043	1/1	0.86	0.66	70,70,70,70	0
56	MG	1A	3493	1/1	0.86	0.16	69,69,69,69	0
56	MG	2A	3072	1/1	0.86	0.18	74,74,74,74	0
56	MG	1a	3213	1/1	0.86	1.10	117,117,117,117	0
56	MG	1a	3058	1/1	0.86	0.30	75,75,75,75	0
56	MG	2A	3286	1/1	0.86	0.15	93,93,93,93	0
56	MG	1A	3556	1/1	0.86	0.18	81,81,81,81	0
56	MG	2a	3168	1/1	0.86	0.15	112,112,112,112	0
56	MG	2A	3084	1/1	0.86	0.26	90,90,90,90	0
56	MG	1A	3425	1/1	0.86	0.31	62,62,62,62	0
56	MG	2A	3188	1/1	0.86	0.12	92,92,92,92	0
56	MG	1A	3237	1/1	0.86	0.33	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3566	1/1	0.86	0.10	93,93,93,93	0
56	MG	1A	3437	1/1	0.87	0.31	79,79,79,79	0
56	MG	1A	3183	1/1	0.87	0.42	74,74,74,74	0
56	MG	1a	3020	1/1	0.87	0.15	74,74,74,74	0
56	MG	1a	3184	1/1	0.87	0.27	71,71,71,71	0
56	MG	1A	3541	1/1	0.87	0.15	72,72,72,72	0
56	MG	1a	3120	1/1	0.87	0.57	87,87,87,87	0
56	MG	2A	3254	1/1	0.87	0.15	78,78,78,78	0
56	MG	1a	3071	1/1	0.87	0.84	75,75,75,75	0
56	MG	2A	3106	1/1	0.87	0.25	73,73,73,73	0
56	MG	2A	3038	1/1	0.87	0.39	65,65,65,65	0
56	MG	1A	3186	1/1	0.87	0.15	95,95,95,95	0
56	MG	1A	3545	1/1	0.87	0.17	67,67,67,67	0
56	MG	2a	3024	1/1	0.87	0.10	90,90,90,90	0
56	MG	1A	3167	1/1	0.87	0.20	90,90,90,90	0
56	MG	2A	3115	1/1	0.87	1.18	80,80,80,80	0
56	MG	1a	3035	1/1	0.87	0.23	81,81,81,81	0
56	MG	1A	3637	1/1	0.87	0.13	100,100,100,100	0
56	MG	2a	3117	1/1	0.87	0.11	92,92,92,92	0
56	MG	1a	3139	1/1	0.87	0.41	81,81,81,81	0
56	MG	2a	3042	1/1	0.87	0.19	82,82,82,82	0
56	MG	1A	3032	1/1	0.87	0.14	75,75,75,75	0
56	MG	2a	3129	1/1	0.87	0.14	92,92,92,92	0
56	MG	1A	3048	1/1	0.87	0.51	74,74,74,74	0
56	MG	1a	3042	1/1	0.87	0.11	74,74,74,74	0
56	MG	2A	3140	1/1	0.87	0.45	81,81,81,81	0
56	MG	1A	3322	1/1	0.87	0.15	92,92,92,92	0
56	MG	1A	3600	1/1	0.87	0.10	77,77,77,77	0
56	MG	1A	3288	1/1	0.87	0.12	70,70,70,70	0
56	MG	1A	3138	1/1	0.87	0.48	82,82,82,82	0
56	MG	2a	3055	1/1	0.87	0.23	95,95,95,95	0
56	MG	1A	3100	1/1	0.87	0.60	61,61,61,61	0
56	MG	1A	3023	1/1	0.87	1.07	88,88,88,88	0
56	MG	1A	3613	1/1	0.87	0.15	64,64,64,64	0
56	MG	2A	3327	1/1	0.87	0.52	96,96,96,96	0
56	MG	1a	3170	1/1	0.87	0.13	76,76,76,76	0
56	MG	1A	3118	1/1	0.87	0.11	60,60,60,60	0
56	MG	2a	3064	1/1	0.87	0.14	99,99,99,99	0
56	MG	2a	3176	1/1	0.87	0.14	83,83,83,83	0
56	MG	1A	3358	1/1	0.87	0.19	83,83,83,83	0
56	MG	2a	3069	1/1	0.87	0.19	103,103,103,103	0
56	MG	2a	3183	1/1	0.87	0.07	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3157	1/1	0.87	0.84	70,70,70,70	0
56	MG	2A	3334	1/1	0.87	0.46	105,105,105,105	0
56	MG	1A	3175	1/1	0.88	0.24	75,75,75,75	0
56	MG	1A	3066	1/1	0.88	0.37	78,78,78,78	0
56	MG	1A	3261	1/1	0.88	0.22	72,72,72,72	0
56	MG	1A	3263	1/1	0.88	0.20	78,78,78,78	0
56	MG	2a	3074	1/1	0.88	0.14	98,98,98,98	0
56	MG	1A	3127	1/1	0.88	0.16	72,72,72,72	0
56	MG	1a	3146	1/1	0.88	0.20	79,79,79,79	0
56	MG	1a	3147	1/1	0.88	0.27	71,71,71,71	0
56	MG	1a	3073	1/1	0.88	0.16	78,78,78,78	0
56	MG	1A	3267	1/1	0.88	0.22	76,76,76,76	0
56	MG	1a	3153	1/1	0.88	0.15	84,84,84,84	0
56	MG	1A	3396	1/1	0.88	0.28	99,99,99,99	0
56	MG	1A	3004	1/1	0.88	0.17	56,56,56,56	0
56	MG	1a	3024	1/1	0.88	0.41	83,83,83,83	0
56	MG	2A	3121	1/1	0.88	0.34	79,79,79,79	0
56	MG	1A	3544	1/1	0.88	0.18	71,71,71,71	0
56	MG	2a	3096	1/1	0.88	0.27	84,84,84,84	0
56	MG	2A	3343	1/1	0.88	0.23	99,99,99,99	0
56	MG	1A	3021	1/1	0.88	1.00	55,55,55,55	0
56	MG	1A	3614	1/1	0.88	0.15	89,89,89,89	0
56	MG	2a	3101	1/1	0.88	0.80	101,101,101,101	0
56	MG	1a	3032	1/1	0.88	0.07	76,76,76,76	0
56	MG	2a	3105	1/1	0.88	0.26	95,95,95,95	0
56	MG	2A	3136	1/1	0.88	0.23	71,71,71,71	0
56	MG	2A	3223	1/1	0.88	0.21	72,72,72,72	0
56	MG	2A	3035	1/1	0.88	0.16	92,92,92,92	0
56	MG	1A	3279	1/1	0.88	0.15	82,82,82,82	0
56	MG	1A	3465	1/1	0.88	0.18	80,80,80,80	0
56	MG	1a	3175	1/1	0.88	0.07	87,87,87,87	0
56	MG	1A	3347	1/1	0.88	0.23	70,70,70,70	0
56	MG	2a	3124	1/1	0.88	0.18	83,83,83,83	0
56	MG	1A	3481	1/1	0.88	0.22	83,83,83,83	0
56	MG	2A	3147	1/1	0.88	0.13	84,84,84,84	0
56	MG	1A	3052	1/1	0.88	0.21	77,77,77,77	0
56	MG	2A	3150	1/1	0.88	0.43	88,88,88,88	0
56	MG	1A	3286	1/1	0.88	0.12	96,96,96,96	0
56	MG	2a	3143	1/1	0.88	0.10	107,107,107,107	0
56	MG	1A	3494	1/1	0.88	0.11	75,75,75,75	0
56	MG	1A	3184	1/1	0.88	1.24	73,73,73,73	0
56	MG	2A	3265	1/1	0.88	0.34	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	3190	1/1	0.88	1.15	95,95,95,95	0
56	MG	1A	3185	1/1	0.88	1.14	80,80,80,80	0
56	MG	1a	3113	1/1	0.88	0.13	86,86,86,86	0
56	MG	1A	3645	1/1	0.88	0.24	82,82,82,82	0
56	MG	2a	3164	1/1	0.88	0.10	114,114,114,114	0
56	MG	1A	3173	1/1	0.88	0.16	74,74,74,74	0
56	MG	1A	3042	1/1	0.88	0.17	64,64,64,64	0
56	MG	1A	3210	1/1	0.88	0.15	71,71,71,71	0
56	MG	1A	3214	1/1	0.88	0.27	96,96,96,96	0
56	MG	1a	3217	1/1	0.88	0.10	85,85,85,85	0
56	MG	2A	3296	1/1	0.88	0.21	102,102,102,102	0
56	MG	2a	3178	1/1	0.88	0.26	96,96,96,96	0
56	MG	1A	3436	1/1	0.88	0.18	68,68,68,68	0
56	MG	2a	3180	1/1	0.88	0.26	102,102,102,102	0
56	MG	1a	3064	1/1	0.88	0.32	87,87,87,87	0
56	MG	2A	3301	1/1	0.88	0.22	83,83,83,83	0
56	MG	1A	3301	1/1	0.88	0.24	85,85,85,85	0
56	MG	1A	3676	1/1	0.89	0.15	84,84,84,84	0
56	MG	2A	3126	1/1	0.89	0.21	80,80,80,80	0
56	MG	1A	3092	1/1	0.89	0.09	70,70,70,70	0
56	MG	2A	3039	1/1	0.89	0.32	88,88,88,88	0
56	MG	1A	3407	1/1	0.89	0.14	91,91,91,91	0
56	MG	2A	3042	1/1	0.89	0.12	89,89,89,89	0
56	MG	2A	3047	1/1	0.89	0.26	89,89,89,89	0
56	MG	1A	3363	1/1	0.89	0.18	79,79,79,79	0
56	MG	2a	3003	1/1	0.89	0.48	69,69,69,69	0
56	MG	2A	3141	1/1	0.89	0.72	81,81,81,81	0
56	MG	2a	3005	1/1	0.89	0.43	96,96,96,96	0
56	MG	1a	3121	1/1	0.89	0.41	88,88,88,88	0
56	MG	1A	3112	1/1	0.89	0.29	66,66,66,66	0
56	MG	1a	3192	1/1	0.89	0.19	85,85,85,85	0
56	MG	1a	3124	1/1	0.89	0.22	70,70,70,70	0
56	MG	1A	3515	1/1	0.89	0.30	63,63,63,63	0
56	MG	1A	3416	1/1	0.89	0.34	82,82,82,82	0
56	MG	2a	3115	1/1	0.89	0.24	103,103,103,103	0
56	MG	1A	3560	1/1	0.89	0.27	88,88,88,88	0
56	MG	1A	3164	1/1	0.89	0.14	72,72,72,72	0
56	MG	1A	3323	1/1	0.89	0.20	81,81,81,81	0
56	MG	1A	3165	1/1	0.89	0.41	86,86,86,86	0
56	MG	1A	3078	1/1	0.89	0.91	79,79,79,79	0
56	MG	1A	3062	1/1	0.89	0.84	92,92,92,92	0
56	MG	2A	3079	1/1	0.89	0.25	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3346	1/1	0.89	0.41	92,92,92,92	0
56	MG	2A	3282	1/1	0.89	0.12	87,87,87,87	0
56	MG	1A	3169	1/1	0.89	0.25	84,84,84,84	0
56	MG	1A	3575	1/1	0.89	0.25	83,83,83,83	0
56	MG	1a	3236	1/1	0.89	0.15	85,85,85,85	0
56	MG	1A	3639	1/1	0.89	0.20	67,67,67,67	0
56	MG	2A	3293	1/1	0.89	0.13	95,95,95,95	0
56	MG	1A	3306	1/1	0.89	0.28	82,82,82,82	0
56	MG	2A	3008	1/1	0.89	0.11	79,79,79,79	0
56	MG	1a	3158	1/1	0.89	0.15	81,81,81,81	0
56	MG	1A	3353	1/1	0.89	0.13	66,66,66,66	0
56	MG	1A	3648	1/1	0.89	0.32	127,127,127,127	0
56	MG	2a	3163	1/1	0.89	0.19	103,103,103,103	0
56	MG	1A	3434	1/1	0.89	0.10	81,81,81,81	0
56	MG	1a	3101	1/1	0.89	0.39	88,88,88,88	0
56	MG	2A	3105	1/1	0.89	0.18	71,71,71,71	0
56	MG	1a	3045	1/1	0.89	0.12	85,85,85,85	0
56	MG	1a	3048	1/1	0.89	0.20	73,73,73,73	0
56	MG	2a	3170	1/1	0.89	0.13	80,80,80,80	0
56	MG	2a	3175	1/1	0.89	0.20	76,76,76,76	0
56	MG	1A	3308	1/1	0.89	0.13	80,80,80,80	0
56	MG	1a	3050	1/1	0.89	0.11	80,80,80,80	0
56	MG	1A	3588	1/1	0.89	0.23	82,82,82,82	0
56	MG	1A	3136	1/1	0.89	0.69	78,78,78,78	0
56	MG	2A	3118	1/1	0.89	0.62	72,72,72,72	0
56	MG	1A	3662	1/1	0.89	0.16	90,90,90,90	0
56	MG	1A	3503	1/1	0.89	0.27	90,90,90,90	0
56	MG	2a	3079	1/1	0.89	0.37	90,90,90,90	0
56	MG	2a	3072	1/1	0.90	0.12	107,107,107,107	0
56	MG	2A	3004	1/1	0.90	0.16	91,91,91,91	0
56	MG	1A	3439	1/1	0.90	0.30	84,84,84,84	0
56	MG	1A	3405	1/1	0.90	0.18	78,78,78,78	0
56	MG	1A	3044	1/1	0.90	0.16	89,89,89,89	0
56	MG	1A	3231	1/1	0.90	0.12	57,57,57,57	0
56	MG	1A	3067	1/1	0.90	0.08	65,65,65,65	0
56	MG	1A	3094	1/1	0.90	0.10	63,63,63,63	0
56	MG	1A	3324	1/1	0.90	0.36	67,67,67,67	0
56	MG	2A	3330	1/1	0.90	0.16	101,101,101,101	0
56	MG	1A	3327	1/1	0.90	0.18	78,78,78,78	0
56	MG	1a	3093	1/1	0.90	0.39	88,88,88,88	0
56	MG	1A	3520	1/1	0.90	0.10	88,88,88,88	0
56	MG	1A	3568	1/1	0.90	0.09	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3096	1/1	0.90	0.09	90,90,90,90	0
56	MG	1A	3374	1/1	0.90	0.20	63,63,63,63	0
56	MG	1A	3188	1/1	0.90	0.27	91,91,91,91	0
56	MG	2A	3213	1/1	0.90	0.14	90,90,90,90	0
56	MG	1A	3070	1/1	0.90	0.23	52,52,52,52	0
56	MG	1A	3468	1/1	0.90	0.73	83,83,83,83	0
56	MG	1A	3577	1/1	0.90	0.12	94,94,94,94	0
56	MG	2A	3130	1/1	0.90	0.24	90,90,90,90	0
56	MG	2A	3040	1/1	0.90	0.14	82,82,82,82	0
56	MG	1a	3046	1/1	0.90	0.24	73,73,73,73	0
56	MG	1a	3109	1/1	0.90	0.61	103,103,103,103	0
56	MG	1A	3531	1/1	0.90	0.20	92,92,92,92	0
56	MG	2a	3011	1/1	0.90	0.10	101,101,101,101	0
56	MG	2A	3139	1/1	0.90	0.25	101,101,101,101	0
56	MG	2a	3014	1/1	0.90	0.30	89,89,89,89	0
56	MG	1A	3472	1/1	0.90	0.14	72,72,72,72	0
56	MG	1A	3049	1/1	0.90	0.20	61,61,61,61	0
56	MG	1A	3584	1/1	0.90	0.16	92,92,92,92	0
56	MG	1A	3009	1/1	0.90	0.28	75,75,75,75	0
56	MG	2a	3139	1/1	0.90	0.15	81,81,81,81	0
56	MG	2a	3029	1/1	0.90	0.20	87,87,87,87	0
56	MG	1A	3665	1/1	0.90	0.21	74,74,74,74	0
56	MG	1a	3118	1/1	0.90	0.75	101,101,101,101	0
56	MG	2A	3256	1/1	0.90	0.08	98,98,98,98	0
56	MG	2a	3151	1/1	0.90	0.20	111,111,111,111	0
56	MG	1A	3270	1/1	0.90	0.41	75,75,75,75	0
56	MG	2a	3155	1/1	0.90	0.11	84,84,84,84	0
56	MG	2a	3157	1/1	0.90	0.29	114,114,114,114	0
56	MG	2a	3040	1/1	0.90	0.14	78,78,78,78	0
56	MG	1a	3209	1/1	0.90	0.33	90,90,90,90	0
56	MG	1A	3489	1/1	0.90	0.34	78,78,78,78	0
56	MG	1A	3679	1/1	0.90	0.59	83,83,83,83	0
56	MG	2A	3273	1/1	0.90	0.20	86,86,86,86	0
56	MG	1A	3156	1/1	0.90	0.14	66,66,66,66	0
56	MG	1a	3215	1/1	0.90	0.15	84,84,84,84	0
56	MG	2A	3076	1/1	0.90	0.47	77,77,77,77	0
56	MG	2A	3077	1/1	0.90	0.42	77,77,77,77	0
56	MG	1A	3547	1/1	0.90	0.18	71,71,71,71	0
56	MG	1a	3065	1/1	0.90	0.19	87,87,87,87	0
56	MG	2A	3159	1/1	0.90	0.14	91,91,91,91	0
56	MG	1a	3066	1/1	0.90	0.11	101,101,101,101	0
56	MG	1A	3607	1/1	0.90	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3250	1/1	0.90	0.30	94,94,94,94	0
56	MG	2A	3089	1/1	0.90	0.15	82,82,82,82	0
56	MG	2A	3173	1/1	0.90	0.11	70,70,70,70	0
56	MG	1a	3009	1/1	0.90	0.36	91,91,91,91	0
56	MG	1a	3012	1/1	0.90	0.49	93,93,93,93	0
56	MG	1a	3014	1/1	0.90	0.10	78,78,78,78	0
57	ZN	2Y	501	1/1	0.90	0.13	138,138,138,138	0
56	MG	1A	3218	1/1	0.90	0.21	96,96,96,96	0
56	MG	1A	3140	1/1	0.91	0.20	89,89,89,89	0
56	MG	1a	3015	1/1	0.91	0.39	90,90,90,90	0
56	MG	1A	3380	1/1	0.91	0.14	67,67,67,67	0
56	MG	2A	3036	1/1	0.91	0.94	87,87,87,87	0
56	MG	2A	3268	1/1	0.91	0.06	82,82,82,82	0
56	MG	1A	3141	1/1	0.91	0.21	70,70,70,70	0
56	MG	1A	3388	1/1	0.91	0.34	69,69,69,69	0
56	MG	1A	3328	1/1	0.91	0.34	94,94,94,94	0
56	MG	1a	3021	1/1	0.91	0.24	102,102,102,102	0
56	MG	1A	3033	1/1	0.91	0.31	86,86,86,86	0
56	MG	2A	3284	1/1	0.91	0.09	79,79,79,79	0
56	MG	1a	3025	1/1	0.91	0.09	85,85,85,85	0
56	MG	2a	3071	1/1	0.91	0.41	88,88,88,88	0
56	MG	2A	3149	1/1	0.91	0.27	84,84,84,84	0
56	MG	1a	3095	1/1	0.91	0.26	62,62,62,62	0
56	MG	1A	3454	1/1	0.91	0.20	66,66,66,66	0
56	MG	1a	3098	1/1	0.91	0.35	87,87,87,87	0
56	MG	2A	3054	1/1	0.91	0.17	89,89,89,89	0
56	MG	1A	3333	1/1	0.91	0.30	73,73,73,73	0
56	MG	1a	3185	1/1	0.91	0.11	90,90,90,90	0
56	MG	1a	3186	1/1	0.91	0.19	85,85,85,85	0
56	MG	1A	3335	1/1	0.91	0.14	66,66,66,66	0
56	MG	1a	3031	1/1	0.91	0.49	103,103,103,103	0
56	MG	2A	3303	1/1	0.91	0.65	98,98,98,98	0
56	MG	1A	3010	1/1	0.91	0.64	65,65,65,65	0
56	MG	1A	3616	1/1	0.91	0.27	84,84,84,84	0
56	MG	2a	3091	1/1	0.91	0.24	92,92,92,92	0
56	MG	2A	3314	1/1	0.91	0.13	94,94,94,94	0
56	MG	2a	3095	1/1	0.91	0.27	75,75,75,75	0
56	MG	1A	3460	1/1	0.91	0.09	55,55,55,55	0
56	MG	1A	3256	1/1	0.91	0.42	84,84,84,84	0
56	MG	2A	3168	1/1	0.91	0.30	98,98,98,98	0
56	MG	2A	3169	1/1	0.91	0.26	79,79,79,79	0
56	MG	2A	3320	1/1	0.91	0.10	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3321	1/1	0.91	0.10	101,101,101,101	0
56	MG	2A	3170	1/1	0.91	0.20	95,95,95,95	0
56	MG	1a	3202	1/1	0.91	0.22	89,89,89,89	0
56	MG	1A	3294	1/1	0.91	0.38	87,87,87,87	0
56	MG	1A	3470	1/1	0.91	0.31	100,100,100,100	0
56	MG	1A	3553	1/1	0.91	0.22	89,89,89,89	0
56	MG	1a	3112	1/1	0.91	0.25	70,70,70,70	0
56	MG	1A	3095	1/1	0.91	0.17	81,81,81,81	0
56	MG	2A	3086	1/1	0.91	0.92	78,78,78,78	0
56	MG	1A	3478	1/1	0.91	0.30	83,83,83,83	0
56	MG	1A	3350	1/1	0.91	0.13	76,76,76,76	0
56	MG	2a	3126	1/1	0.91	0.31	86,86,86,86	0
56	MG	2a	3127	1/1	0.91	0.10	100,100,100,100	0
56	MG	1a	3216	1/1	0.91	0.14	81,81,81,81	0
56	MG	2A	3091	1/1	0.91	0.28	74,74,74,74	0
56	MG	2A	3348	1/1	0.91	0.25	79,79,79,79	0
56	MG	1A	3232	1/1	0.91	0.24	52,52,52,52	0
56	MG	2a	3001	1/1	0.91	0.12	74,74,74,74	0
56	MG	1A	3559	1/1	0.91	0.10	115,115,115,115	0
56	MG	1A	3300	1/1	0.91	0.19	77,77,77,77	0
56	MG	1A	3178	1/1	0.91	0.43	82,82,82,82	0
56	MG	2a	3145	1/1	0.91	0.20	90,90,90,90	0
56	MG	1a	3226	1/1	0.91	0.27	89,89,89,89	0
56	MG	1A	3357	1/1	0.91	0.32	76,76,76,76	0
56	MG	1a	3232	1/1	0.91	0.19	76,76,76,76	0
56	MG	1A	3652	1/1	0.91	0.13	86,86,86,86	0
56	MG	1A	3035	1/1	0.91	0.15	70,70,70,70	0
56	MG	2A	3210	1/1	0.91	0.12	75,75,75,75	0
56	MG	1A	3006	1/1	0.91	0.45	69,69,69,69	0
56	MG	1a	3061	1/1	0.91	0.35	79,79,79,79	0
56	MG	1A	3426	1/1	0.91	0.25	72,72,72,72	0
56	MG	2a	3023	1/1	0.91	0.47	80,80,80,80	0
56	MG	1A	3504	1/1	0.91	0.19	77,77,77,77	0
56	MG	2A	3009	1/1	0.91	0.90	89,89,89,89	0
56	MG	1A	3427	1/1	0.91	0.20	78,78,78,78	0
56	MG	1A	3361	1/1	0.91	0.27	71,71,71,71	0
56	MG	1A	3060	1/1	0.91	0.17	75,75,75,75	0
56	MG	1A	3201	1/1	0.91	0.29	68,68,68,68	0
56	MG	1A	3310	1/1	0.91	0.14	76,76,76,76	0
56	MG	2A	3124	1/1	0.91	0.20	86,86,86,86	0
56	MG	1A	3243	1/1	0.91	0.12	81,81,81,81	0
56	MG	2A	3246	1/1	0.91	0.88	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3119	1/1	0.91	0.23	107,107,107,107	0
56	MG	1A	3024	1/1	0.91	0.82	83,83,83,83	0
56	MG	1a	3154	1/1	0.91	0.32	78,78,78,78	0
56	MG	1A	3050	1/1	0.91	0.16	76,76,76,76	0
56	MG	1A	3285	1/1	0.91	0.26	56,56,56,56	0
56	MG	2A	3257	1/1	0.91	0.26	76,76,76,76	0
56	MG	1a	3079	1/1	0.92	0.19	73,73,73,73	0
56	MG	2A	3252	1/1	0.92	0.13	73,73,73,73	0
56	MG	1A	3124	1/1	0.92	0.79	86,86,86,86	0
56	MG	1A	3207	1/1	0.92	0.11	74,74,74,74	0
56	MG	2A	3135	1/1	0.92	0.25	78,78,78,78	0
56	MG	1a	3084	1/1	0.92	0.20	94,94,94,94	0
56	MG	1A	3340	1/1	0.92	0.32	78,78,78,78	0
56	MG	1A	3283	1/1	0.92	0.25	58,58,58,58	0
56	MG	1A	3115	1/1	0.92	0.23	87,87,87,87	0
56	MG	1a	3091	1/1	0.92	0.57	83,83,83,83	0
56	MG	1a	3178	1/1	0.92	0.32	81,81,81,81	0
56	MG	1A	3384	1/1	0.92	0.46	75,75,75,75	0
56	MG	1a	3022	1/1	0.92	0.21	89,89,89,89	0
56	MG	2A	3145	1/1	0.92	0.11	77,77,77,77	0
56	MG	2A	3043	1/1	0.92	0.21	82,82,82,82	0
56	MG	2A	3044	1/1	0.92	0.22	78,78,78,78	0
56	MG	2A	3046	1/1	0.92	0.13	68,68,68,68	0
56	MG	1A	3488	1/1	0.92	0.16	80,80,80,80	0
56	MG	2a	3073	1/1	0.92	0.19	113,113,113,113	0
56	MG	1A	3550	1/1	0.92	0.31	101,101,101,101	0
56	MG	2a	3075	1/1	0.92	0.30	98,98,98,98	0
56	MG	2A	3050	1/1	0.92	0.36	81,81,81,81	0
56	MG	1a	3026	1/1	0.92	0.22	80,80,80,80	0
56	MG	1A	3551	1/1	0.92	0.24	97,97,97,97	0
56	MG	1A	3126	1/1	0.92	0.64	76,76,76,76	0
56	MG	1A	3491	1/1	0.92	0.23	84,84,84,84	0
56	MG	1A	3618	1/1	0.92	0.19	98,98,98,98	0
56	MG	1A	3313	1/1	0.92	0.29	72,72,72,72	0
56	MG	2a	3086	1/1	0.92	0.14	87,87,87,87	0
56	MG	1A	3389	1/1	0.92	0.49	75,75,75,75	0
56	MG	1a	3197	1/1	0.92	0.12	102,102,102,102	0
56	MG	2A	3066	1/1	0.92	0.13	92,92,92,92	0
56	MG	2A	3305	1/1	0.92	0.11	85,85,85,85	0
56	MG	2A	3164	1/1	0.92	0.16	82,82,82,82	0
56	MG	2A	3312	1/1	0.92	0.10	74,74,74,74	0
56	MG	2A	3068	1/1	0.92	0.18	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	3034	1/1	0.92	0.12	73,73,73,73	0
56	MG	1A	3495	1/1	0.92	0.23	66,66,66,66	0
56	MG	1A	3211	1/1	0.92	0.30	88,88,88,88	0
56	MG	1A	3500	1/1	0.92	0.17	86,86,86,86	0
56	MG	1a	3207	1/1	0.92	0.20	96,96,96,96	0
56	MG	2A	3180	1/1	0.92	0.15	74,74,74,74	0
56	MG	1A	3143	1/1	0.92	0.32	84,84,84,84	0
56	MG	2A	3182	1/1	0.92	0.23	81,81,81,81	0
56	MG	2A	3326	1/1	0.92	0.16	91,91,91,91	0
56	MG	2a	3113	1/1	0.92	0.08	111,111,111,111	0
56	MG	1A	3563	1/1	0.92	0.17	97,97,97,97	0
56	MG	1A	3638	1/1	0.92	0.13	80,80,80,80	0
56	MG	2A	3187	1/1	0.92	0.14	81,81,81,81	0
56	MG	1A	3290	1/1	0.92	0.35	90,90,90,90	0
56	MG	2a	3119	1/1	0.92	0.12	107,107,107,107	0
56	MG	2A	3081	1/1	0.92	0.10	79,79,79,79	0
56	MG	1A	3642	1/1	0.92	0.29	74,74,74,74	0
56	MG	2a	3123	1/1	0.92	0.16	79,79,79,79	0
56	MG	1A	3356	1/1	0.92	0.67	61,61,61,61	0
56	MG	2A	3335	1/1	0.92	0.09	100,100,100,100	0
56	MG	1A	3187	1/1	0.92	0.14	75,75,75,75	0
56	MG	1A	3110	1/1	0.92	0.67	82,82,82,82	0
56	MG	1A	3171	1/1	0.92	0.14	77,77,77,77	0
56	MG	1A	3449	1/1	0.92	0.27	76,76,76,76	0
56	MG	1a	3123	1/1	0.92	0.16	72,72,72,72	0
56	MG	1a	3229	1/1	0.92	0.24	85,85,85,85	0
56	MG	1A	3325	1/1	0.92	0.19	69,69,69,69	0
56	MG	1A	3409	1/1	0.92	0.33	70,70,70,70	0
56	MG	1a	3059	1/1	0.92	0.68	82,82,82,82	0
56	MG	1A	3411	1/1	0.92	0.17	66,66,66,66	0
56	MG	1A	3055	1/1	0.92	0.22	79,79,79,79	0
56	MG	2a	3152	1/1	0.92	0.19	111,111,111,111	0
56	MG	1A	3274	1/1	0.92	0.24	78,78,78,78	0
56	MG	1A	3672	1/1	0.92	0.28	68,68,68,68	0
56	MG	2a	3156	1/1	0.92	0.08	104,104,104,104	0
56	MG	2A	3211	1/1	0.92	0.29	81,81,81,81	0
56	MG	2A	3007	1/1	0.92	0.14	80,80,80,80	0
56	MG	1A	3365	1/1	0.92	0.31	75,75,75,75	0
56	MG	1A	3581	1/1	0.92	0.13	84,84,84,84	0
56	MG	1A	3582	1/1	0.92	0.20	73,73,73,73	0
56	MG	1A	3329	1/1	0.92	0.20	77,77,77,77	0
56	MG	1A	3461	1/1	0.92	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3116	1/1	0.92	0.35	91,91,91,91	0
56	MG	2a	3026	1/1	0.92	0.15	90,90,90,90	0
56	MG	2A	3229	1/1	0.92	0.18	90,90,90,90	0
56	MG	2A	3231	1/1	0.92	0.17	74,74,74,74	0
56	MG	1A	3275	1/1	0.92	0.19	61,61,61,61	0
56	MG	2a	3033	1/1	0.92	0.13	86,86,86,86	0
56	MG	1A	3466	1/1	0.92	0.16	92,92,92,92	0
56	MG	2A	3238	1/1	0.92	0.17	93,93,93,93	0
56	MG	2A	3242	1/1	0.92	0.18	70,70,70,70	0
56	MG	2a	3039	1/1	0.92	0.13	89,89,89,89	0
56	MG	2A	3020	1/1	0.92	0.29	69,69,69,69	0
56	MG	1A	3204	1/1	0.92	0.19	60,60,60,60	0
56	MG	1a	3010	1/1	0.92	0.26	85,85,85,85	0
56	MG	2a	3046	1/1	0.92	0.10	85,85,85,85	0
56	MG	1A	3596	1/1	0.92	0.16	81,81,81,81	0
56	MG	1A	3599	1/1	0.92	0.30	100,100,100,100	0
56	MG	1A	3221	1/1	0.93	0.31	79,79,79,79	0
56	MG	2A	3308	1/1	0.93	0.13	103,103,103,103	0
56	MG	2A	3309	1/1	0.93	0.12	85,85,85,85	0
56	MG	1A	3223	1/1	0.93	0.16	59,59,59,59	0
56	MG	2A	3311	1/1	0.93	0.22	106,106,106,106	0
56	MG	2A	3107	1/1	0.93	0.27	92,92,92,92	0
56	MG	1A	3523	1/1	0.93	0.11	96,96,96,96	0
56	MG	1a	3041	1/1	0.93	0.14	81,81,81,81	0
56	MG	1a	3102	1/1	0.93	0.13	72,72,72,72	0
56	MG	1A	3229	1/1	0.93	0.21	74,74,74,74	0
56	MG	1A	3255	1/1	0.93	0.26	59,59,59,59	0
56	MG	2A	3202	1/1	0.93	0.32	88,88,88,88	0
56	MG	1A	3289	1/1	0.93	0.71	92,92,92,92	0
56	MG	2a	3084	1/1	0.93	0.14	78,78,78,78	0
56	MG	1A	3038	1/1	0.93	0.16	74,74,74,74	0
56	MG	2A	3322	1/1	0.93	0.15	86,86,86,86	0
56	MG	1A	3530	1/1	0.93	0.79	79,79,79,79	0
56	MG	1A	3469	1/1	0.93	0.37	84,84,84,84	0
56	MG	2A	3037	1/1	0.93	0.26	75,75,75,75	0
56	MG	2A	3208	1/1	0.93	0.12	71,71,71,71	0
56	MG	1A	3202	1/1	0.93	0.28	73,73,73,73	0
56	MG	1A	3670	1/1	0.93	0.13	76,76,76,76	0
56	MG	1A	3233	1/1	0.93	0.09	58,58,58,58	0
56	MG	2A	3129	1/1	0.93	0.32	73,73,73,73	0
56	MG	1A	3537	1/1	0.93	1.62	113,113,113,113	0
56	MG	1A	3476	1/1	0.93	0.11	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3133	1/1	0.93	0.19	65,65,65,65	0
56	MG	2A	3219	1/1	0.93	0.13	80,80,80,80	0
56	MG	2A	3341	1/1	0.93	0.15	94,94,94,94	0
56	MG	2a	3104	1/1	0.93	0.11	100,100,100,100	0
56	MG	1A	3592	1/1	0.93	0.25	84,84,84,84	0
56	MG	1a	3196	1/1	0.93	0.15	85,85,85,85	0
56	MG	1a	3003	1/1	0.93	0.11	92,92,92,92	0
56	MG	2A	3137	1/1	0.93	0.28	91,91,91,91	0
56	MG	2a	3114	1/1	0.93	0.34	92,92,92,92	0
56	MG	2A	3230	1/1	0.93	0.35	82,82,82,82	0
56	MG	1a	3198	1/1	0.93	0.28	89,89,89,89	0
56	MG	1A	3542	1/1	0.93	0.42	77,77,77,77	0
56	MG	1A	3331	1/1	0.93	0.12	75,75,75,75	0
56	MG	1A	3132	1/1	0.93	0.22	82,82,82,82	0
56	MG	1a	3204	1/1	0.93	0.17	80,80,80,80	0
56	MG	2a	3008	1/1	0.93	0.10	85,85,85,85	0
56	MG	1A	3334	1/1	0.93	0.18	64,64,64,64	0
56	MG	1a	3206	1/1	0.93	0.10	89,89,89,89	0
56	MG	1A	3235	1/1	0.93	0.13	73,73,73,73	0
56	MG	1A	3189	1/1	0.93	0.49	78,78,78,78	0
56	MG	1a	3125	1/1	0.93	0.21	106,106,106,106	0
56	MG	1A	3025	1/1	0.93	0.29	87,87,87,87	0
56	MG	1A	3166	1/1	0.93	0.33	77,77,77,77	0
56	MG	2a	3020	1/1	0.93	0.08	98,98,98,98	0
56	MG	1a	3132	1/1	0.93	0.12	101,101,101,101	0
56	MG	1A	3241	1/1	0.93	0.32	68,68,68,68	0
56	MG	2a	3025	1/1	0.93	0.08	86,86,86,86	0
56	MG	1A	3438	1/1	0.93	0.10	71,71,71,71	0
56	MG	2a	3027	1/1	0.93	0.12	83,83,83,83	0
56	MG	2a	3148	1/1	0.93	0.13	92,92,92,92	0
56	MG	1A	3273	1/1	0.93	0.23	62,62,62,62	0
56	MG	1A	3496	1/1	0.93	0.24	72,72,72,72	0
56	MG	2A	3260	1/1	0.93	0.24	87,87,87,87	0
56	MG	2A	3075	1/1	0.93	0.34	83,83,83,83	0
56	MG	1A	3074	1/1	0.93	0.14	81,81,81,81	0
56	MG	1a	3141	1/1	0.93	0.20	59,59,59,59	0
56	MG	1A	3047	1/1	0.93	0.99	68,68,68,68	0
56	MG	2A	3271	1/1	0.93	0.18	83,83,83,83	0
56	MG	1A	3029	1/1	0.93	0.21	65,65,65,65	0
56	MG	1A	3312	1/1	0.93	0.30	62,62,62,62	0
56	MG	1A	3355	1/1	0.93	0.23	68,68,68,68	0
56	MG	2A	3280	1/1	0.93	0.83	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	3235	1/1	0.93	0.32	93,93,93,93	0
56	MG	1a	3151	1/1	0.93	0.21	80,80,80,80	0
56	MG	1A	3624	1/1	0.93	0.29	64,64,64,64	0
56	MG	2A	3285	1/1	0.93	0.11	82,82,82,82	0
56	MG	2A	3001	1/1	0.93	0.14	75,75,75,75	0
56	MG	1A	3278	1/1	0.93	0.28	59,59,59,59	0
56	MG	2a	3173	1/1	0.93	0.35	115,115,115,115	0
56	MG	1A	3158	1/1	0.93	0.19	67,67,67,67	0
56	MG	2A	3177	1/1	0.93	0.22	74,74,74,74	0
56	MG	1A	3512	1/1	0.93	0.29	82,82,82,82	0
56	MG	1a	3159	1/1	0.93	0.28	72,72,72,72	0
56	MG	1a	3160	1/1	0.93	0.23	76,76,76,76	0
56	MG	1A	3081	1/1	0.93	0.17	60,60,60,60	0
56	MG	1A	3120	1/1	0.93	0.23	111,111,111,111	0
56	MG	1A	3413	1/1	0.93	0.24	71,71,71,71	0
56	MG	1A	3640	1/1	0.93	0.26	81,81,81,81	0
56	MG	1A	3414	1/1	0.93	0.36	82,82,82,82	0
56	MG	1A	3017	1/1	0.94	0.27	64,64,64,64	0
56	MG	1A	3039	1/1	0.94	0.12	70,70,70,70	0
56	MG	1A	3326	1/1	0.94	0.20	83,83,83,83	0
56	MG	1A	3677	1/1	0.94	0.23	55,55,55,55	0
56	MG	1a	3078	1/1	0.94	0.18	65,65,65,65	0
56	MG	1A	3586	1/1	0.94	0.32	71,71,71,71	0
56	MG	2A	3261	1/1	0.94	0.40	98,98,98,98	0
56	MG	1A	3418	1/1	0.94	0.35	75,75,75,75	0
56	MG	1A	3473	1/1	0.94	0.12	86,86,86,86	0
56	MG	2a	3056	1/1	0.94	0.11	97,97,97,97	0
56	MG	1A	3264	1/1	0.94	0.43	67,67,67,67	0
56	MG	1a	3006	1/1	0.94	0.21	90,90,90,90	0
56	MG	1A	3593	1/1	0.94	0.17	65,65,65,65	0
56	MG	1A	3595	1/1	0.94	0.32	69,69,69,69	0
56	MG	2A	3045	1/1	0.94	0.21	76,76,76,76	0
56	MG	1A	3366	1/1	0.94	0.14	72,72,72,72	0
56	MG	1A	3422	1/1	0.94	0.32	67,67,67,67	0
56	MG	1A	3134	1/1	0.94	0.30	63,63,63,63	0
56	MG	2a	3067	1/1	0.94	0.09	112,112,112,112	0
56	MG	1A	3266	1/1	0.94	0.30	65,65,65,65	0
56	MG	1A	3603	1/1	0.94	0.21	67,67,67,67	0
56	MG	1A	3605	1/1	0.94	0.20	93,93,93,93	0
56	MG	1a	3017	1/1	0.94	0.12	81,81,81,81	0
56	MG	1A	3370	1/1	0.94	0.17	82,82,82,82	0
56	MG	2A	3289	1/1	0.94	0.07	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3056	1/1	0.94	0.67	73,73,73,73	0
56	MG	1a	3193	1/1	0.94	0.24	88,88,88,88	0
56	MG	1A	3088	1/1	0.94	0.18	71,71,71,71	0
56	MG	1A	3220	1/1	0.94	0.18	71,71,71,71	0
56	MG	1A	3610	1/1	0.94	0.21	79,79,79,79	0
56	MG	1a	3199	1/1	0.94	0.31	93,93,93,93	0
56	MG	2a	3081	1/1	0.94	0.10	61,61,61,61	0
56	MG	1A	3332	1/1	0.94	0.24	77,77,77,77	0
56	MG	2a	3083	1/1	0.94	0.52	76,76,76,76	0
56	MG	1A	3077	1/1	0.94	0.30	93,93,93,93	0
56	MG	1A	3272	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3245	1/1	0.94	0.31	56,56,56,56	0
56	MG	2A	3304	1/1	0.94	0.46	92,92,92,92	0
56	MG	1A	3381	1/1	0.94	0.27	68,68,68,68	0
56	MG	2A	3171	1/1	0.94	0.19	86,86,86,86	0
56	MG	1A	3383	1/1	0.94	0.24	69,69,69,69	0
56	MG	2A	3174	1/1	0.94	0.13	79,79,79,79	0
56	MG	1A	3337	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3558	1/1	0.94	0.14	97,97,97,97	0
56	MG	1A	3116	1/1	0.94	0.41	113,113,113,113	0
56	MG	1A	3387	1/1	0.94	0.17	80,80,80,80	0
56	MG	1A	3623	1/1	0.94	0.15	87,87,87,87	0
56	MG	2A	3185	1/1	0.94	0.32	76,76,76,76	0
56	MG	1A	3561	1/1	0.94	0.17	64,64,64,64	0
56	MG	2A	3082	1/1	0.94	0.05	85,85,85,85	0
56	MG	1A	3305	1/1	0.94	0.20	65,65,65,65	0
56	MG	1A	3564	1/1	0.94	0.10	97,97,97,97	0
56	MG	1a	3218	1/1	0.94	0.21	80,80,80,80	0
56	MG	2A	3088	1/1	0.94	0.17	77,77,77,77	0
56	MG	2a	3109	1/1	0.94	0.11	82,82,82,82	0
56	MG	2a	3110	1/1	0.94	0.13	80,80,80,80	0
56	MG	2a	3111	1/1	0.94	0.13	86,86,86,86	0
56	MG	2a	3112	1/1	0.94	0.14	87,87,87,87	0
56	MG	1A	3224	1/1	0.94	0.22	65,65,65,65	0
56	MG	1A	3227	1/1	0.94	0.18	72,72,72,72	0
56	MG	1A	3051	1/1	0.94	0.10	68,68,68,68	0
56	MG	1A	3079	1/1	0.94	0.12	96,96,96,96	0
56	MG	1A	3351	1/1	0.94	0.24	58,58,58,58	0
56	MG	2A	3095	1/1	0.94	0.43	89,89,89,89	0
56	MG	1A	3206	1/1	0.94	0.07	76,76,76,76	0
56	MG	1A	3644	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3316	1/1	0.94	0.29	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	3234	1/1	0.94	0.18	85,85,85,85	0
56	MG	1A	3254	1/1	0.94	0.14	78,78,78,78	0
56	MG	2A	3103	1/1	0.94	0.24	83,83,83,83	0
56	MG	2A	3342	1/1	0.94	0.26	78,78,78,78	0
56	MG	2a	3128	1/1	0.94	0.17	74,74,74,74	0
56	MG	1A	3574	1/1	0.94	0.23	77,77,77,77	0
56	MG	1A	3649	1/1	0.94	0.05	86,86,86,86	0
56	MG	2a	3131	1/1	0.94	0.13	84,84,84,84	0
56	MG	2a	3132	1/1	0.94	0.20	83,83,83,83	0
56	MG	2a	3136	1/1	0.94	0.27	85,85,85,85	0
56	MG	2a	3137	1/1	0.94	0.09	81,81,81,81	0
56	MG	2A	3346	1/1	0.94	0.27	78,78,78,78	0
56	MG	1a	3137	1/1	0.94	0.10	79,79,79,79	0
56	MG	1A	3650	1/1	0.94	1.24	90,90,90,90	0
56	MG	2A	3212	1/1	0.94	0.52	83,83,83,83	0
56	MG	2A	3108	1/1	0.94	0.25	72,72,72,72	0
56	MG	2A	3214	1/1	0.94	0.49	92,92,92,92	0
56	MG	2A	3109	1/1	0.94	0.14	93,93,93,93	0
56	MG	1a	3055	1/1	0.94	0.18	83,83,83,83	0
56	MG	1a	3056	1/1	0.94	0.11	83,83,83,83	0
56	MG	2A	3218	1/1	0.94	0.23	83,83,83,83	0
56	MG	2a	3153	1/1	0.94	0.13	106,106,106,106	0
56	MG	1A	3152	1/1	0.94	0.67	84,84,84,84	0
56	MG	2A	3220	1/1	0.94	0.33	74,74,74,74	0
56	MG	2A	3113	1/1	0.94	0.20	73,73,73,73	0
56	MG	1A	3576	1/1	0.94	0.14	76,76,76,76	0
56	MG	2a	3013	1/1	0.94	0.28	85,85,85,85	0
56	MG	2A	3226	1/1	0.94	0.11	73,73,73,73	0
56	MG	1A	3656	1/1	0.94	0.20	70,70,70,70	0
56	MG	2A	3228	1/1	0.94	0.10	68,68,68,68	0
56	MG	2a	3018	1/1	0.94	0.13	71,71,71,71	0
56	MG	2A	3012	1/1	0.94	0.30	92,92,92,92	0
56	MG	1A	3080	1/1	0.94	0.19	66,66,66,66	0
56	MG	1A	3578	1/1	0.94	0.12	86,86,86,86	0
56	MG	2A	3233	1/1	0.94	0.25	71,71,71,71	0
56	MG	1A	3659	1/1	0.94	0.18	80,80,80,80	0
56	MG	2A	3235	1/1	0.94	0.19	69,69,69,69	0
56	MG	1A	3321	1/1	0.94	0.21	62,62,62,62	0
56	MG	1A	3412	1/1	0.94	0.45	79,79,79,79	0
56	MG	2a	3174	1/1	0.94	0.12	101,101,101,101	0
56	MG	1a	3155	1/1	0.94	0.08	74,74,74,74	0
56	MG	2a	3032	1/1	0.94	0.17	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3663	1/1	0.94	0.23	89,89,89,89	0
56	MG	2A	3128	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	3209	1/1	0.94	0.19	56,56,56,56	0
56	MG	1A	3666	1/1	0.94	0.17	92,92,92,92	0
56	MG	2a	3182	1/1	0.94	0.17	106,106,106,106	0
56	MG	1A	3668	1/1	0.94	0.11	82,82,82,82	0
56	MG	1A	3130	1/1	0.94	0.36	81,81,81,81	0
56	MG	2A	3251	1/1	0.94	0.13	73,73,73,73	0
56	MG	2A	3032	1/1	0.94	0.25	78,78,78,78	0
56	MG	2A	3200	1/1	0.95	0.26	86,86,86,86	0
56	MG	1A	3546	1/1	0.95	0.21	69,69,69,69	0
56	MG	2A	3010	1/1	0.95	0.14	85,85,85,85	0
56	MG	1a	3157	1/1	0.95	0.45	89,89,89,89	0
56	MG	1A	3373	1/1	0.95	0.35	54,54,54,54	0
56	MG	1A	3341	1/1	0.95	0.21	70,70,70,70	0
56	MG	2A	3015	1/1	0.95	0.53	84,84,84,84	0
56	MG	2A	3016	1/1	0.95	0.14	82,82,82,82	0
56	MG	1A	3342	1/1	0.95	0.20	64,64,64,64	0
56	MG	1a	3081	1/1	0.95	0.16	81,81,81,81	0
56	MG	1A	3131	1/1	0.95	0.18	84,84,84,84	0
56	MG	1a	3164	1/1	0.95	0.73	81,81,81,81	0
56	MG	2A	3324	1/1	0.95	0.27	83,83,83,83	0
56	MG	1A	3484	1/1	0.95	0.25	80,80,80,80	0
56	MG	1A	3260	1/1	0.95	0.26	62,62,62,62	0
56	MG	1A	3487	1/1	0.95	0.11	81,81,81,81	0
56	MG	1A	3238	1/1	0.95	0.13	60,60,60,60	0
56	MG	2A	3027	1/1	0.95	0.16	87,87,87,87	0
56	MG	1A	3382	1/1	0.95	0.23	60,60,60,60	0
56	MG	1a	3172	1/1	0.95	0.14	90,90,90,90	0
56	MG	2A	3125	1/1	0.95	0.28	88,88,88,88	0
56	MG	1A	3349	1/1	0.95	0.25	72,72,72,72	0
56	MG	1A	3083	1/1	0.95	0.21	71,71,71,71	0
56	MG	1A	3162	1/1	0.95	0.09	83,83,83,83	0
56	MG	2A	3338	1/1	0.95	0.64	97,97,97,97	0
56	MG	1A	3432	1/1	0.95	0.32	57,57,57,57	0
56	MG	1A	3386	1/1	0.95	0.49	68,68,68,68	0
56	MG	1A	3054	1/1	0.95	0.24	86,86,86,86	0
56	MG	1a	3181	1/1	0.95	0.28	66,66,66,66	0
56	MG	1A	3182	1/1	0.95	0.69	72,72,72,72	0
56	MG	2A	3347	1/1	0.95	0.16	86,86,86,86	0
56	MG	1A	3626	1/1	0.95	0.16	86,86,86,86	0
56	MG	2A	3349	1/1	0.95	0.26	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3501	1/1	0.95	0.28	71,71,71,71	0
56	MG	1A	3631	1/1	0.95	0.08	82,82,82,82	0
56	MG	2a	3002	1/1	0.95	0.13	98,98,98,98	0
56	MG	1A	3076	1/1	0.95	0.60	54,54,54,54	0
56	MG	1a	3104	1/1	0.95	0.15	74,74,74,74	0
56	MG	1A	3091	1/1	0.95	0.29	75,75,75,75	0
56	MG	1A	3108	1/1	0.95	0.43	84,84,84,84	0
56	MG	1A	3393	1/1	0.95	0.18	82,82,82,82	0
56	MG	1A	3225	1/1	0.95	0.38	65,65,65,65	0
56	MG	2A	3049	1/1	0.95	0.15	81,81,81,81	0
56	MG	1a	3195	1/1	0.95	0.22	80,80,80,80	0
56	MG	1A	3570	1/1	0.95	0.32	99,99,99,99	0
56	MG	2a	3122	1/1	0.95	0.09	114,114,114,114	0
56	MG	2A	3248	1/1	0.95	0.11	85,85,85,85	0
56	MG	2A	3052	1/1	0.95	0.15	72,72,72,72	0
56	MG	1A	3395	1/1	0.95	0.14	72,72,72,72	0
56	MG	1A	3109	1/1	0.95	0.16	78,78,78,78	0
56	MG	1A	3446	1/1	0.95	0.16	65,65,65,65	0
56	MG	1a	3040	1/1	0.95	0.08	89,89,89,89	0
56	MG	2a	3019	1/1	0.95	0.13	95,95,95,95	0
56	MG	2A	3255	1/1	0.95	0.60	91,91,91,91	0
56	MG	2a	3021	1/1	0.95	0.09	101,101,101,101	0
56	MG	2a	3134	1/1	0.95	0.19	100,100,100,100	0
56	MG	2a	3135	1/1	0.95	0.14	108,108,108,108	0
56	MG	1a	3114	1/1	0.95	0.09	86,86,86,86	0
56	MG	1A	3397	1/1	0.95	0.09	83,83,83,83	0
56	MG	1A	3302	1/1	0.95	0.26	59,59,59,59	0
56	MG	1A	3402	1/1	0.95	0.21	51,51,51,51	0
56	MG	2A	3062	1/1	0.95	0.12	84,84,84,84	0
56	MG	2A	3262	1/1	0.95	0.66	84,84,84,84	0
56	MG	1A	3403	1/1	0.95	0.36	59,59,59,59	0
56	MG	2a	3030	1/1	0.95	0.12	77,77,77,77	0
56	MG	1A	3522	1/1	0.95	0.10	69,69,69,69	0
56	MG	2a	3147	1/1	0.95	0.36	89,89,89,89	0
56	MG	1A	3404	1/1	0.95	0.16	62,62,62,62	0
56	MG	1A	3360	1/1	0.95	0.14	68,68,68,68	0
56	MG	1a	3212	1/1	0.95	0.10	71,71,71,71	0
56	MG	1A	3020	1/1	0.95	0.36	89,89,89,89	0
56	MG	2A	3274	1/1	0.95	0.23	92,92,92,92	0
56	MG	1A	3458	1/1	0.95	0.14	82,82,82,82	0
56	MG	1A	3528	1/1	0.95	0.28	78,78,78,78	0
56	MG	1A	3230	1/1	0.95	0.20	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3281	1/1	0.95	0.10	88,88,88,88	0
56	MG	1A	3031	1/1	0.95	0.10	62,62,62,62	0
56	MG	1a	3128	1/1	0.95	0.22	98,98,98,98	0
56	MG	1A	3008	1/1	0.95	0.13	74,74,74,74	0
56	MG	1A	3664	1/1	0.95	0.21	82,82,82,82	0
56	MG	1A	3587	1/1	0.95	0.18	80,80,80,80	0
56	MG	1A	3462	1/1	0.95	0.11	64,64,64,64	0
56	MG	1a	3228	1/1	0.95	0.19	72,72,72,72	0
56	MG	1A	3018	1/1	0.95	0.56	84,84,84,84	0
56	MG	2A	3183	1/1	0.95	0.15	80,80,80,80	0
56	MG	1A	3669	1/1	0.95	0.19	79,79,79,79	0
56	MG	2a	3057	1/1	0.95	0.13	74,74,74,74	0
56	MG	2a	3172	1/1	0.95	0.38	89,89,89,89	0
56	MG	1A	3536	1/1	0.95	0.22	74,74,74,74	0
56	MG	1A	3309	1/1	0.95	0.10	67,67,67,67	0
56	MG	1A	3540	1/1	0.95	0.10	94,94,94,94	0
56	MG	1a	3145	1/1	0.95	0.48	97,97,97,97	0
56	MG	1A	3675	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3336	1/1	0.95	0.41	81,81,81,81	0
56	MG	1A	3369	1/1	0.95	0.31	86,86,86,86	0
56	MG	1A	3003	1/1	0.95	0.39	60,60,60,60	0
56	MG	1A	3082	1/1	0.95	0.15	69,69,69,69	0
56	MG	2a	3068	1/1	0.95	0.16	83,83,83,83	0
56	MG	2A	3005	1/1	0.95	0.09	84,84,84,84	0
56	MG	1A	3602	1/1	0.95	0.22	67,67,67,67	0
56	MG	1A	3236	1/1	0.95	0.29	60,60,60,60	0
56	MG	1A	3222	1/1	0.96	0.22	64,64,64,64	0
56	MG	1A	3163	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3170	1/1	0.96	0.30	99,99,99,99	0
56	MG	1A	3421	1/1	0.96	0.22	68,68,68,68	0
56	MG	1A	3467	1/1	0.96	0.11	73,73,73,73	0
56	MG	1A	3641	1/1	0.96	0.17	68,68,68,68	0
56	MG	1a	3208	1/1	0.96	0.14	80,80,80,80	0
56	MG	1A	3027	1/1	0.96	1.18	68,68,68,68	0
56	MG	2A	3176	1/1	0.96	0.22	89,89,89,89	0
56	MG	1a	3210	1/1	0.96	0.23	91,91,91,91	0
56	MG	1A	3226	1/1	0.96	0.22	62,62,62,62	0
56	MG	1A	3172	1/1	0.96	0.26	94,94,94,94	0
56	MG	2A	3299	1/1	0.96	0.48	66,66,66,66	0
56	MG	1A	3471	1/1	0.96	0.19	88,88,88,88	0
56	MG	1A	3281	1/1	0.96	0.17	64,64,64,64	0
56	MG	1A	3282	1/1	0.96	0.29	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3535	1/1	0.96	0.34	90,90,90,90	0
56	MG	1a	3044	1/1	0.96	0.29	90,90,90,90	0
56	MG	2A	3307	1/1	0.96	0.17	79,79,79,79	0
56	MG	1A	3392	1/1	0.96	0.36	80,80,80,80	0
56	MG	2A	3083	1/1	0.96	0.10	80,80,80,80	0
56	MG	2A	3189	1/1	0.96	0.23	89,89,89,89	0
56	MG	1A	3362	1/1	0.96	0.21	53,53,53,53	0
56	MG	1A	3653	1/1	0.96	0.17	95,95,95,95	0
56	MG	1a	3223	1/1	0.96	0.24	84,84,84,84	0
56	MG	1A	3654	1/1	0.96	0.16	89,89,89,89	0
56	MG	1a	3225	1/1	0.96	0.57	85,85,85,85	0
56	MG	1a	3130	1/1	0.96	0.27	99,99,99,99	0
56	MG	1A	3538	1/1	0.96	0.09	87,87,87,87	0
56	MG	1A	3539	1/1	0.96	0.33	85,85,85,85	0
56	MG	2A	3199	1/1	0.96	0.37	74,74,74,74	0
56	MG	1A	3430	1/1	0.96	0.24	61,61,61,61	0
56	MG	1A	3480	1/1	0.96	0.27	104,104,104,104	0
56	MG	2a	3093	1/1	0.96	0.23	87,87,87,87	0
56	MG	2a	3094	1/1	0.96	0.29	89,89,89,89	0
56	MG	2A	3096	1/1	0.96	0.17	90,90,90,90	0
56	MG	1A	3590	1/1	0.96	0.21	68,68,68,68	0
56	MG	2A	3325	1/1	0.96	0.20	91,91,91,91	0
56	MG	1A	3591	1/1	0.96	0.34	83,83,83,83	0
56	MG	1a	3057	1/1	0.96	0.24	92,92,92,92	0
56	MG	1A	3228	1/1	0.96	0.17	59,59,59,59	0
56	MG	2A	3329	1/1	0.96	0.29	100,100,100,100	0
56	MG	1a	3237	1/1	0.96	0.06	106,106,106,106	0
56	MG	1a	3142	1/1	0.96	0.16	85,85,85,85	0
56	MG	1A	3284	1/1	0.96	0.16	86,86,86,86	0
56	MG	1A	3059	1/1	0.96	0.13	81,81,81,81	0
56	MG	2a	3108	1/1	0.96	0.05	98,98,98,98	0
56	MG	1A	3213	1/1	0.96	0.16	66,66,66,66	0
56	MG	1A	3597	1/1	0.96	0.16	87,87,87,87	0
56	MG	2A	3006	1/1	0.96	0.24	71,71,71,71	0
56	MG	1A	3598	1/1	0.96	0.27	74,74,74,74	0
56	MG	1a	3150	1/1	0.96	0.15	83,83,83,83	0
56	MG	2A	3340	1/1	0.96	0.19	67,67,67,67	0
56	MG	1A	3398	1/1	0.96	0.14	67,67,67,67	0
56	MG	1A	3671	1/1	0.96	0.16	79,79,79,79	0
56	MG	1A	3399	1/1	0.96	0.28	68,68,68,68	0
56	MG	1A	3673	1/1	0.96	0.30	77,77,77,77	0
56	MG	1A	3037	1/1	0.96	0.18	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3221	1/1	0.96	0.14	107,107,107,107	0
56	MG	2A	3014	1/1	0.96	0.38	72,72,72,72	0
56	MG	1A	3315	1/1	0.96	0.12	57,57,57,57	0
56	MG	1A	3440	1/1	0.96	0.14	77,77,77,77	0
56	MG	1A	3248	1/1	0.96	0.20	76,76,76,76	0
56	MG	1A	3678	1/1	0.96	0.23	75,75,75,75	0
56	MG	1a	3161	1/1	0.96	0.10	82,82,82,82	0
56	MG	1A	3317	1/1	0.96	0.30	56,56,56,56	0
56	MG	1a	3074	1/1	0.96	0.12	88,88,88,88	0
56	MG	1a	3001	1/1	0.96	0.25	90,90,90,90	0
56	MG	1A	3216	1/1	0.96	0.32	50,50,50,50	0
56	MG	1A	3406	1/1	0.96	0.22	59,59,59,59	0
56	MG	2a	3133	1/1	0.96	0.23	92,92,92,92	0
56	MG	2A	3236	1/1	0.96	0.18	69,69,69,69	0
56	MG	1A	3445	1/1	0.96	0.20	80,80,80,80	0
56	MG	1a	3168	1/1	0.96	0.14	111,111,111,111	0
56	MG	2A	3240	1/1	0.96	0.12	84,84,84,84	0
56	MG	2A	3132	1/1	0.96	0.19	97,97,97,97	0
56	MG	2A	3029	1/1	0.96	0.21	94,94,94,94	0
56	MG	1A	3344	1/1	0.96	0.19	79,79,79,79	0
56	MG	2a	3016	1/1	0.96	0.29	91,91,91,91	0
56	MG	1A	3117	1/1	0.96	0.10	98,98,98,98	0
56	MG	1a	3171	1/1	0.96	0.23	86,86,86,86	0
56	MG	1A	3269	1/1	0.96	0.15	69,69,69,69	0
56	MG	2a	3146	1/1	0.96	0.17	100,100,100,100	0
56	MG	1A	3450	1/1	0.96	0.38	76,76,76,76	0
56	MG	1a	3087	1/1	0.96	0.13	100,100,100,100	0
56	MG	1A	3508	1/1	0.96	0.12	86,86,86,86	0
56	MG	1a	3176	1/1	0.96	0.10	84,84,84,84	0
56	MG	1a	3011	1/1	0.96	0.20	94,94,94,94	0
56	MG	1A	3410	1/1	0.96	0.17	77,77,77,77	0
56	MG	1a	3013	1/1	0.96	0.09	77,77,77,77	0
56	MG	1A	3562	1/1	0.96	0.10	60,60,60,60	0
56	MG	1A	3348	1/1	0.96	0.34	74,74,74,74	0
56	MG	1A	3193	1/1	0.96	0.17	62,62,62,62	0
56	MG	2A	3259	1/1	0.96	0.21	76,76,76,76	0
56	MG	1a	3096	1/1	0.96	0.10	95,95,95,95	0
56	MG	1A	3514	1/1	0.96	0.12	94,94,94,94	0
56	MG	1A	3378	1/1	0.96	0.43	73,73,73,73	0
56	MG	2a	3035	1/1	0.96	0.15	94,94,94,94	0
56	MG	1A	3516	1/1	0.96	0.07	81,81,81,81	0
56	MG	2A	3264	1/1	0.96	0.10	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3038	1/1	0.96	0.20	101,101,101,101	0
56	MG	1a	3100	1/1	0.96	0.13	78,78,78,78	0
56	MG	1A	3625	1/1	0.96	0.17	66,66,66,66	0
56	MG	1A	3090	1/1	0.96	0.50	84,84,84,84	0
56	MG	2a	3171	1/1	0.96	0.07	115,115,115,115	0
56	MG	2A	3269	1/1	0.96	0.75	74,74,74,74	0
56	MG	2A	3270	1/1	0.96	0.11	80,80,80,80	0
56	MG	2A	3155	1/1	0.96	0.07	66,66,66,66	0
56	MG	2A	3272	1/1	0.96	0.15	89,89,89,89	0
56	MG	1A	3627	1/1	0.96	0.20	60,60,60,60	0
56	MG	1a	3023	1/1	0.96	0.23	87,87,87,87	0
56	MG	1A	3195	1/1	0.96	0.33	78,78,78,78	0
56	MG	2a	3052	1/1	0.96	0.09	95,95,95,95	0
56	MG	1A	3630	1/1	0.96	0.17	77,77,77,77	0
56	MG	2a	3181	1/1	0.96	0.17	90,90,90,90	0
56	MG	2A	3279	1/1	0.96	0.25	70,70,70,70	0
56	MG	1A	3297	1/1	0.96	0.13	77,77,77,77	0
56	MG	2A	3161	1/1	0.96	0.11	69,69,69,69	0
57	ZN	16	501	1/1	0.96	0.23	87,87,87,87	0
56	MG	1A	3298	1/1	0.96	0.42	83,83,83,83	0
56	MG	1A	3634	1/1	0.96	0.19	83,83,83,83	0
57	ZN	29	501	1/1	0.96	0.19	105,105,105,105	0
56	MG	2A	3275	1/1	0.97	0.34	81,81,81,81	0
56	MG	2a	3098	1/1	0.97	0.37	101,101,101,101	0
56	MG	2A	3276	1/1	0.97	0.12	82,82,82,82	0
56	MG	1A	3635	1/1	0.97	0.20	78,78,78,78	0
56	MG	1A	3271	1/1	0.97	0.17	49,49,49,49	0
56	MG	1A	3594	1/1	0.97	0.17	77,77,77,77	0
56	MG	2a	3103	1/1	0.97	0.27	73,73,73,73	0
56	MG	1a	3054	1/1	0.97	0.21	85,85,85,85	0
56	MG	1A	3483	1/1	0.97	0.07	77,77,77,77	0
56	MG	1A	3424	1/1	0.97	1.40	81,81,81,81	0
56	MG	1A	3401	1/1	0.97	0.27	90,90,90,90	0
56	MG	1A	3526	1/1	0.97	0.12	76,76,76,76	0
56	MG	1a	3231	1/1	0.97	0.16	82,82,82,82	0
56	MG	1A	3040	1/1	0.97	0.24	115,115,115,115	0
56	MG	2a	3022	1/1	0.97	0.15	83,83,83,83	0
56	MG	1A	3643	1/1	0.97	0.13	86,86,86,86	0
56	MG	1A	3311	1/1	0.97	0.34	61,61,61,61	0
56	MG	1A	3071	1/1	0.97	0.21	74,74,74,74	0
56	MG	2A	3291	1/1	0.97	0.10	87,87,87,87	0
56	MG	2A	3292	1/1	0.97	0.08	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3490	1/1	0.97	0.19	79,79,79,79	0
56	MG	1A	3292	1/1	0.97	0.13	50,50,50,50	0
56	MG	2A	3063	1/1	0.97	0.07	67,67,67,67	0
56	MG	2A	3065	1/1	0.97	0.36	88,88,88,88	0
56	MG	1A	3492	1/1	0.97	0.12	77,77,77,77	0
56	MG	1a	3119	1/1	0.97	0.58	88,88,88,88	0
56	MG	2A	3002	1/1	0.97	0.22	81,81,81,81	0
56	MG	1A	3606	1/1	0.97	0.47	71,71,71,71	0
56	MG	1A	3043	1/1	0.97	0.13	74,74,74,74	0
56	MG	2A	3073	1/1	0.97	0.16	85,85,85,85	0
56	MG	1A	3061	1/1	0.97	0.21	77,77,77,77	0
56	MG	1A	3338	1/1	0.97	0.21	45,45,45,45	0
56	MG	1A	3005	1/1	0.97	0.13	74,74,74,74	0
56	MG	2a	3041	1/1	0.97	0.20	69,69,69,69	0
56	MG	1A	3611	1/1	0.97	0.30	75,75,75,75	0
56	MG	1a	3183	1/1	0.97	0.34	78,78,78,78	0
56	MG	2a	3044	1/1	0.97	0.29	86,86,86,86	0
56	MG	1A	3296	1/1	0.97	0.12	76,76,76,76	0
56	MG	1A	3499	1/1	0.97	0.09	72,72,72,72	0
56	MG	1A	3463	1/1	0.97	0.29	75,75,75,75	0
56	MG	1A	3660	1/1	0.97	0.25	65,65,65,65	0
56	MG	1a	3131	1/1	0.97	0.25	107,107,107,107	0
56	MG	1A	3464	1/1	0.97	0.15	73,73,73,73	0
56	MG	2A	3232	1/1	0.97	0.24	53,53,53,53	0
56	MG	2A	3085	1/1	0.97	0.66	101,101,101,101	0
56	MG	1A	3155	1/1	0.97	0.15	65,65,65,65	0
56	MG	2A	3319	1/1	0.97	0.14	78,78,78,78	0
56	MG	1a	3029	1/1	0.97	0.12	64,64,64,64	0
56	MG	1a	3135	1/1	0.97	0.10	82,82,82,82	0
56	MG	1a	3194	1/1	0.97	0.22	102,102,102,102	0
56	MG	2a	3149	1/1	0.97	0.09	74,74,74,74	0
56	MG	2a	3150	1/1	0.97	0.21	87,87,87,87	0
56	MG	1A	3106	1/1	0.97	0.26	63,63,63,63	0
56	MG	2A	3239	1/1	0.97	0.08	77,77,77,77	0
56	MG	2A	3021	1/1	0.97	0.43	98,98,98,98	0
56	MG	2A	3241	1/1	0.97	0.12	89,89,89,89	0
56	MG	1A	3093	1/1	0.97	0.15	73,73,73,73	0
56	MG	2A	3093	1/1	0.97	0.16	71,71,71,71	0
56	MG	2A	3023	1/1	0.97	0.07	71,71,71,71	0
56	MG	1a	3138	1/1	0.97	0.20	91,91,91,91	0
56	MG	1A	3619	1/1	0.97	0.15	86,86,86,86	0
56	MG	1A	3212	1/1	0.97	0.21	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3068	1/1	0.97	0.08	74,74,74,74	0
56	MG	1A	3510	1/1	0.97	0.17	64,64,64,64	0
56	MG	2A	3172	1/1	0.97	0.23	80,80,80,80	0
56	MG	1A	3146	1/1	0.97	0.17	62,62,62,62	0
56	MG	1a	3144	1/1	0.97	0.18	71,71,71,71	0
56	MG	2A	3175	1/1	0.97	0.16	65,65,65,65	0
56	MG	2A	3102	1/1	0.97	0.55	72,72,72,72	0
56	MG	1A	3215	1/1	0.97	0.15	49,49,49,49	0
56	MG	2A	3179	1/1	0.97	0.14	74,74,74,74	0
56	MG	1a	3038	1/1	0.97	0.12	88,88,88,88	0
56	MG	1A	3084	1/1	0.97	0.28	71,71,71,71	0
56	MG	2A	3345	1/1	0.97	0.60	77,77,77,77	0
56	MG	1a	3148	1/1	0.97	0.21	112,112,112,112	0
56	MG	1A	3217	1/1	0.97	0.11	60,60,60,60	0
56	MG	1A	3474	1/1	0.97	0.24	74,74,74,74	0
56	MG	1A	3628	1/1	0.97	0.16	56,56,56,56	0
56	MG	2A	3350	1/1	0.97	0.33	70,70,70,70	0
56	MG	1A	3475	1/1	0.97	0.30	88,88,88,88	0
56	MG	1A	3085	1/1	0.97	0.37	92,92,92,92	0
56	MG	1A	3307	1/1	0.97	0.28	60,60,60,60	0
56	MG	1A	3086	1/1	0.97	0.17	70,70,70,70	0
56	MG	1a	3156	1/1	0.97	0.19	73,73,73,73	0
56	MG	2A	3191	1/1	0.97	0.36	74,74,74,74	0
56	MG	1A	3680	1/1	0.97	0.19	85,85,85,85	0
57	ZN	1n	501	1/1	0.97	0.20	105,105,105,105	0
56	MG	1A	3448	1/1	0.97	0.15	78,78,78,78	0
56	MG	2A	3117	1/1	0.97	0.17	83,83,83,83	0
56	MG	1a	3002	1/1	0.97	0.12	83,83,83,83	0
57	ZN	2n	501	1/1	0.97	0.10	117,117,117,117	0
56	MG	1A	3604	1/1	0.98	0.14	67,67,67,67	0
56	MG	1A	3482	1/1	0.98	0.22	75,75,75,75	0
56	MG	2A	3064	1/1	0.98	0.34	82,82,82,82	0
56	MG	1a	3219	1/1	0.98	0.20	74,74,74,74	0
56	MG	1A	3632	1/1	0.98	0.16	63,63,63,63	0
56	MG	2A	3067	1/1	0.98	0.14	82,82,82,82	0
56	MG	1a	3221	1/1	0.98	0.20	79,79,79,79	0
56	MG	2A	3069	1/1	0.98	0.15	82,82,82,82	0
56	MG	1A	3069	1/1	0.98	0.90	67,67,67,67	0
56	MG	2a	3140	1/1	0.98	0.14	88,88,88,88	0
56	MG	2A	3163	1/1	0.98	0.22	79,79,79,79	0
56	MG	2A	3267	1/1	0.98	0.21	93,93,93,93	0
56	MG	1A	3507	1/1	0.98	0.25	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	3075	1/1	0.98	0.24	72,72,72,72	0
56	MG	1a	3076	1/1	0.98	0.21	58,58,58,58	0
56	MG	2A	3167	1/1	0.98	0.12	87,87,87,87	0
56	MG	1A	3532	1/1	0.98	0.09	88,88,88,88	0
56	MG	2A	3120	1/1	0.98	0.13	94,94,94,94	0
56	MG	2A	3030	1/1	0.98	0.11	81,81,81,81	0
56	MG	2A	3122	1/1	0.98	0.21	86,86,86,86	0
56	MG	1A	3259	1/1	0.98	0.20	54,54,54,54	0
56	MG	1a	3188	1/1	0.98	0.12	81,81,81,81	0
56	MG	2A	3224	1/1	0.98	0.18	62,62,62,62	0
56	MG	1A	3509	1/1	0.98	0.28	75,75,75,75	0
56	MG	1a	3080	1/1	0.98	0.17	88,88,88,88	0
56	MG	1a	3047	1/1	0.98	0.20	82,82,82,82	0
56	MG	1A	3667	1/1	0.98	0.45	68,68,68,68	0
56	MG	2A	3178	1/1	0.98	0.17	63,63,63,63	0
56	MG	2A	3339	1/1	0.98	0.14	92,92,92,92	0
56	MG	1A	3101	1/1	0.98	0.23	86,86,86,86	0
56	MG	2a	3045	1/1	0.98	0.08	102,102,102,102	0
56	MG	1A	3179	1/1	0.98	0.34	90,90,90,90	0
56	MG	1A	3262	1/1	0.98	0.22	64,64,64,64	0
56	MG	1A	3314	1/1	0.98	0.29	54,54,54,54	0
56	MG	2a	3165	1/1	0.98	0.08	116,116,116,116	0
56	MG	1a	3088	1/1	0.98	0.18	96,96,96,96	0
56	MG	1A	3451	1/1	0.98	0.11	85,85,85,85	0
56	MG	1A	3435	1/1	0.98	0.17	59,59,59,59	0
56	MG	1a	3200	1/1	0.98	0.17	83,83,83,83	0
56	MG	1A	3129	1/1	0.98	0.16	93,93,93,93	0
56	MG	1A	3517	1/1	0.98	0.20	77,77,77,77	0
56	MG	1A	3646	1/1	0.98	0.31	92,92,92,92	0
56	MG	1a	3129	1/1	0.98	0.11	88,88,88,88	0
56	MG	1A	3276	1/1	0.98	0.24	64,64,64,64	0
56	MG	1A	3345	1/1	0.98	0.15	66,66,66,66	0
56	MG	1A	3456	1/1	0.98	0.25	96,96,96,96	0
56	MG	2A	3300	1/1	0.98	0.35	79,79,79,79	0
56	MG	1A	3072	1/1	0.98	0.47	67,67,67,67	0
56	MG	1A	3097	1/1	0.98	0.11	94,94,94,94	0
56	MG	1A	3477	1/1	0.98	0.15	56,56,56,56	0
56	MG	1A	3089	1/1	0.98	0.66	59,59,59,59	0
56	MG	2a	3065	1/1	0.98	0.17	83,83,83,83	0
56	MG	1A	3200	1/1	0.98	0.22	63,63,63,63	0
57	ZN	1Y	501	1/1	0.98	0.18	100,100,100,100	0
56	MG	2A	3306	1/1	0.98	0.19	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3125	1/1	0.98	0.14	75,75,75,75	0
56	MG	1A	3655	1/1	0.98	0.35	67,67,67,67	0
56	MG	1A	3502	1/1	0.98	0.27	61,61,61,61	0
56	MG	2A	3059	1/1	0.98	0.12	93,93,93,93	0
56	MG	1A	3046	1/1	0.98	0.09	54,54,54,54	0
56	MG	1A	3247	1/1	0.98	0.10	55,55,55,55	0
56	MG	1a	3177	1/1	0.99	0.14	73,73,73,73	0
56	MG	2A	3225	1/1	0.99	0.27	75,75,75,75	0
56	MG	1A	3375	1/1	0.99	0.24	62,62,62,62	0
56	MG	1A	3057	1/1	0.99	0.16	79,79,79,79	0
56	MG	1A	3102	1/1	0.99	0.12	78,78,78,78	0
56	MG	1A	3064	1/1	0.99	0.17	84,84,84,84	0
56	MG	1a	3227	1/1	0.99	0.33	64,64,64,64	0
56	MG	1A	3379	1/1	0.99	0.26	55,55,55,55	0
56	MG	1A	3135	1/1	0.99	0.10	59,59,59,59	0
56	MG	2A	3250	1/1	0.99	0.24	65,65,65,65	0
56	MG	1A	3111	1/1	0.99	0.10	83,83,83,83	0
56	MG	2A	3288	1/1	0.99	0.19	71,71,71,71	0
56	MG	1a	3086	1/1	0.99	0.33	76,76,76,76	0
57	ZN	15	501	1/1	0.99	0.21	87,87,87,87	0
56	MG	1A	3073	1/1	0.99	0.25	81,81,81,81	0
57	ZN	19	501	1/1	0.99	0.25	77,77,77,77	0
56	MG	1A	3013	1/1	0.99	0.25	69,69,69,69	0
56	MG	1A	3028	1/1	0.99	0.23	68,68,68,68	0
56	MG	1A	3107	1/1	0.99	0.27	81,81,81,81	0
57	ZN	25	501	1/1	0.99	0.23	97,97,97,97	0
57	ZN	26	501	1/1	0.99	0.26	98,98,98,98	0
56	MG	1A	3485	1/1	0.99	0.18	61,61,61,61	0
56	MG	1A	3498	1/1	0.99	0.14	85,85,85,85	0
58	SF4	1d	501	8/8	0.99	0.23	76,91,99,101	0
58	SF4	2d	501	8/8	0.99	0.18	95,106,118,119	0

6.5 Other polymers (i)

There are no such residues in this entry.