Full wwPDB X-ray Structure Validation Report

Jul 29, 2024 – 07:28 PM EDT

PDB ID	:	8UVS
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with spectinomycin derivative 2694, mRNA, deacylated A- and E-site tRNAphe, and deacylated P-site tRNAmet at 2.75A resolution
Authors	:	Killam, B.Y.; Phelps, G.A.; Lee, R.E.; Polikanov, Y.S.
Deposited on	:	2023-11-03
Resolution	:	2.75 Å(reported)

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

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

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

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

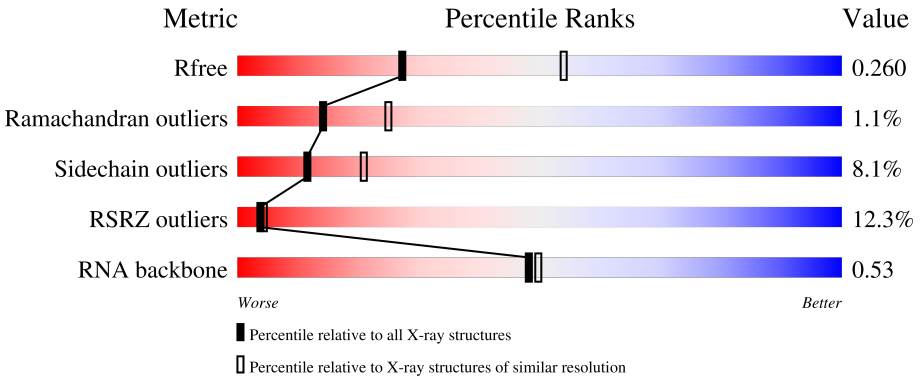
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.75 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	1235 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)
RNA backbone	3102	1060 (3.02-2.50)

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% 82% 16%
1	2A	2915	4% 79% 16%
2	1B	121	93% 7%
2	2B	121	69% 30%

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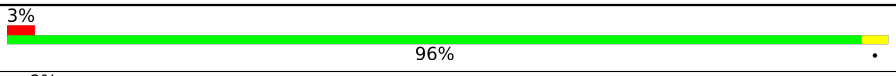
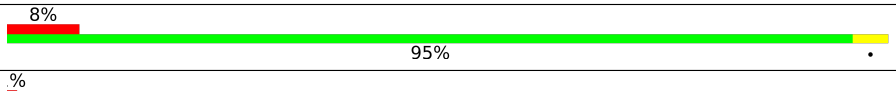
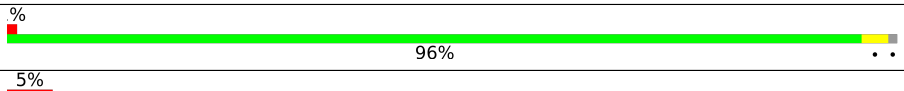
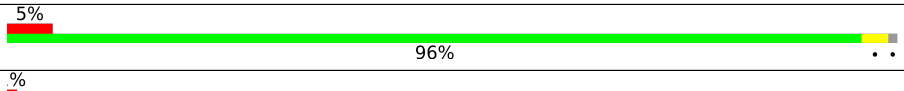
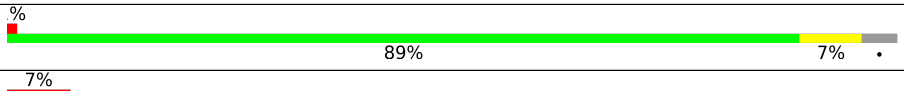
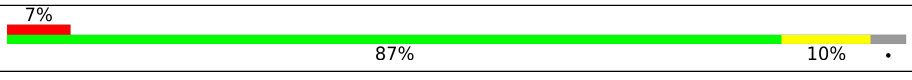
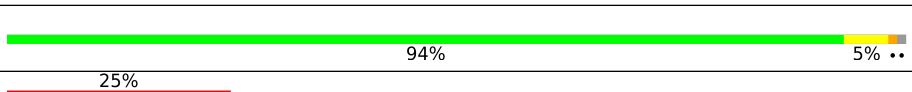
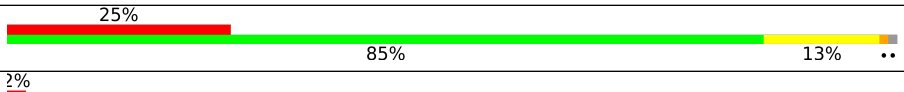
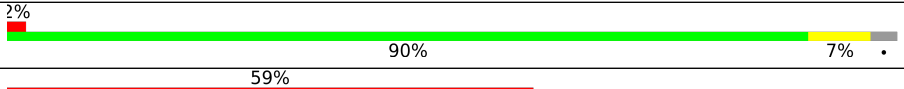
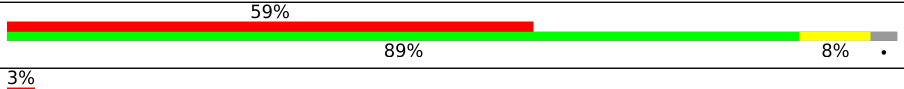
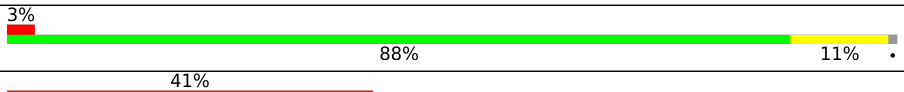
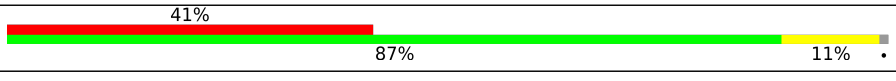
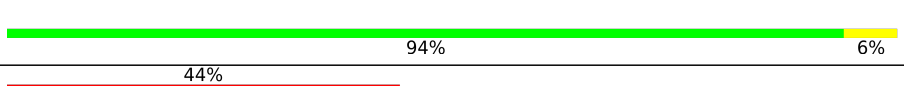
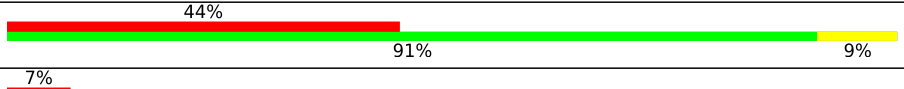
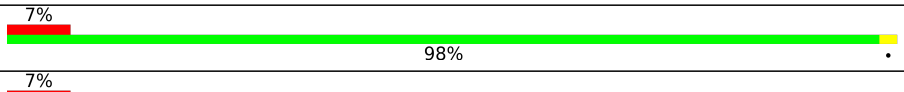
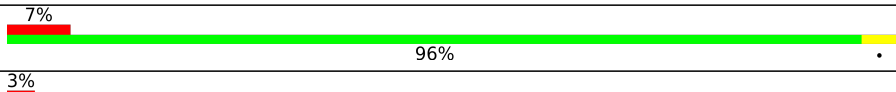
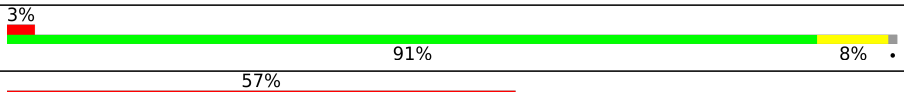
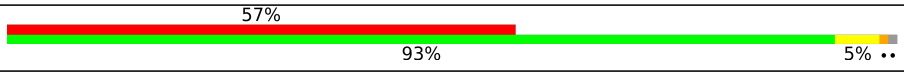
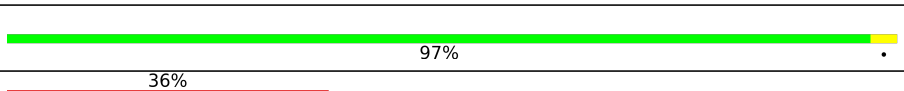
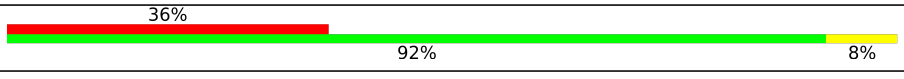
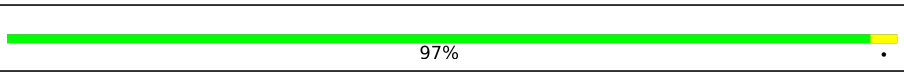
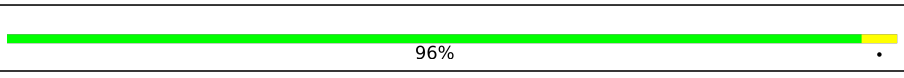
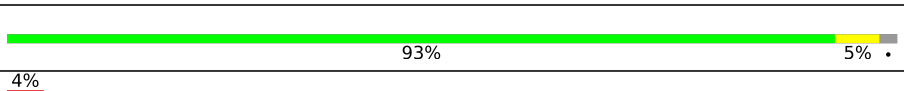
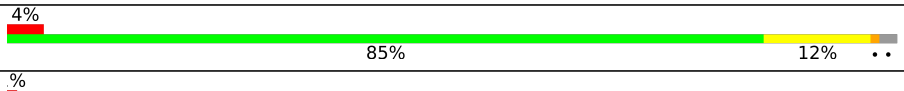
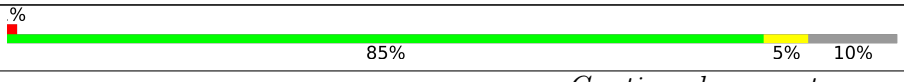
Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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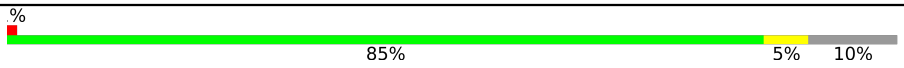
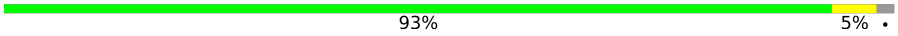
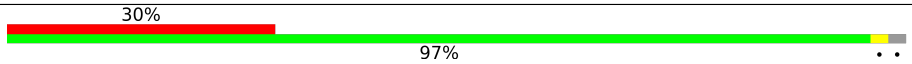
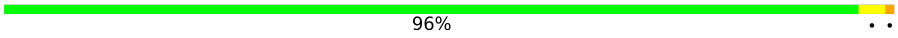
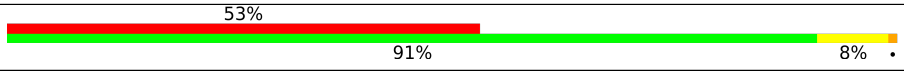
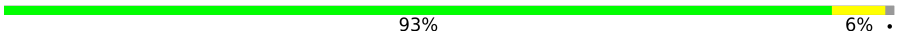
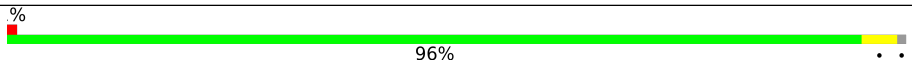
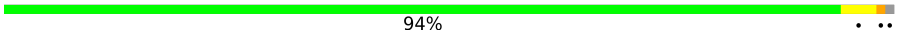
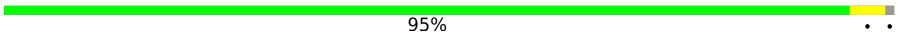
Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
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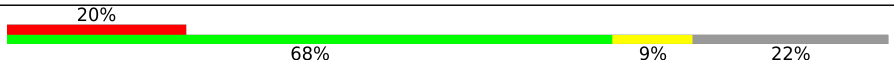
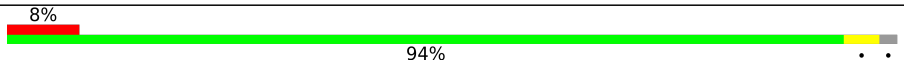
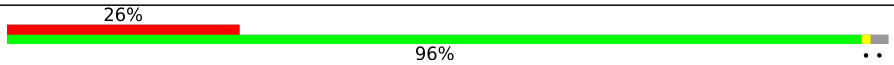
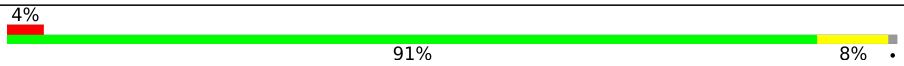
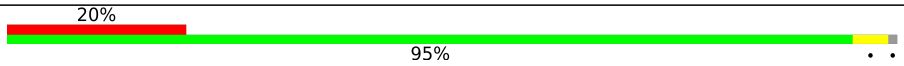
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
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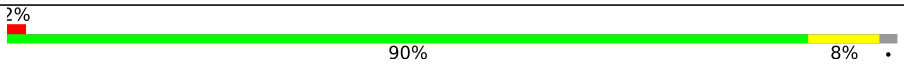
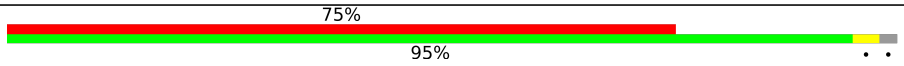
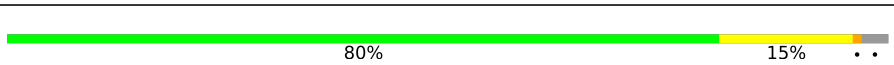
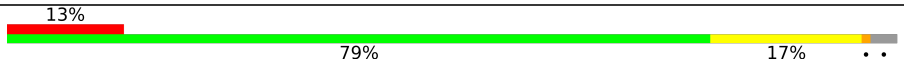
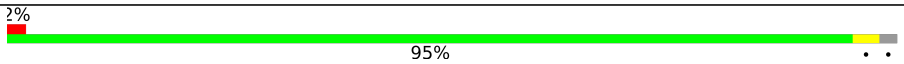
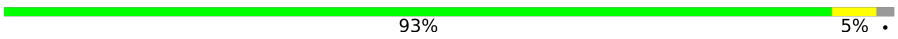
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	

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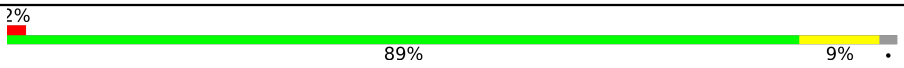
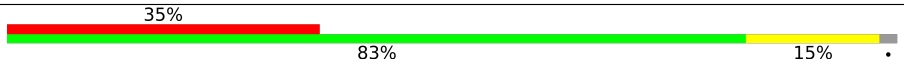
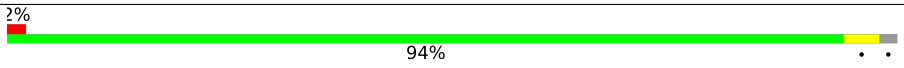
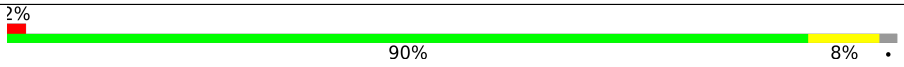
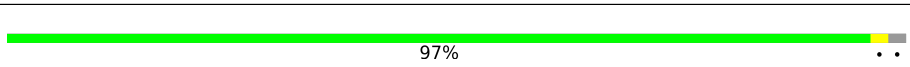
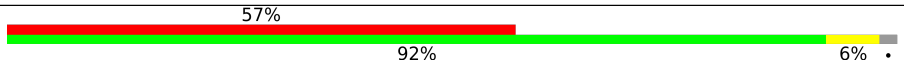
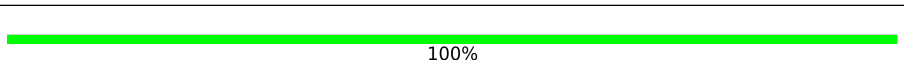
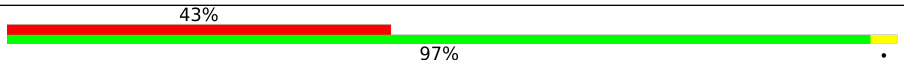
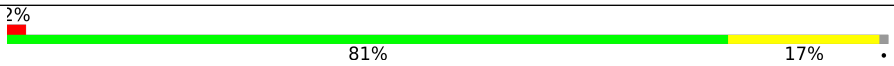
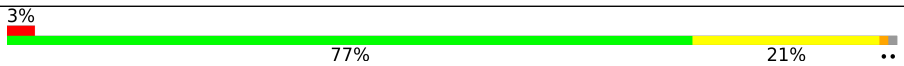
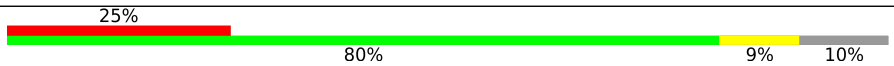
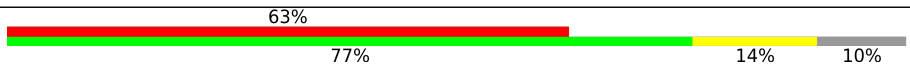
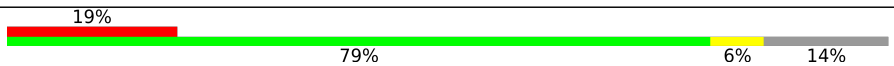
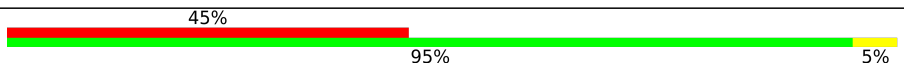
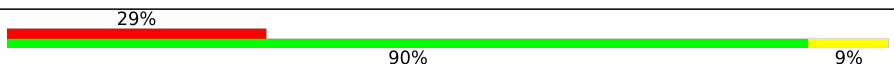
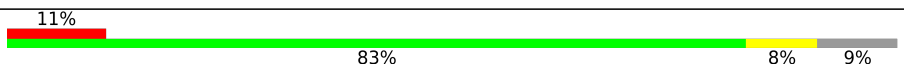
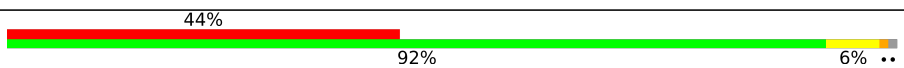
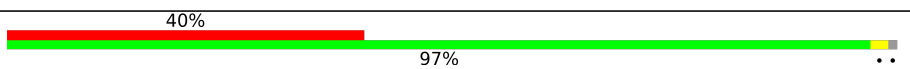
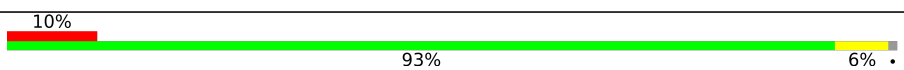
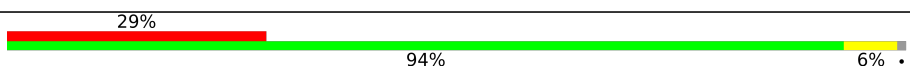
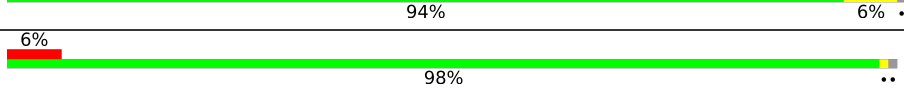
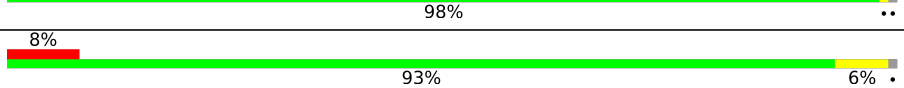
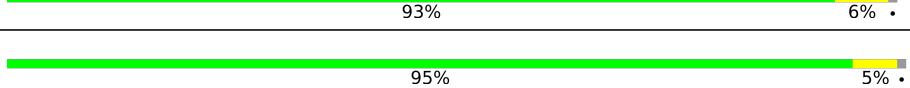
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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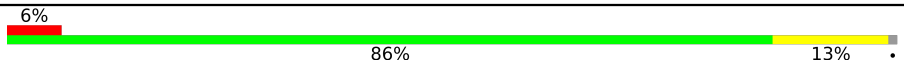
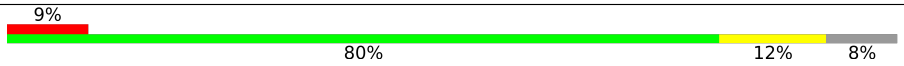
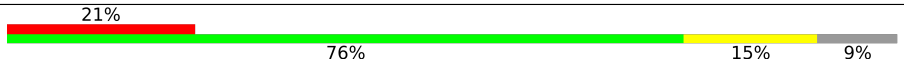
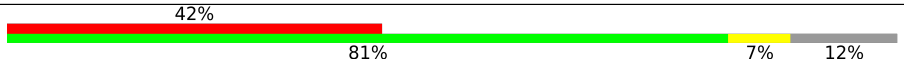
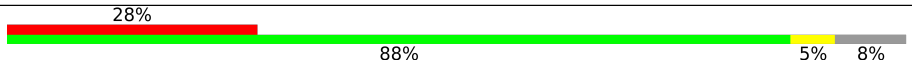
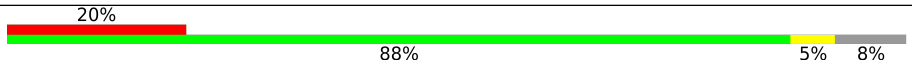
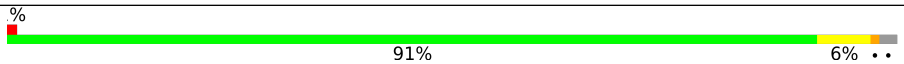
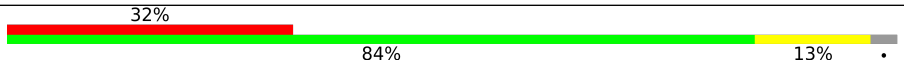
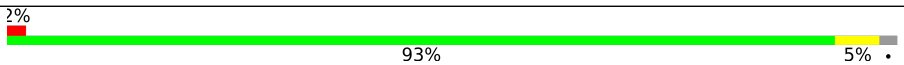
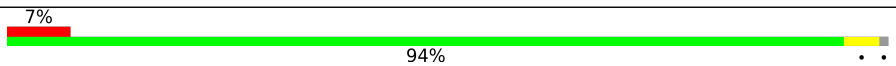
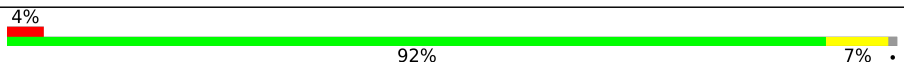
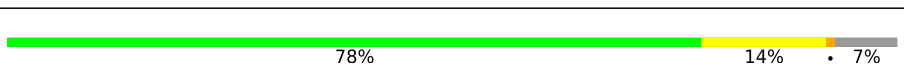
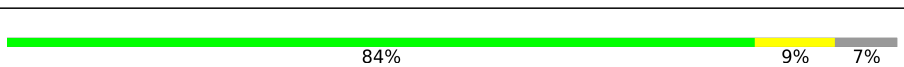
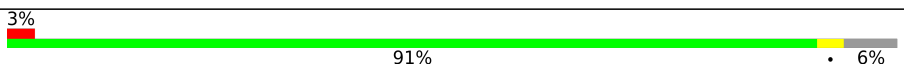
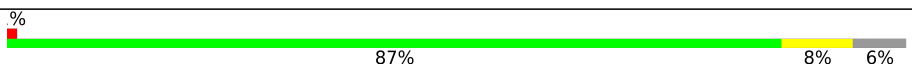
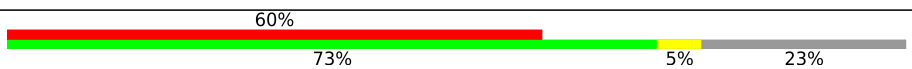
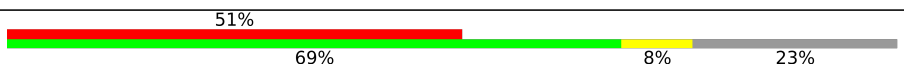
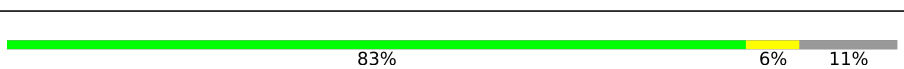
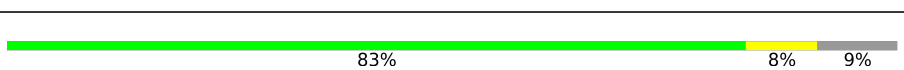
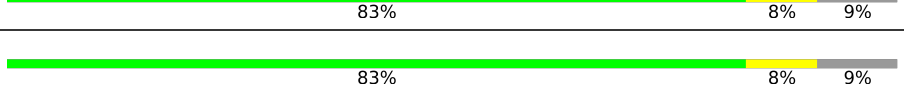
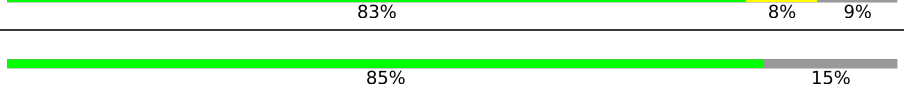
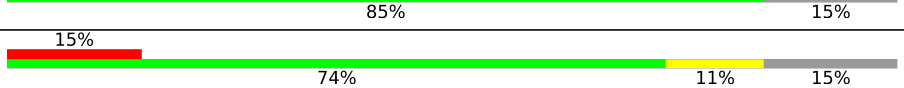
Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1v	24	17% 50% 46%
53	2v	24	33% 42% 12% 46%
54	1w	76	45% 57% 37%
54	1y	76	38% 53% 36% 9%
54	2w	76	76% 53% 39% 5%
54	2y	76	70% 58% 32% 7%
55	1x	77	4% 74% 23%
55	2x	77	25% 77% 21%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	G7M	2w	46	-	-	-	X
54	PSU	2w	55	-	-	-	X
54	4SU	2w	8	-	-	-	X
54	G7M	2y	46	-	-	-	X
54	5MU	2y	54	-	-	-	X
56	MG	10	102	-	-	-	X
56	MG	1A	3056	-	-	-	X
56	MG	1A	3125	-	-	-	X
56	MG	1A	3140	-	-	-	X
56	MG	1A	3263	-	-	-	X
56	MG	1A	3292	-	-	-	X
56	MG	1A	3325	-	-	-	X
56	MG	1A	3363	-	-	-	X
56	MG	1A	3368	-	-	-	X
56	MG	1A	3375	-	-	-	X
56	MG	1A	3391	-	-	-	X
56	MG	1A	3408	-	-	-	X
56	MG	1A	3409	-	-	-	X
56	MG	1A	3992	-	-	-	X
56	MG	1A	4035	-	-	-	X
56	MG	1A	4078	-	-	-	X
56	MG	1D	313	-	-	-	X
56	MG	1O	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1w	107	-	-	-	X
56	MG	28	101	-	-	-	X
56	MG	2A	3025	-	-	-	X
56	MG	2A	3067	-	-	-	X
56	MG	2A	3145	-	-	-	X
56	MG	2A	3162	-	-	-	X
56	MG	2A	3185	-	-	-	X
56	MG	2A	3192	-	-	-	X
56	MG	2A	3194	-	-	-	X
56	MG	2A	3212	-	-	-	X
56	MG	2A	3215	-	-	-	X
56	MG	2A	3218	-	-	-	X
56	MG	2A	3220	-	-	-	X
56	MG	2A	3230	-	-	-	X
56	MG	2A	3234	-	-	-	X
56	MG	2A	3235	-	-	-	X
56	MG	2A	3249	-	-	-	X
56	MG	2A	3271	-	-	-	X
56	MG	2A	3274	-	-	-	X
56	MG	2A	3283	-	-	-	X
56	MG	2A	3319	-	-	-	X
56	MG	2A	3325	-	-	-	X
56	MG	2A	3341	-	-	-	X
56	MG	2A	3354	-	-	-	X
56	MG	2A	3395	-	-	-	X
56	MG	2A	3499	-	-	-	X
56	MG	2A	3581	-	-	-	X
56	MG	2A	3591	-	-	-	X
56	MG	2A	3619	-	-	-	X
56	MG	2A	3648	-	-	-	X
56	MG	2A	3664	-	-	-	X
56	MG	2A	3763	-	-	-	X
56	MG	2A	3880	-	-	-	X
56	MG	2A	3884	-	-	-	X
56	MG	2B	202	-	-	-	X
56	MG	2Q	202	-	-	-	X
56	MG	2a	1621	-	-	-	X
56	MG	2a	1704	-	-	-	X
56	MG	2a	1822	-	-	-	X
56	MG	2g	201	-	-	-	X
56	MG	2w	105	-	-	-	X
56	MG	2w	107	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2y	101	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 300806 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	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	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 MF-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	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 Deacylated tRNAmet.

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	1139	Total	Mg	0	0
			1139	1139		
56	1B	37	Total	Mg	0	0
			37	37		
56	1D	13	Total	Mg	0	0
			13	13		
56	1E	14	Total	Mg	0	0
			14	14		
56	1F	13	Total	Mg	0	0
			13	13		
56	1G	5	Total	Mg	0	0
			5	5		
56	1I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1N	6	Total Mg 6 6	0	0
56	1O	6	Total Mg 6 6	0	0
56	1P	5	Total Mg 5 5	0	0
56	1Q	7	Total Mg 7 7	0	0
56	1R	3	Total Mg 3 3	0	0
56	1S	3	Total Mg 3 3	0	0
56	1T	4	Total Mg 4 4	0	0
56	1U	10	Total Mg 10 10	0	0
56	1V	7	Total Mg 7 7	0	0
56	1W	7	Total Mg 7 7	0	0
56	1X	5	Total Mg 5 5	0	0
56	1Y	4	Total Mg 4 4	0	0
56	1Z	3	Total Mg 3 3	0	0
56	10	8	Total Mg 8 8	0	0
56	11	4	Total Mg 4 4	0	0
56	12	2	Total Mg 2 2	0	0
56	13	6	Total Mg 6 6	0	0
56	15	4	Total Mg 4 4	0	0
56	16	2	Total Mg 2 2	0	0
56	17	4	Total Mg 4 4	0	0
56	18	7	Total Mg 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	19	1	Total Mg 1 1	0	0
56	1a	241	Total Mg 241 241	0	0
56	1b	2	Total Mg 2 2	0	0
56	1e	2	Total Mg 2 2	0	0
56	1f	2	Total Mg 2 2	0	0
56	1h	1	Total Mg 1 1	0	0
56	1l	2	Total Mg 2 2	0	0
56	1m	1	Total Mg 1 1	0	0
56	1n	1	Total Mg 1 1	0	0
56	1s	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1v	2	Total Mg 2 2	0	0
56	1w	9	Total Mg 9 9	0	0
56	1x	14	Total Mg 14 14	0	0
56	1y	2	Total Mg 2 2	0	0
56	2A	884	Total Mg 884 884	0	0
56	2B	20	Total Mg 20 20	0	0
56	2D	7	Total Mg 7 7	0	0
56	2E	6	Total Mg 6 6	0	0
56	2F	6	Total Mg 6 6	0	0
56	2G	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2N	1	Total Mg 1 1	0	0
56	2O	2	Total Mg 2 2	0	0
56	2P	2	Total Mg 2 2	0	0
56	2Q	3	Total Mg 3 3	0	0
56	2R	3	Total Mg 3 3	0	0
56	2T	3	Total Mg 3 3	0	0
56	2U	2	Total Mg 2 2	0	0
56	2V	2	Total Mg 2 2	0	0
56	2W	2	Total Mg 2 2	0	0
56	2X	3	Total Mg 3 3	0	0
56	2Y	1	Total Mg 1 1	0	0
56	2Z	1	Total Mg 1 1	0	0
56	20	3	Total Mg 3 3	0	0
56	21	2	Total Mg 2 2	0	0
56	23	2	Total Mg 2 2	0	0
56	25	5	Total Mg 5 5	0	0
56	26	1	Total Mg 1 1	0	0
56	27	4	Total Mg 4 4	0	0
56	28	3	Total Mg 3 3	0	0
56	2a	240	Total Mg 240 240	0	0
56	2d	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2e	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	2g	1	Total Mg 1 1	0	0
56	2j	1	Total Mg 1 1	0	0
56	2k	1	Total Mg 1 1	0	0
56	2l	4	Total Mg 4 4	0	0
56	2m	1	Total Mg 1 1	0	0
56	2p	1	Total Mg 1 1	0	0
56	2q	2	Total Mg 2 2	0	0
56	2r	1	Total Mg 1 1	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	1	Total Mg 1 1	0	0
56	2w	9	Total Mg 9 9	0	0
56	2x	7	Total Mg 7 7	0	0
56	2y	7	Total Mg 7 7	0	0

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

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

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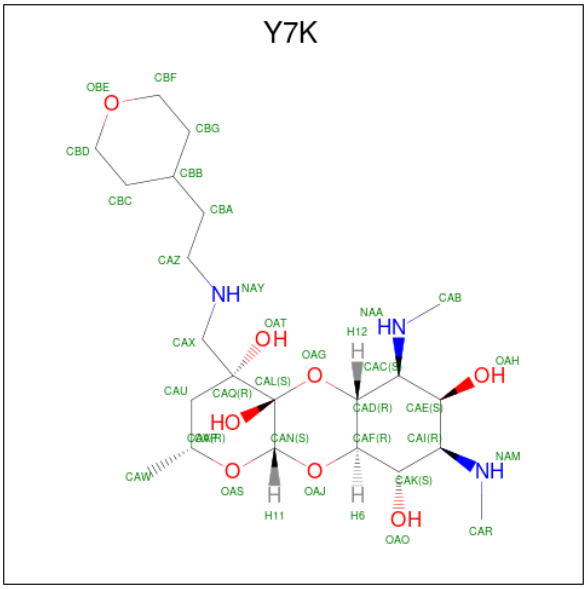
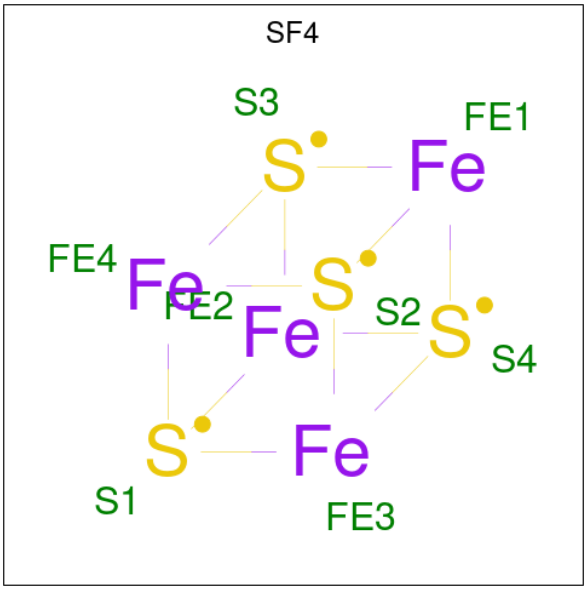
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	19	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	2Y	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0
57	25	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0
57	29	1	Total Zn 1 1	0	0
57	2n	1	Total Zn 1 1	0	0

- Molecule 58 is (2R,4R,4aS,5aR,6S,7S,8R,9S,9aR,10aS)-2-methyl-6,8-bis(methylamino)-4-({[2-(oxan-4-yl)ethyl]amino}methyl)octahydro-2H-pyrano[2,3-b][1,4]benzodioxine-4,4a,7,9(10aH)-tetrol (three-letter code: Y7K) (formula: $C_{22}H_{41}N_3O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1a	1	Total C N O 33 22 3 8	0	0
58	2a	1	Total C N O 33 22 3 8	0	0

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



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

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1x	1	Total K 1 1	0	0
60	2A	1	Total K 1 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2188	Total O 2188 2188	0	0
61	1B	68	Total O 68 68	0	0
61	1D	33	Total O 33 33	0	0
61	1E	30	Total O 30 30	0	0
61	1F	18	Total O 18 18	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	3	Total O 3 3	0	0
61	1H	2	Total O 2 2	0	0
61	1I	1	Total O 1 1	0	0
61	1N	8	Total O 8 8	0	0
61	1O	4	Total O 4 4	0	0
61	1P	20	Total O 20 20	0	0
61	1Q	10	Total O 10 10	0	0
61	1R	12	Total O 12 12	0	0
61	1S	6	Total O 6 6	0	0
61	1T	8	Total O 8 8	0	0
61	1U	17	Total O 17 17	0	0
61	1V	11	Total O 11 11	0	0
61	1W	8	Total O 8 8	0	0
61	1X	7	Total O 7 7	0	0
61	1Y	2	Total O 2 2	0	0
61	1Z	1	Total O 1 1	0	0
61	10	13	Total O 13 13	0	0
61	11	11	Total O 11 11	0	0
61	12	4	Total O 4 4	0	0
61	13	3	Total O 3 3	0	0
61	14	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	15	8	Total O 8 8	0	0
61	16	1	Total O 1 1	0	0
61	17	9	Total O 9 9	0	0
61	18	11	Total O 11 11	0	0
61	1a	498	Total O 498 498	0	0
61	1c	2	Total O 2 2	0	0
61	1d	1	Total O 1 1	0	0
61	1e	4	Total O 4 4	0	0
61	1f	1	Total O 1 1	0	0
61	1g	3	Total O 3 3	0	0
61	1i	1	Total O 1 1	0	0
61	1j	1	Total O 1 1	0	0
61	1l	8	Total O 8 8	0	0
61	1m	1	Total O 1 1	0	0
61	1n	1	Total O 1 1	0	0
61	1o	1	Total O 1 1	0	0
61	1p	1	Total O 1 1	0	0
61	1q	3	Total O 3 3	0	0
61	1u	1	Total O 1 1	0	0
61	1v	7	Total O 7 7	0	0
61	1w	14	Total O 14 14	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1x	19	Total O 19 19	0	0
61	1y	1	Total O 1 1	0	0
61	2A	1294	Total O 1294 1294	0	0
61	2B	27	Total O 27 27	0	0
61	2D	24	Total O 24 24	0	0
61	2E	15	Total O 15 15	0	0
61	2F	13	Total O 13 13	0	0
61	2I	3	Total O 3 3	0	0
61	2N	1	Total O 1 1	0	0
61	2O	2	Total O 2 2	0	0
61	2P	16	Total O 16 16	0	0
61	2Q	2	Total O 2 2	0	0
61	2R	3	Total O 3 3	0	0
61	2T	6	Total O 6 6	0	0
61	2U	4	Total O 4 4	0	0
61	2W	3	Total O 3 3	0	0
61	2X	2	Total O 2 2	0	0
61	2Y	1	Total O 1 1	0	0
61	2Z	1	Total O 1 1	0	0
61	20	3	Total O 3 3	0	0
61	21	8	Total O 8 8	0	0

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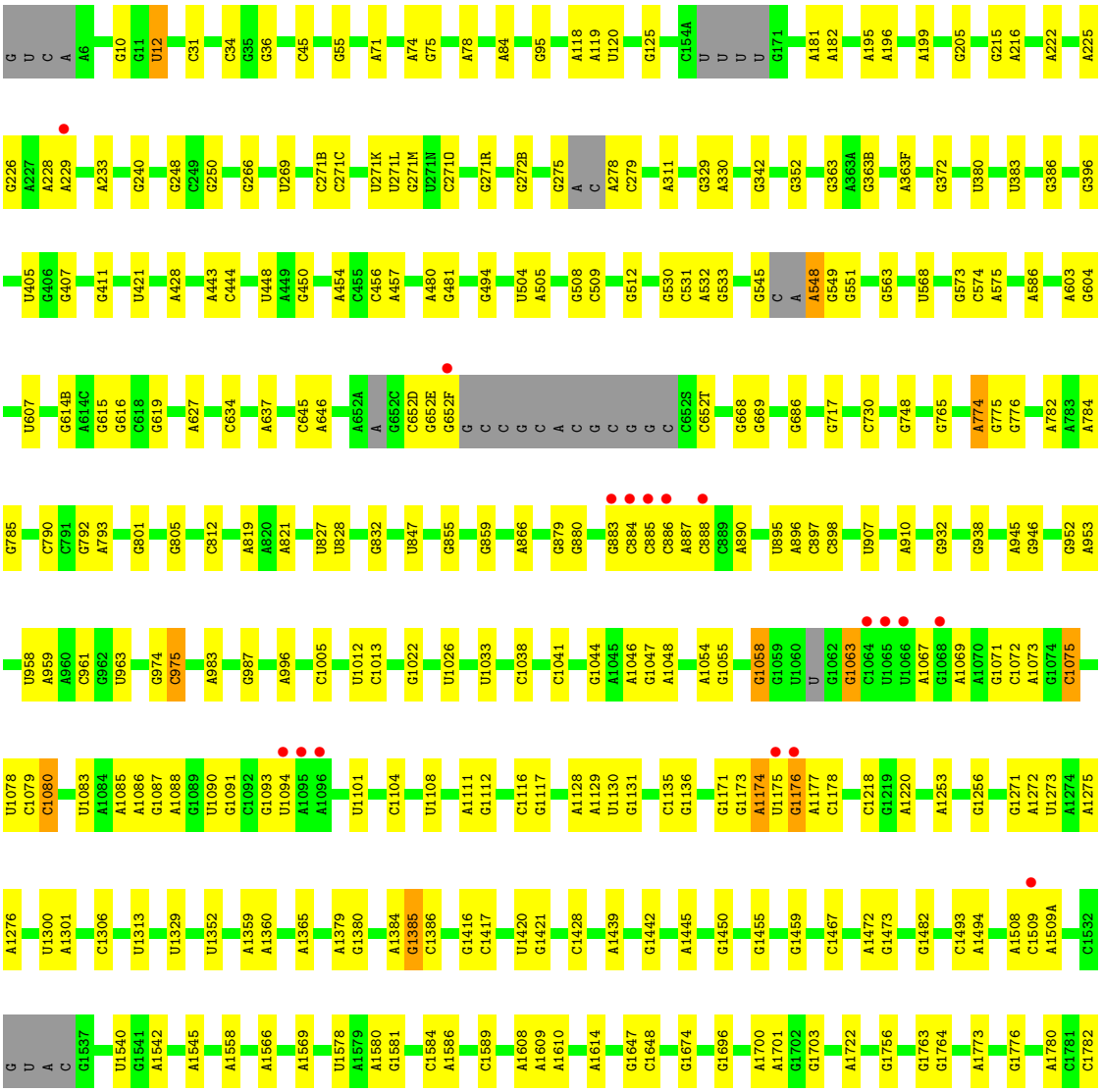
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	23	3	Total O 3 3	0	0
61	25	1	Total O 1 1	0	0
61	26	1	Total O 1 1	0	0
61	27	3	Total O 3 3	0	0
61	28	3	Total O 3 3	0	0
61	29	1	Total O 1 1	0	0
61	2a	296	Total O 296 296	0	0
61	2c	1	Total O 1 1	0	0
61	2d	2	Total O 2 2	0	0
61	2e	1	Total O 1 1	0	0
61	2f	1	Total O 1 1	0	0
61	2j	3	Total O 3 3	0	0
61	2l	4	Total O 4 4	0	0
61	2n	1	Total O 1 1	0	0
61	2p	2	Total O 2 2	0	0
61	2r	1	Total O 1 1	0	0
61	2t	2	Total O 2 2	0	0
61	2v	1	Total O 1 1	0	0
61	2w	4	Total O 4 4	0	0
61	2x	5	Total O 5 5	0	0
61	2y	15	Total O 15 15	0	0

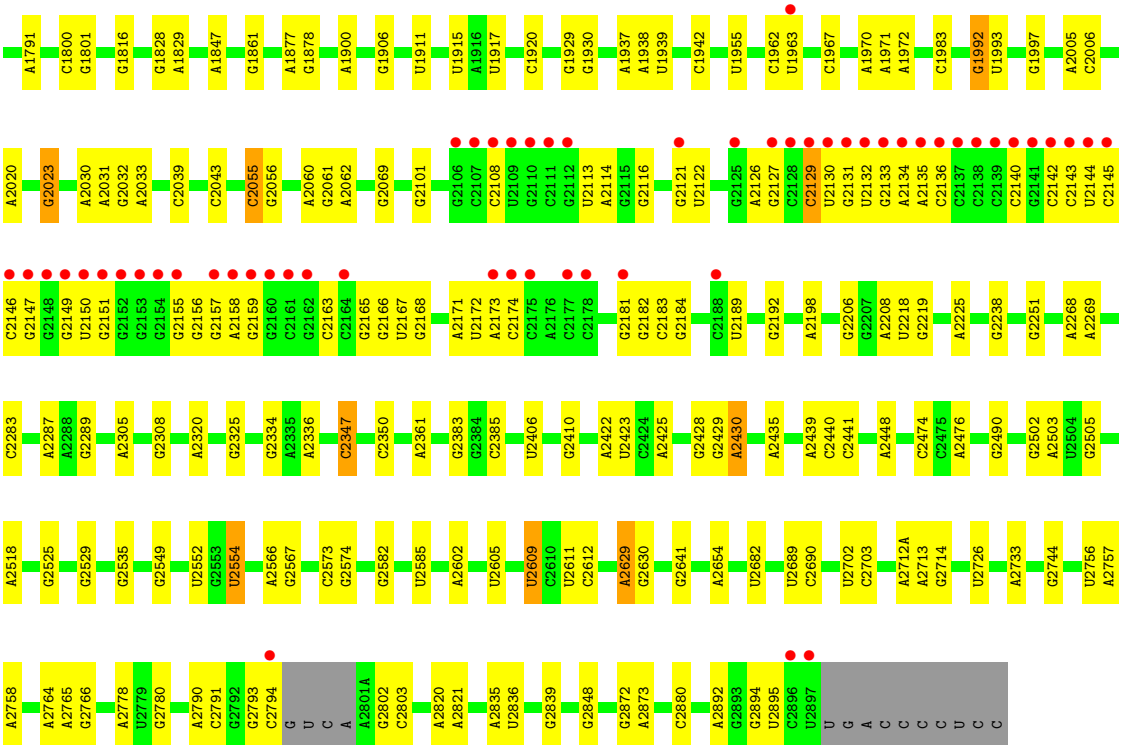
3 Residue-property plots (i)

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

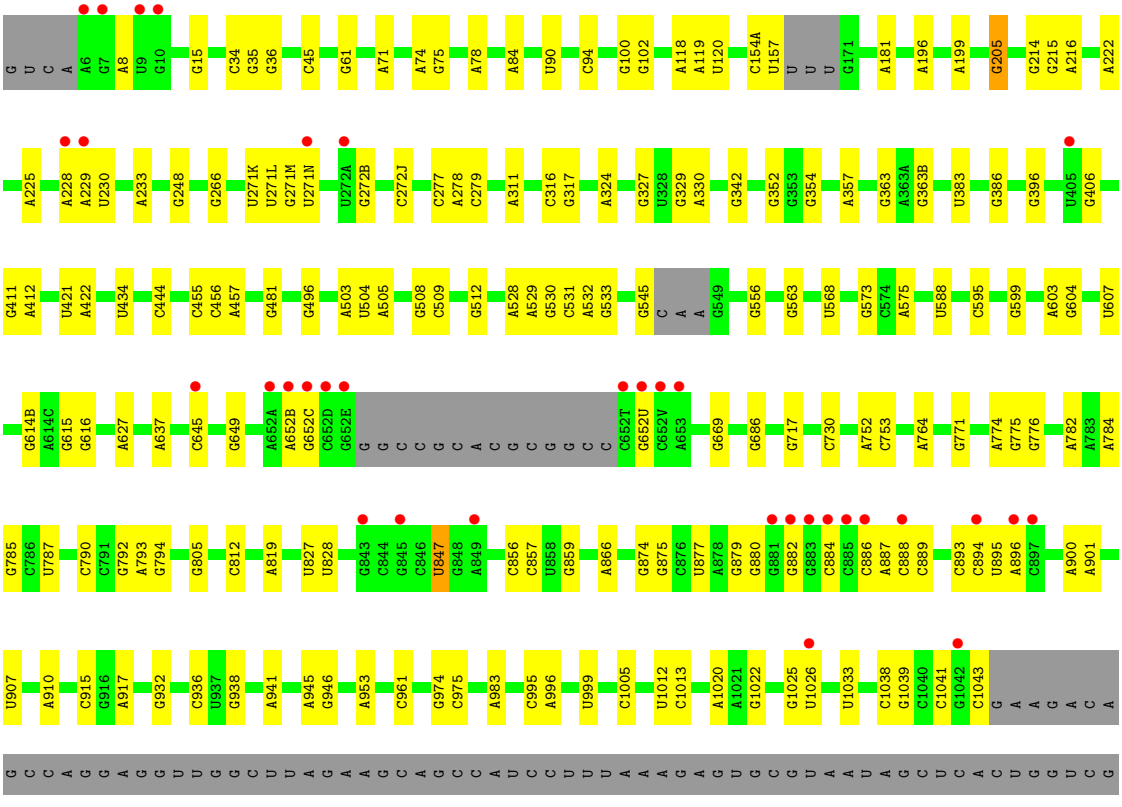
Chain 1A:

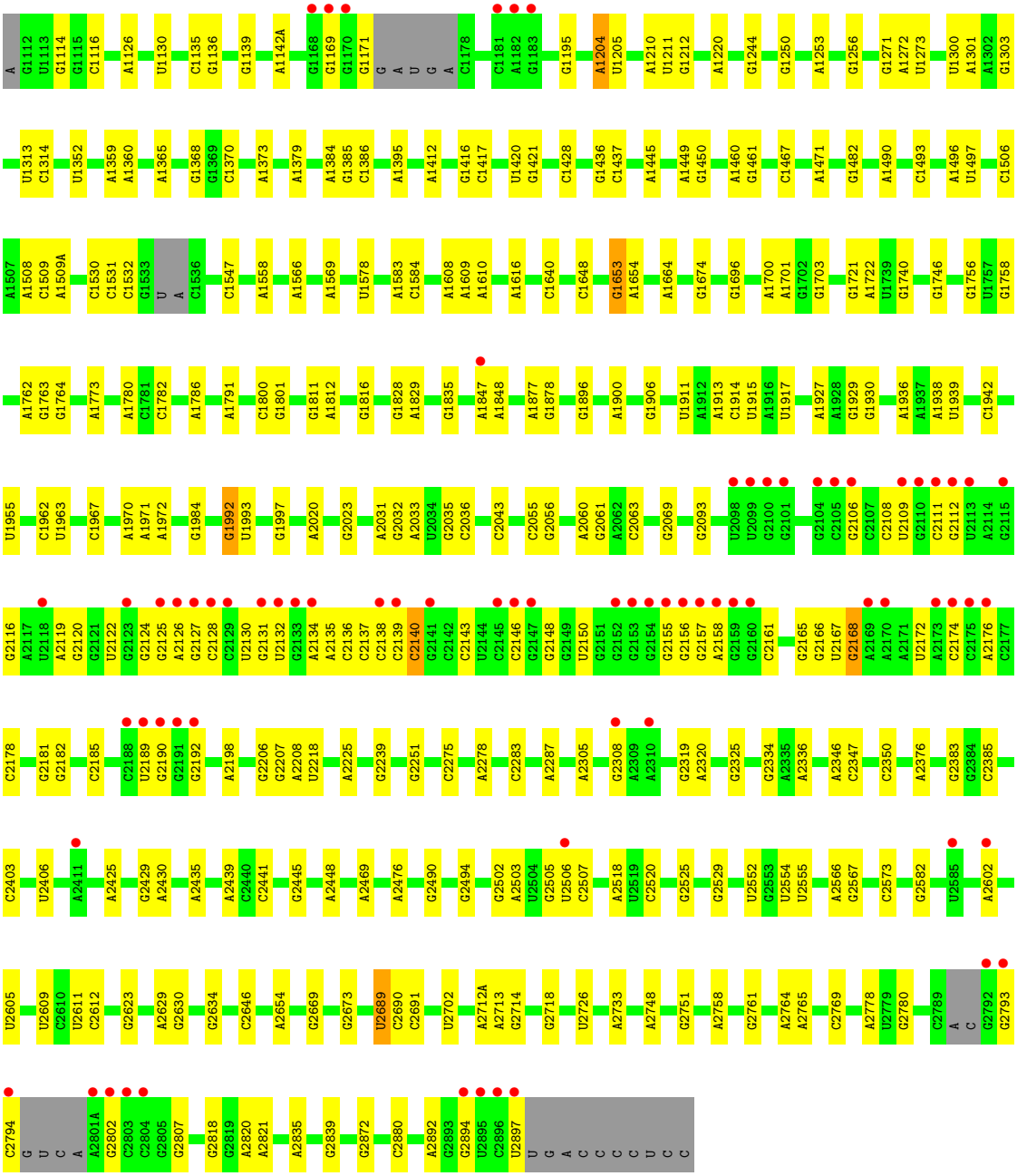




• Molecule 1: 23S Ribosomal RNA

Chain 2A:



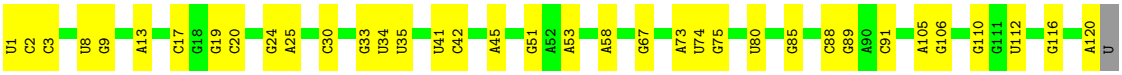


• Molecule 2: 5S Ribosomal RNA

Chain 1B:

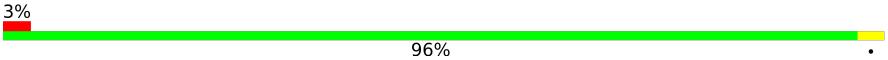
• Molecule 2: 5S Ribosomal RNA

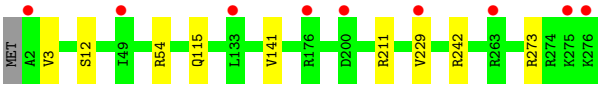
Chain 2B:



• Molecule 3: 50S ribosomal protein L2

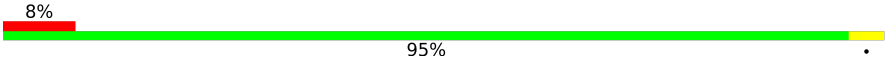
Chain 1D:

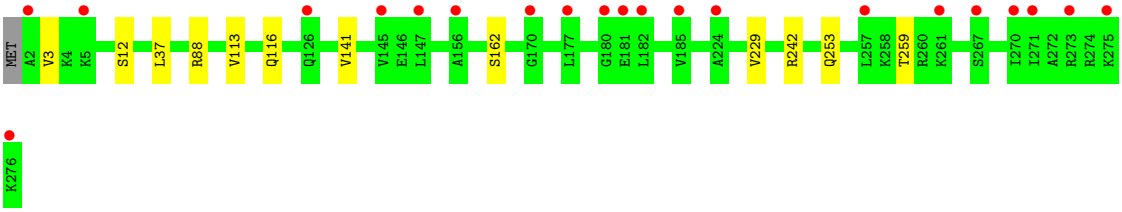




• Molecule 3: 50S ribosomal protein L2

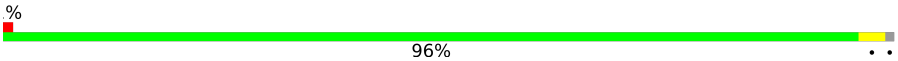
Chain 2D:





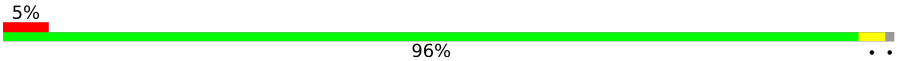
• Molecule 4: 50S ribosomal protein L3

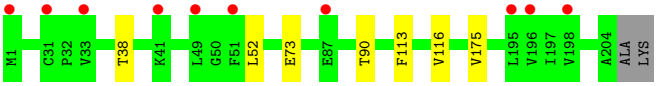
Chain 1E:



• Molecule 4: 50S ribosomal protein L3

Chain 2E:



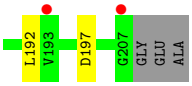


• Molecule 5: 50S ribosomal protein L4

Chain 1F:

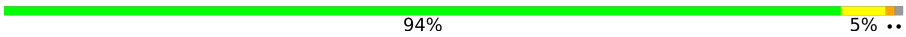
• Molecule 5: 50S ribosomal protein L4

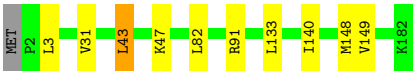
Chain 2F:



• Molecule 6: 50S ribosomal protein L5

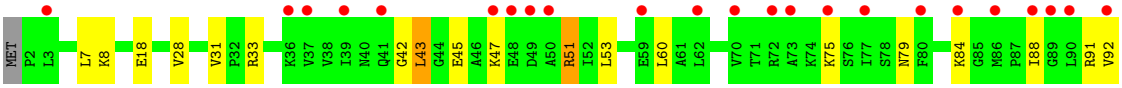
Chain 1G:

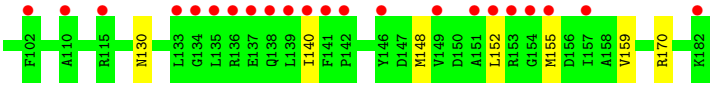




• Molecule 6: 50S ribosomal protein L5

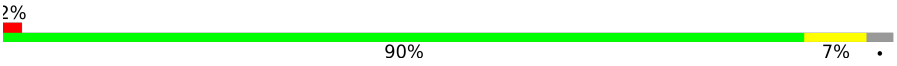
Chain 2G:

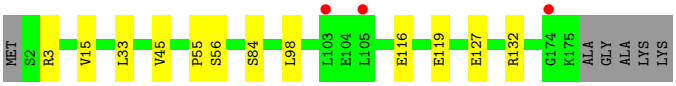




• Molecule 7: 50S ribosomal protein L6

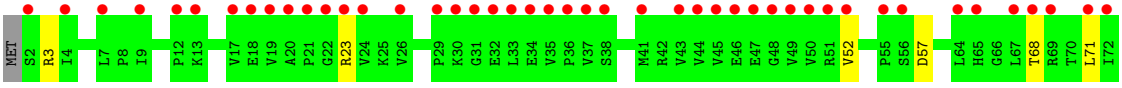
Chain 1H:

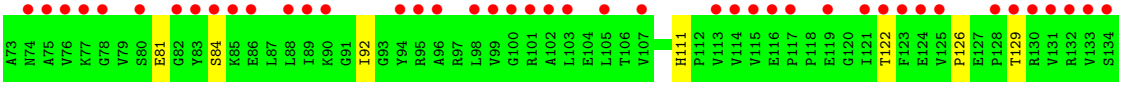


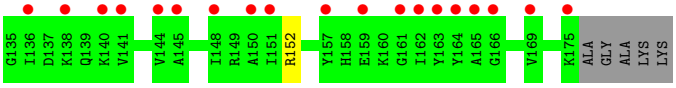


• Molecule 7: 50S ribosomal protein L6

Chain 2H:





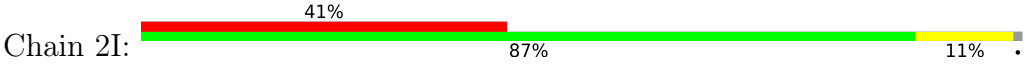


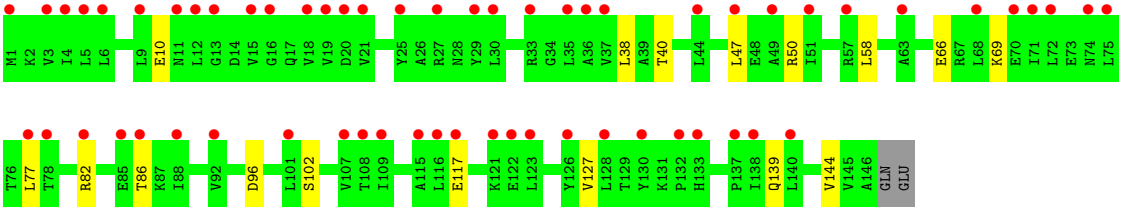
• Molecule 8: 50S ribosomal protein L9

Chain 1I:

• Molecule 8: 50S ribosomal protein L9

Chain 2I:



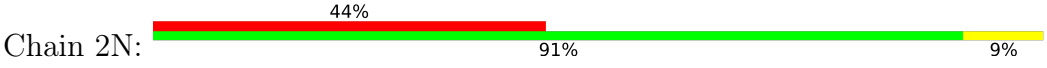


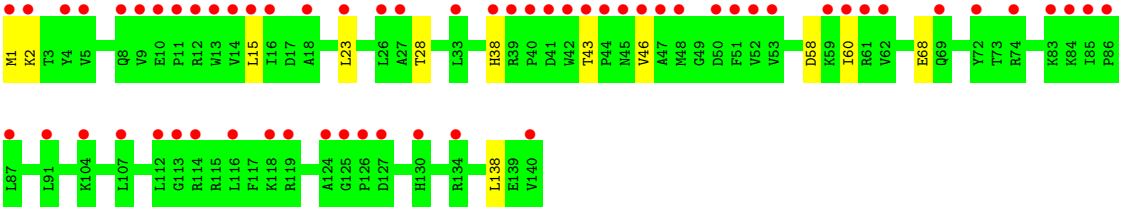
• Molecule 9: 50S ribosomal protein L13

Chain 1N:

• Molecule 9: 50S ribosomal protein L13

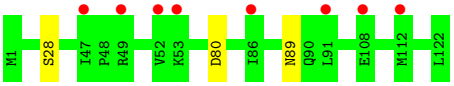
Chain 2N:





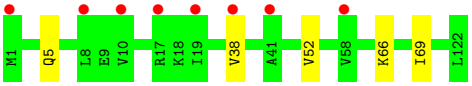
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



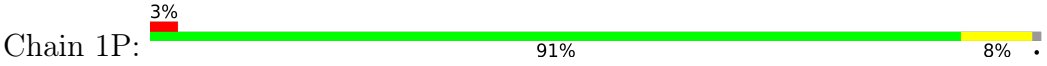
• Molecule 10: 50S ribosomal protein L14

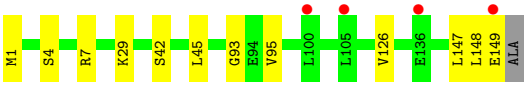
Chain 2O:



• Molecule 11: 50S ribosomal protein L15

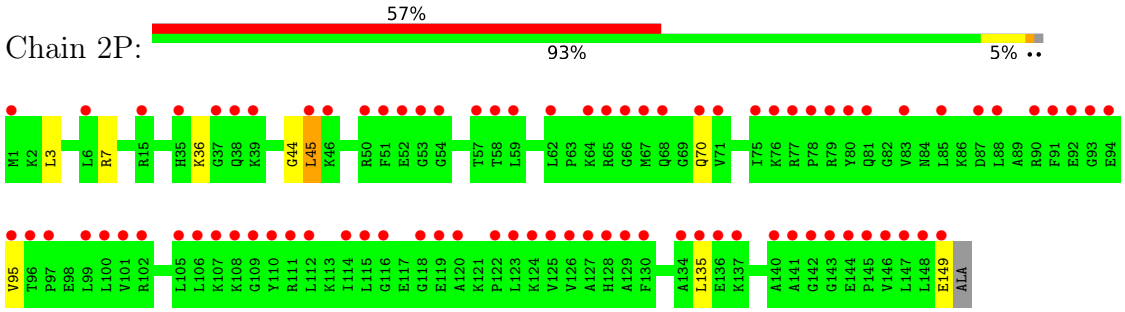
Chain 1P:





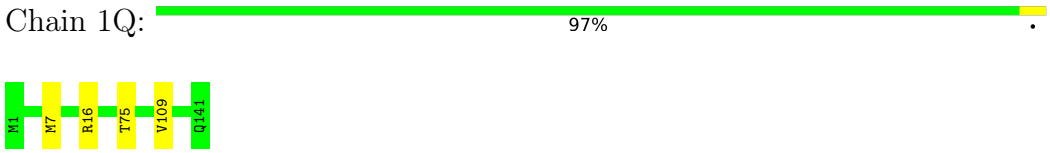
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



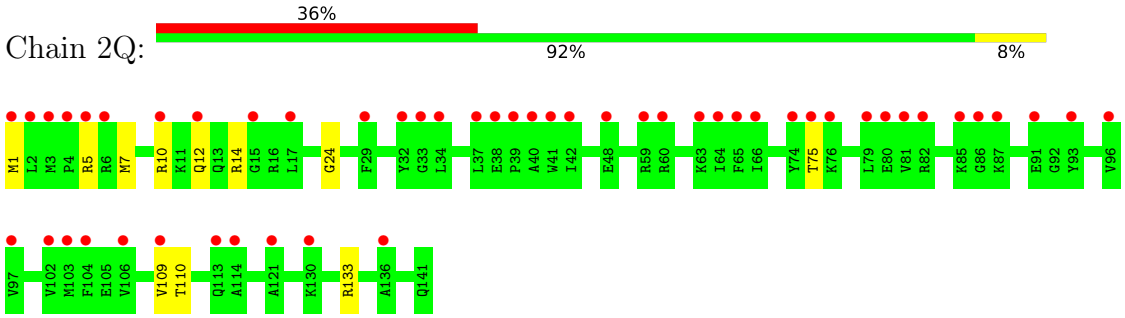
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



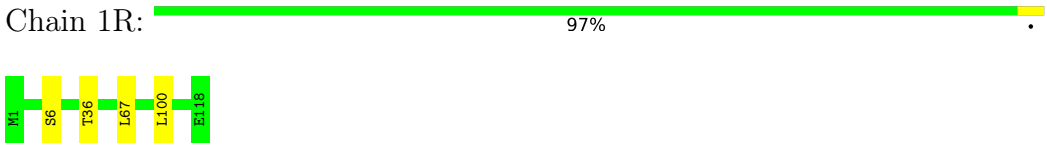
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



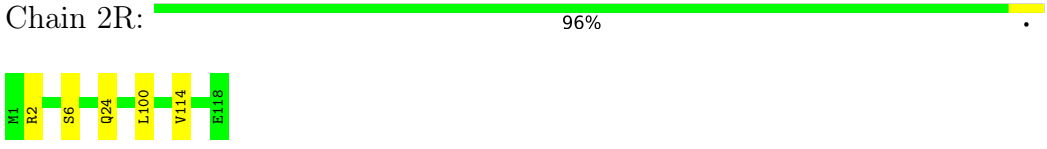
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



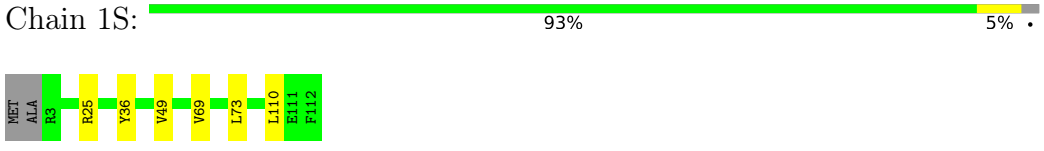
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



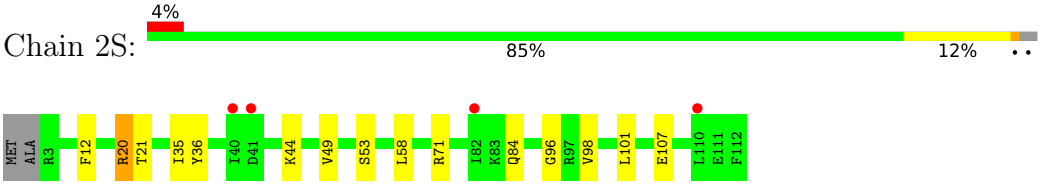
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



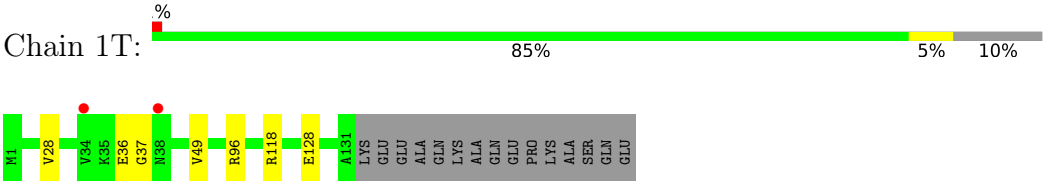
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



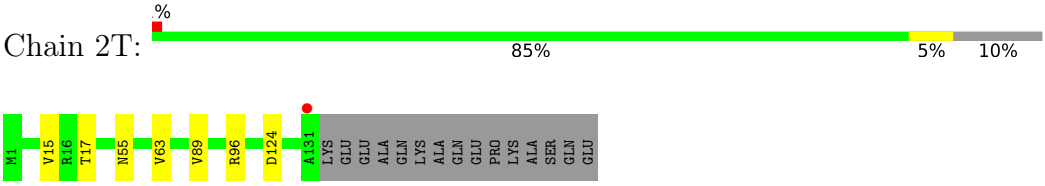
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



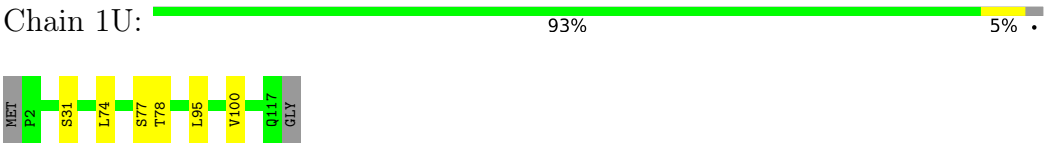
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



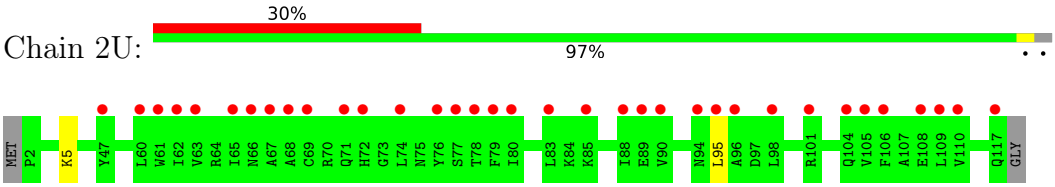
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



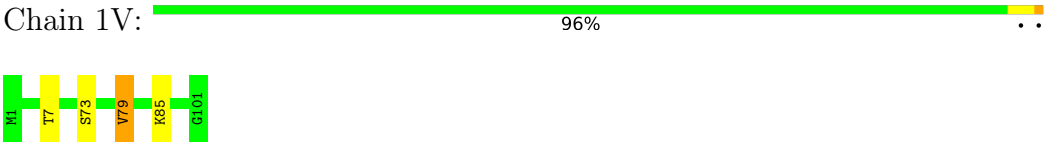
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



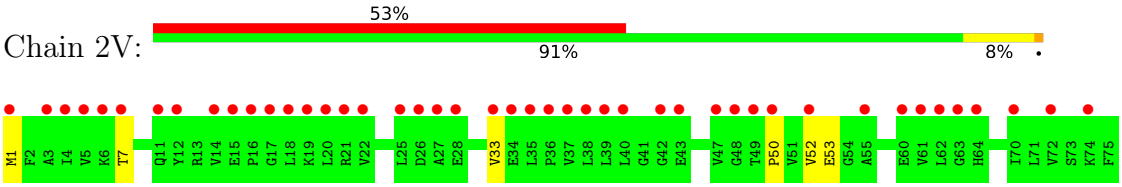
• Molecule 17: 50S ribosomal protein L21

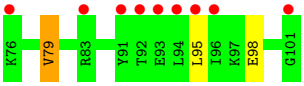
Chain 1V:



• Molecule 17: 50S ribosomal protein L21

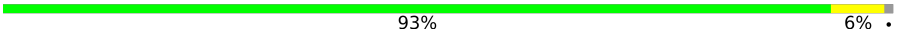
Chain 2V:

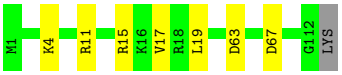




• Molecule 18: 50S ribosomal protein L22

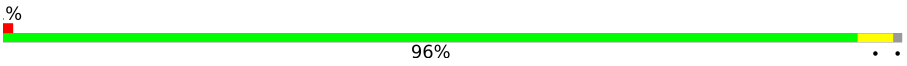
Chain 1W:





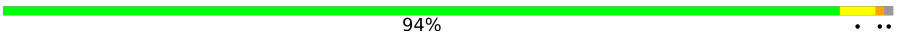
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



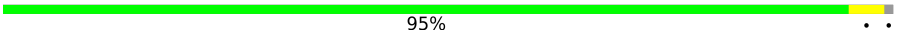
• Molecule 19: 50S ribosomal protein L23

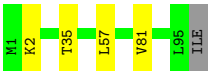
Chain 1X:



• Molecule 19: 50S ribosomal protein L23

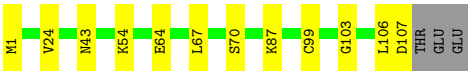
Chain 2X:





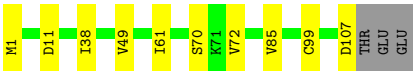
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



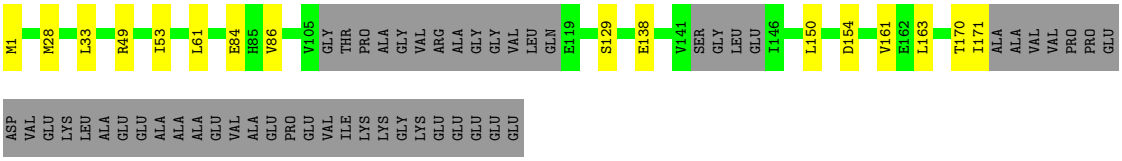
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



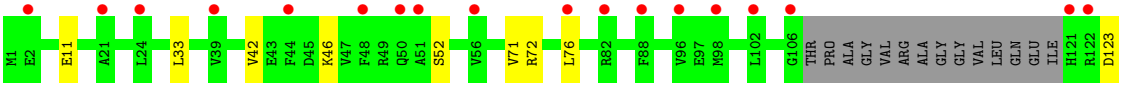
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



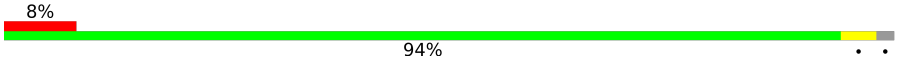
• Molecule 21: 50S ribosomal protein L25

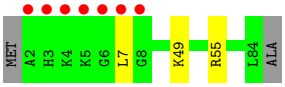
Chain 2Z:



• Molecule 22: 50S ribosomal protein L27

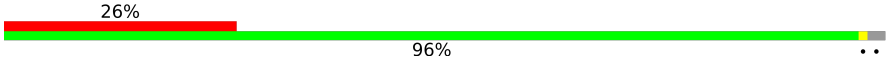
Chain 10:

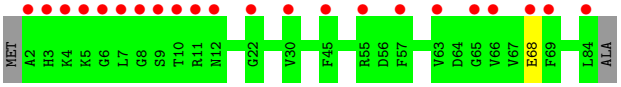




• Molecule 22: 50S ribosomal protein L27

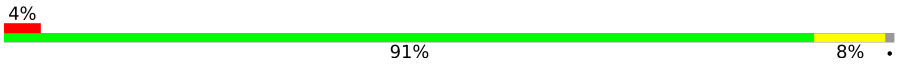
Chain 20:

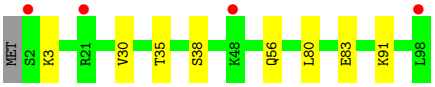




• Molecule 23: 50S ribosomal protein L28

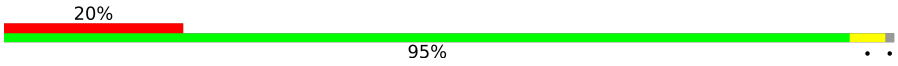
Chain 11:

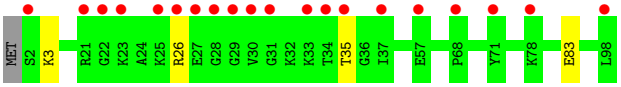




• Molecule 23: 50S ribosomal protein L28

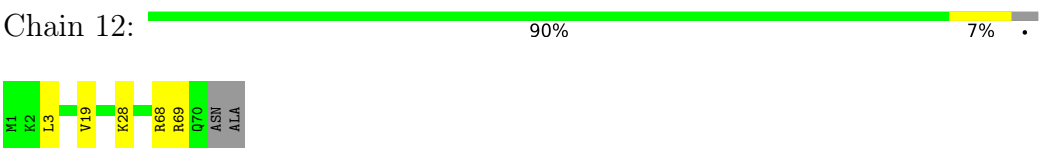
Chain 21:





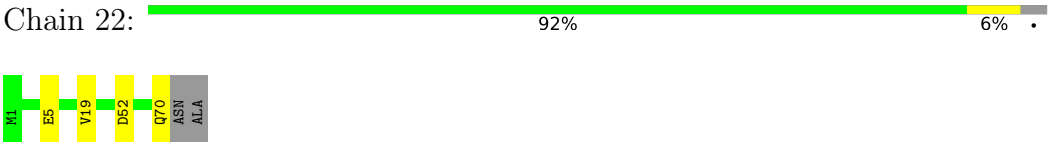
• Molecule 24: 50S ribosomal protein L29

Chain 12:



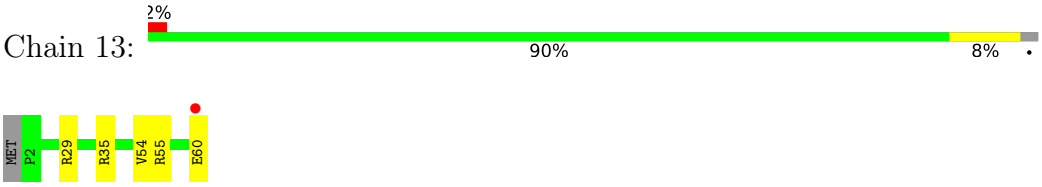
• Molecule 24: 50S ribosomal protein L29

Chain 22:



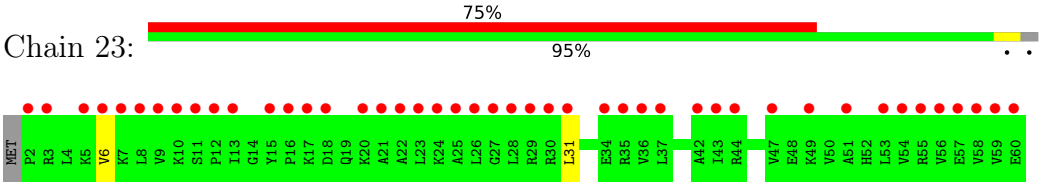
• Molecule 25: 50S ribosomal protein L30

Chain 13:



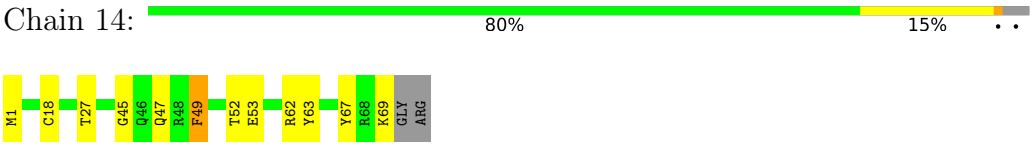
• Molecule 25: 50S ribosomal protein L30

Chain 23:



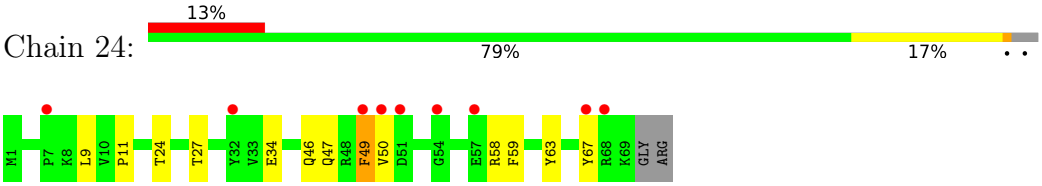
• Molecule 26: 50S ribosomal protein L31

Chain 14:



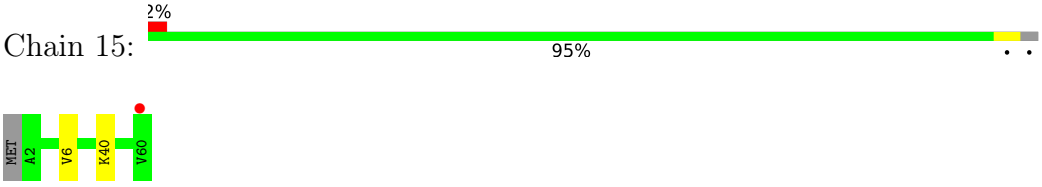
• Molecule 26: 50S ribosomal protein L31

Chain 24:



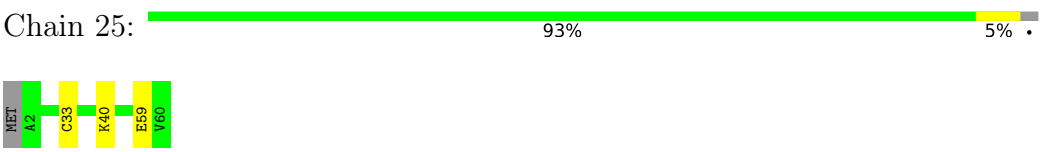
• Molecule 27: 50S ribosomal protein L32

Chain 15:



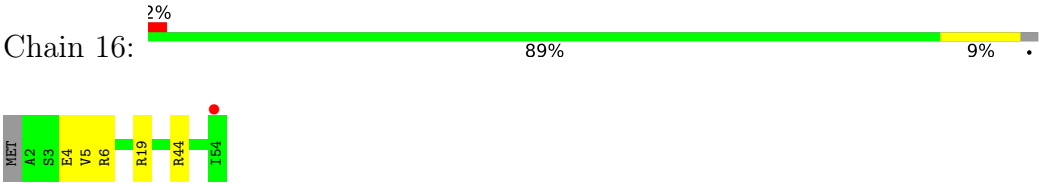
• Molecule 27: 50S ribosomal protein L32

Chain 25:



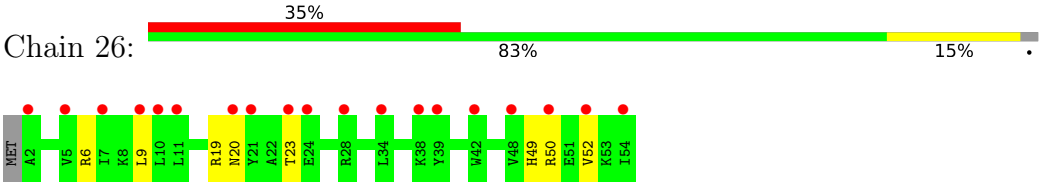
• Molecule 28: 50S ribosomal protein L33

Chain 16:



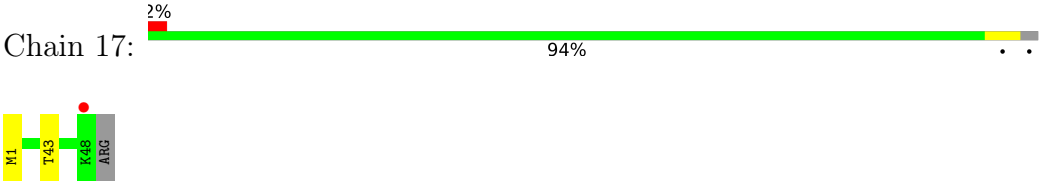
• Molecule 28: 50S ribosomal protein L33

Chain 26:



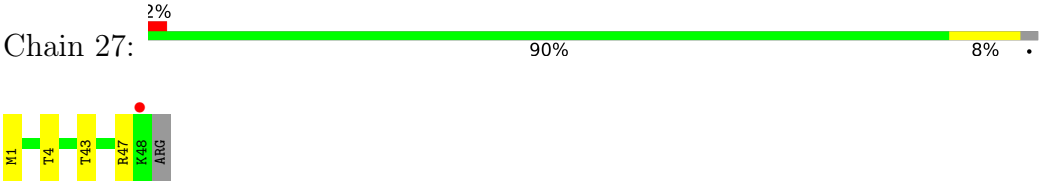
• Molecule 29: 50S ribosomal protein L34

Chain 17:



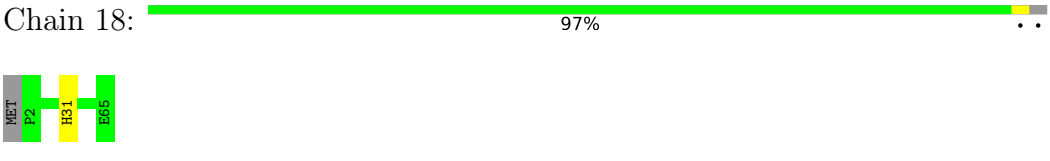
• Molecule 29: 50S ribosomal protein L34

Chain 27:



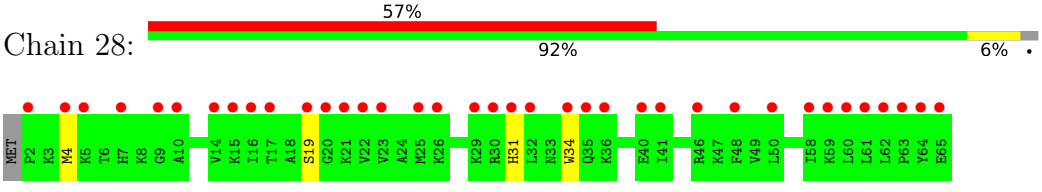
• Molecule 30: 50S ribosomal protein L35

Chain 18:



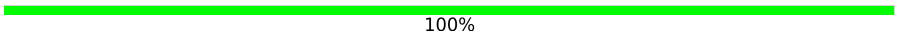
• Molecule 30: 50S ribosomal protein L35

Chain 28:



• Molecule 31: 50S ribosomal protein L36

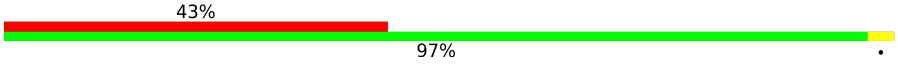
Chain 19:

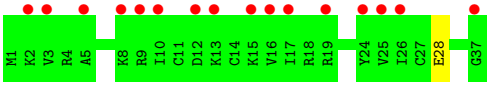


There are no outlier residues recorded for this chain.

• Molecule 31: 50S ribosomal protein L36

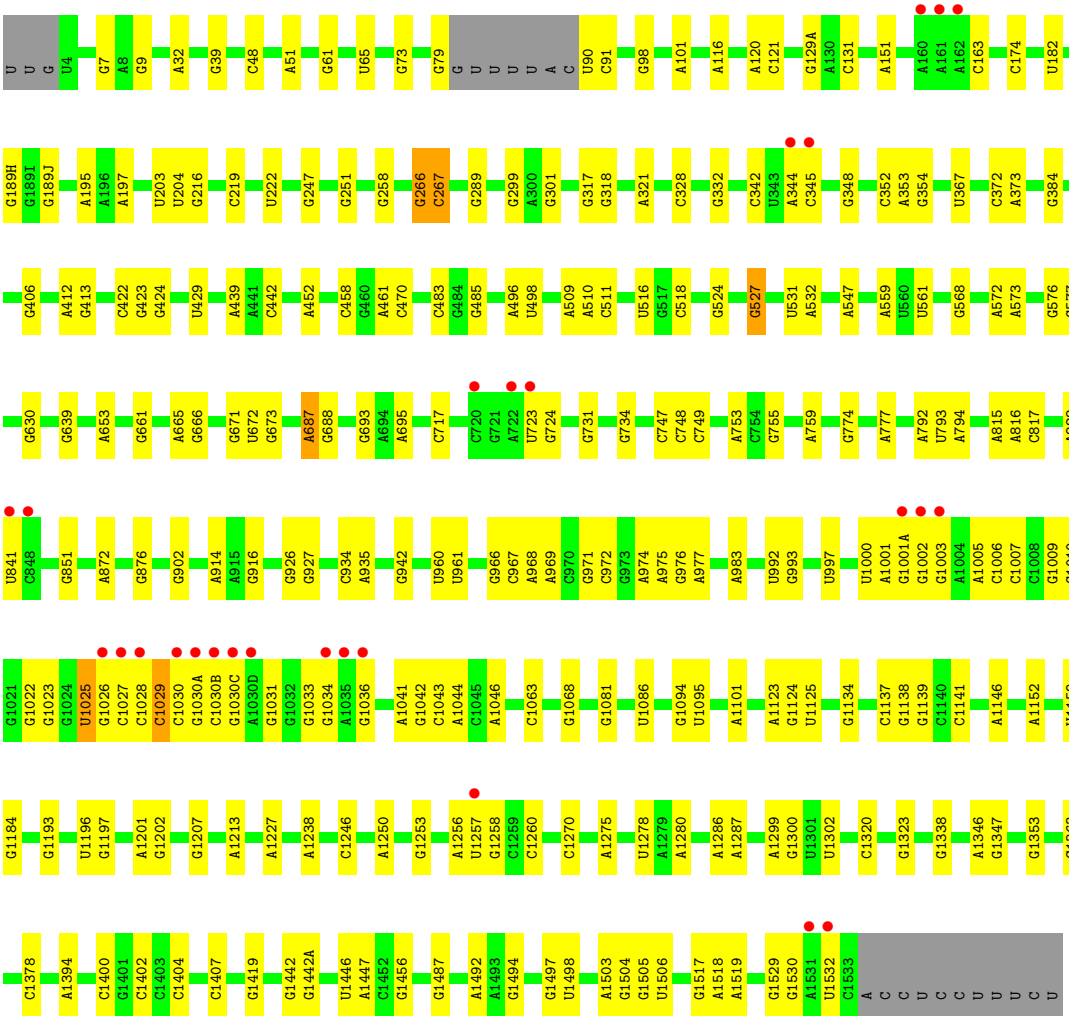
Chain 29:





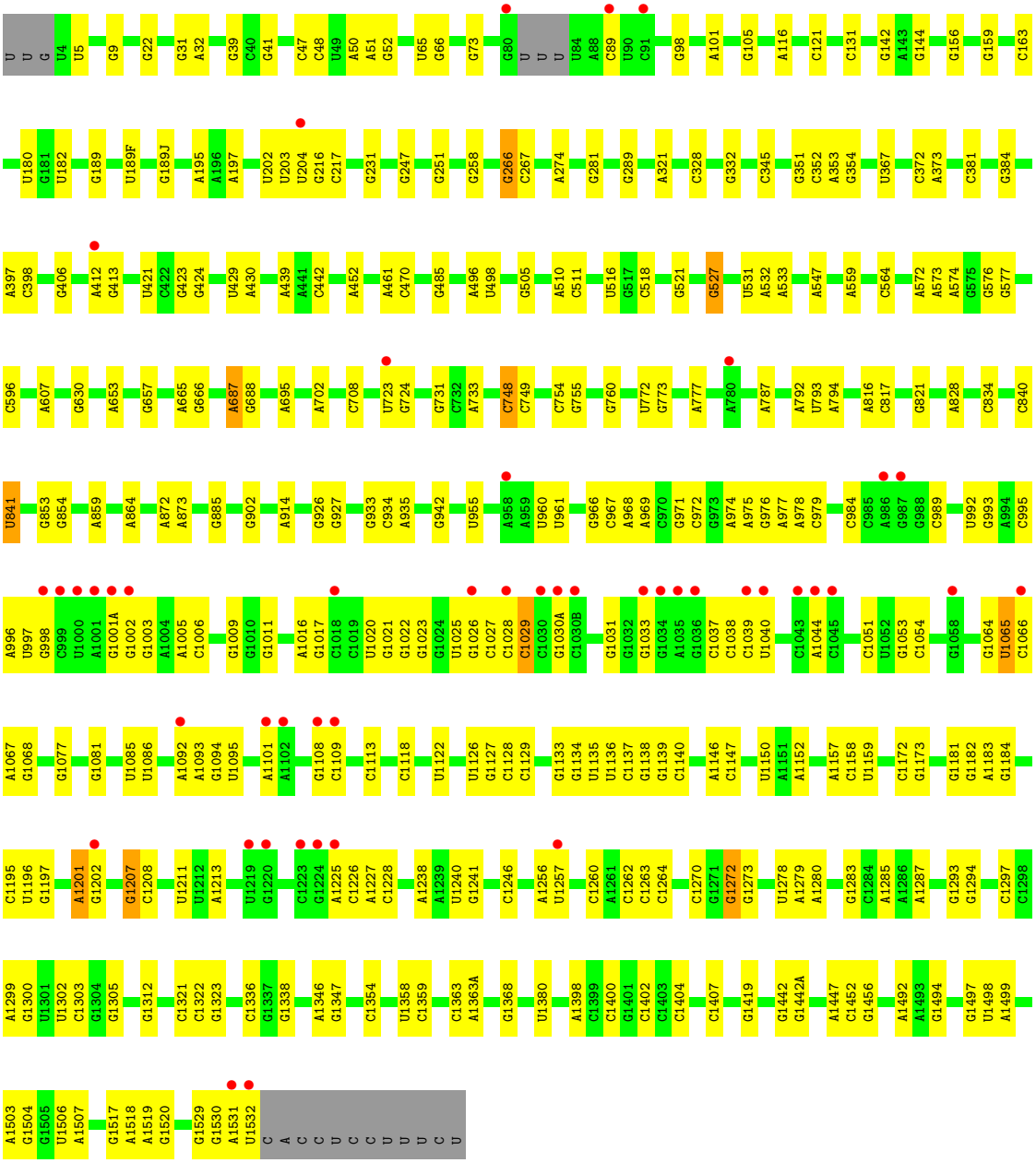
• Molecule 32: 16S Ribosomal RNA

Chain 1a:



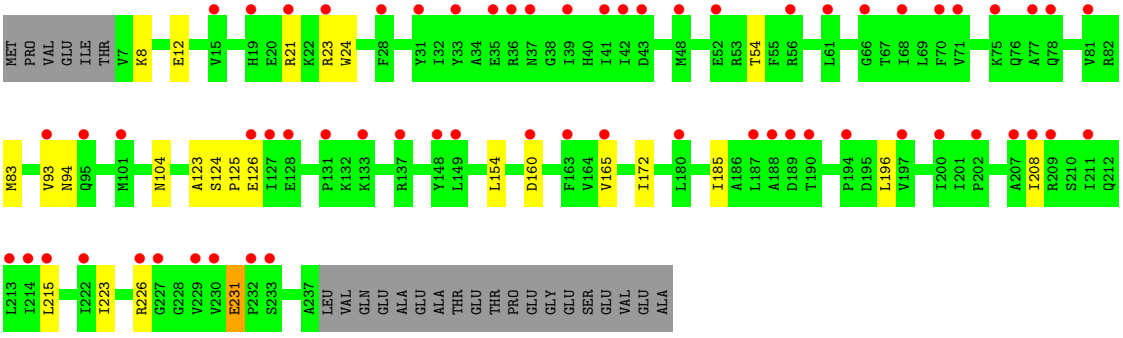
• Molecule 32: 16S Ribosomal RNA

Chain 2a:



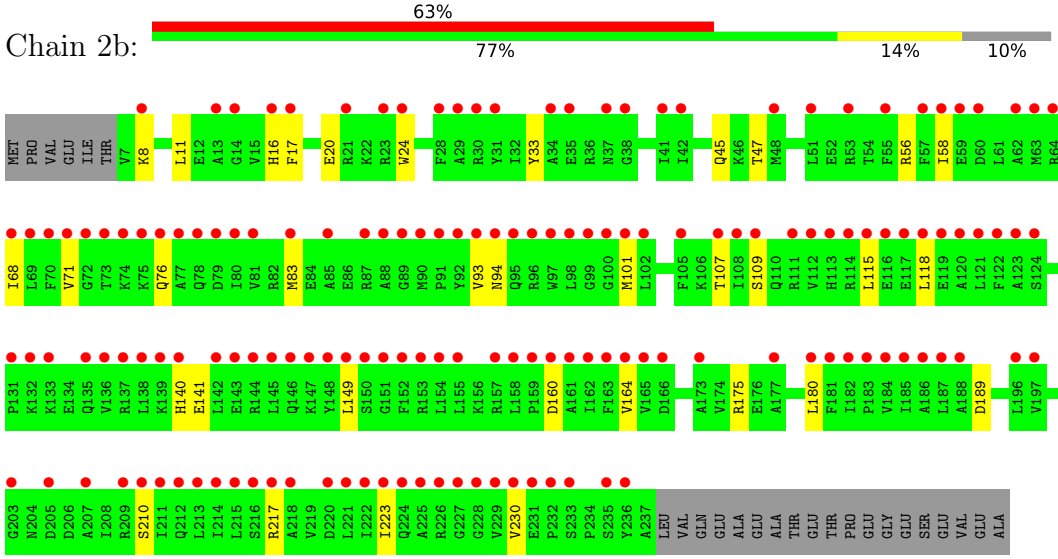
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



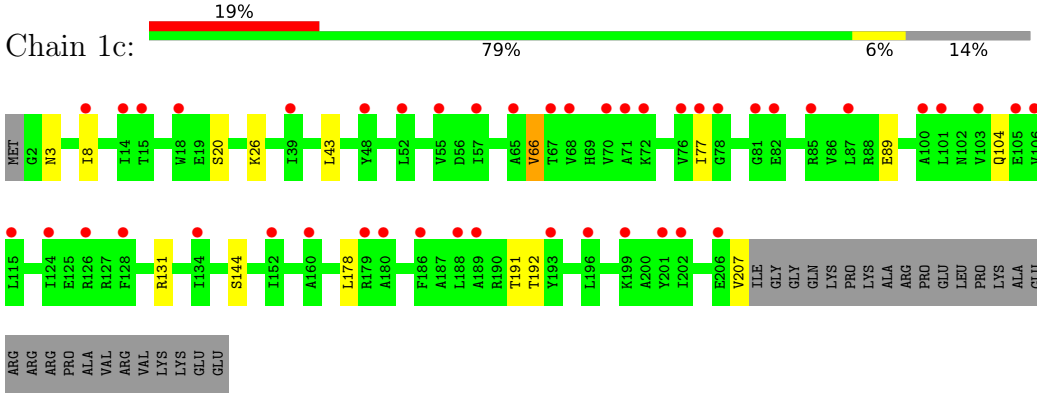
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



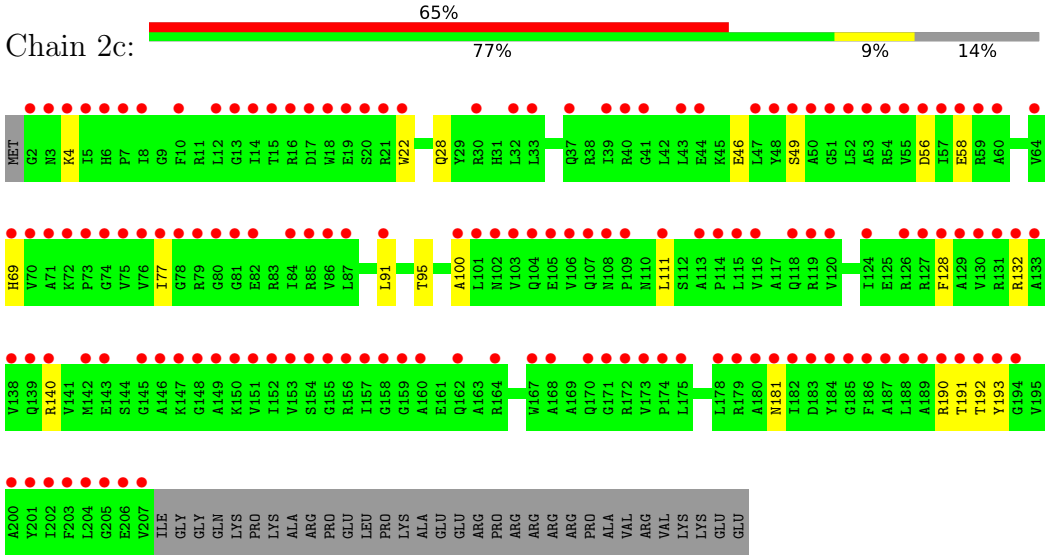
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



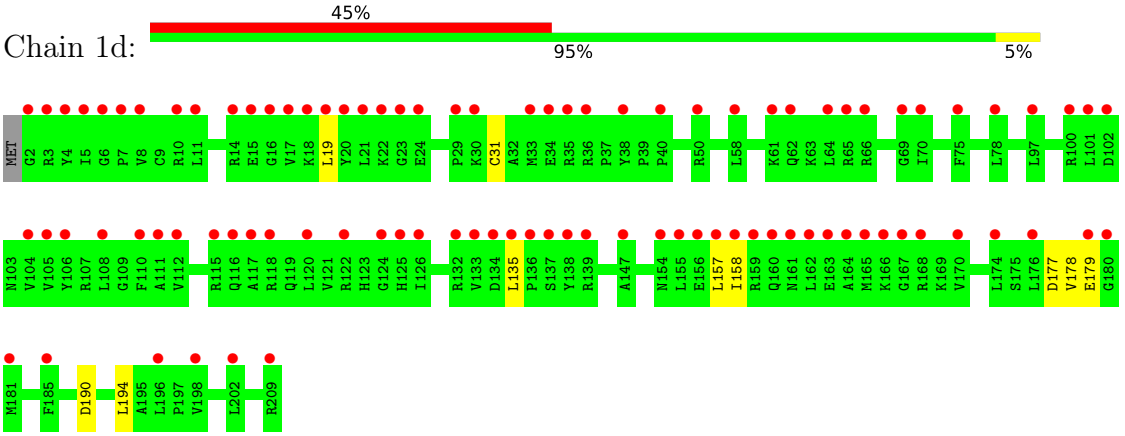
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



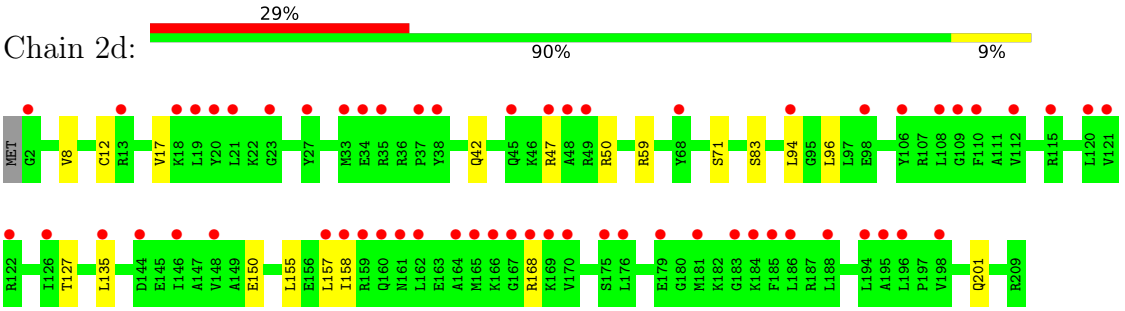
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



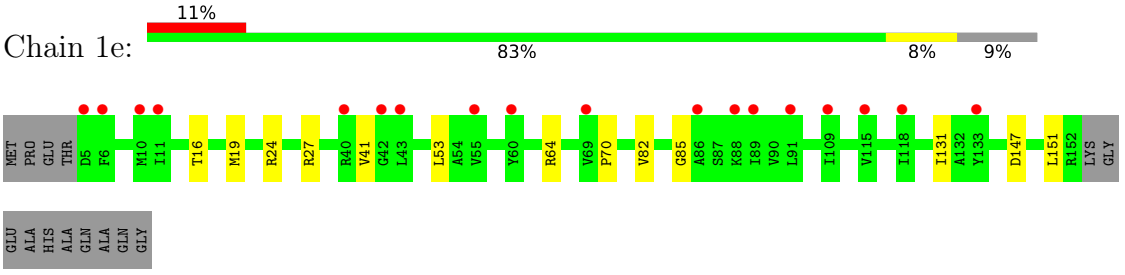
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



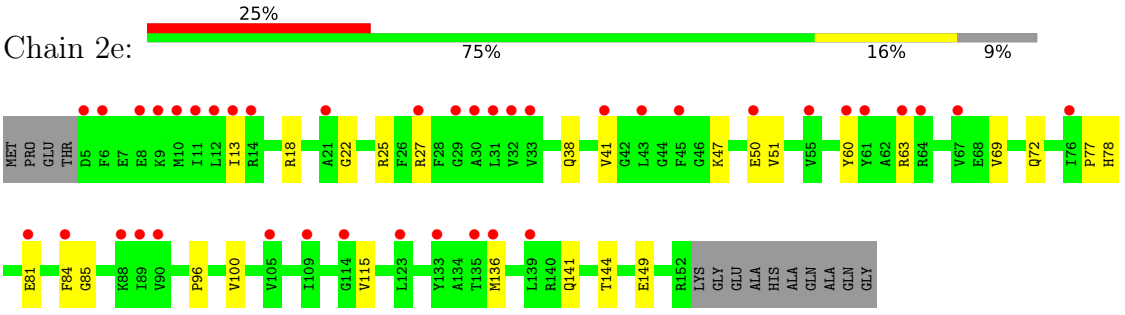
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



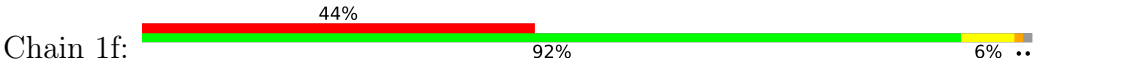
• Molecule 36: 30S ribosomal protein S5

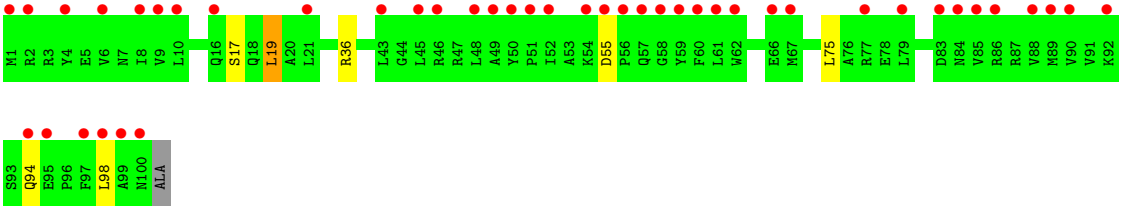
Chain 2e:



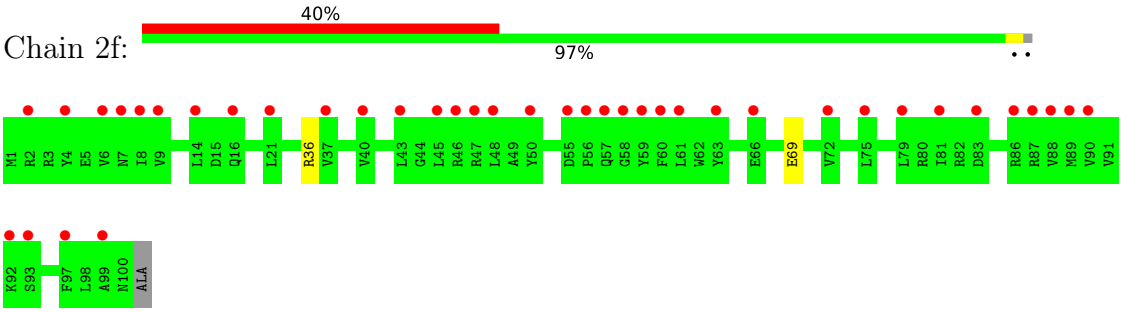
• Molecule 37: 30S ribosomal protein S6

Chain 1f:

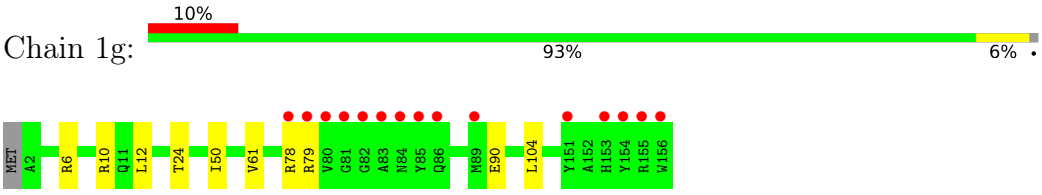




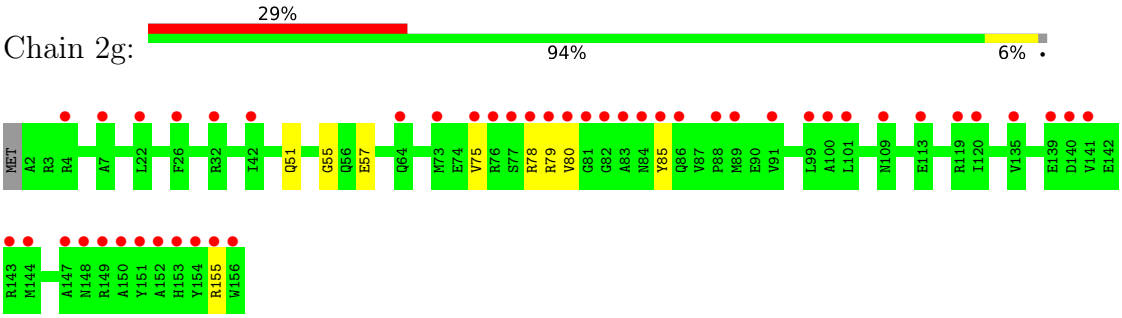
• Molecule 37: 30S ribosomal protein S6



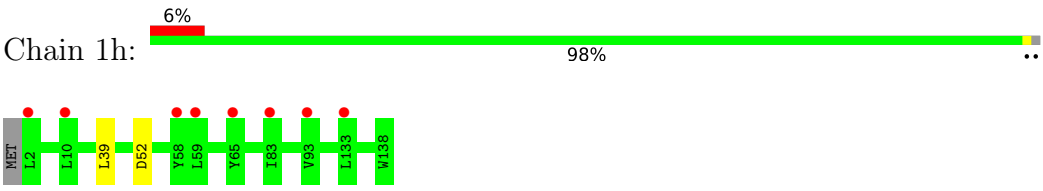
• Molecule 38: 30S ribosomal protein S7



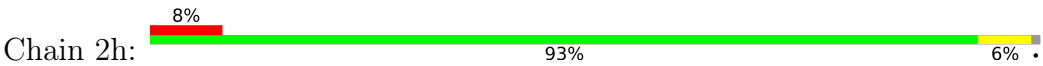
• Molecule 38: 30S ribosomal protein S7

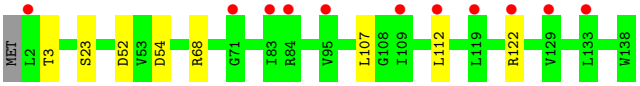


• Molecule 39: 30S ribosomal protein S8



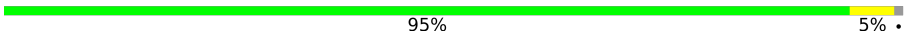
• Molecule 39: 30S ribosomal protein S8





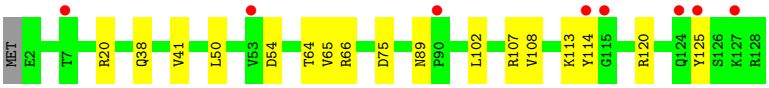
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



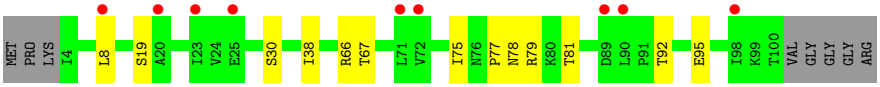
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



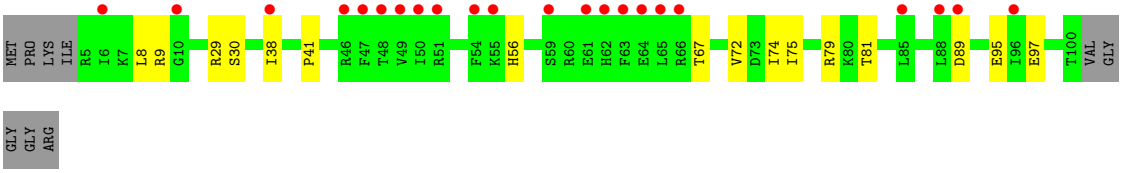
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



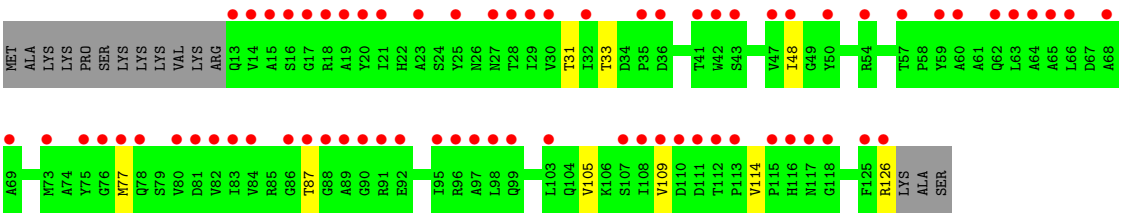
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



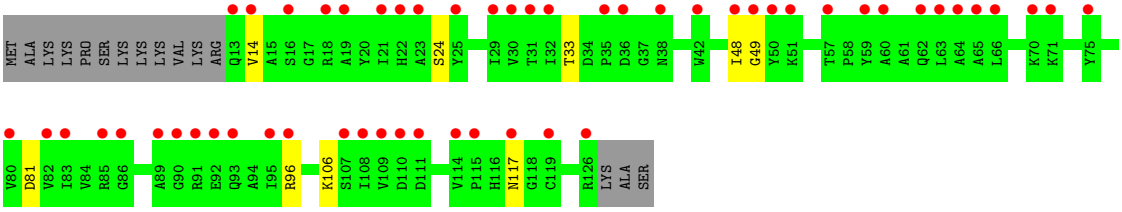
• Molecule 42: 30S ribosomal protein S11

Chain 1k:

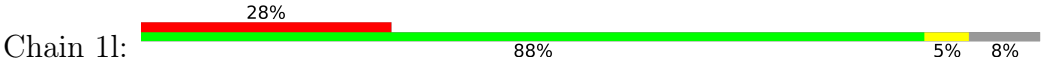


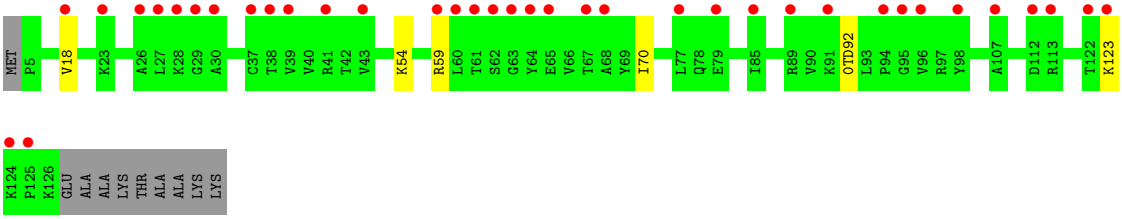
• Molecule 42: 30S ribosomal protein S11

Chain 2k:

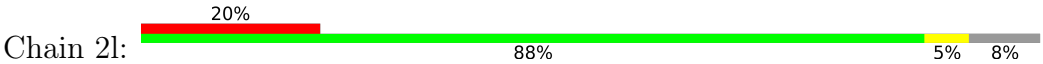


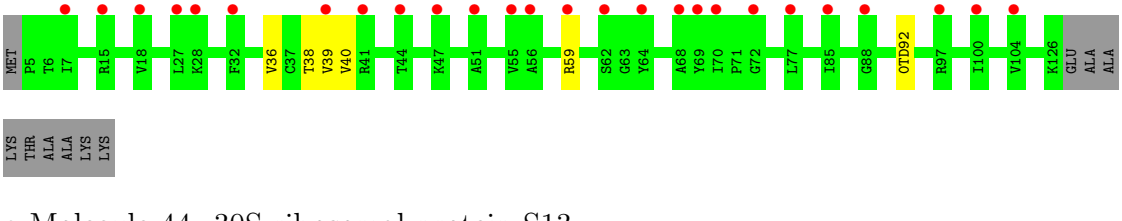
• Molecule 43: 30S ribosomal protein S12



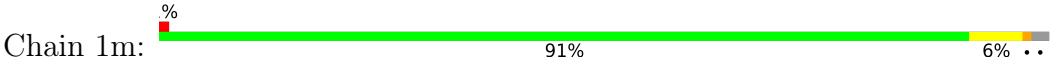


• Molecule 43: 30S ribosomal protein S12

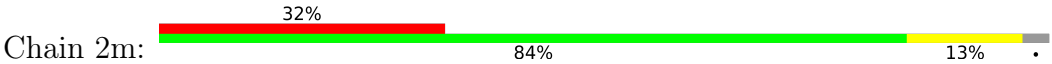


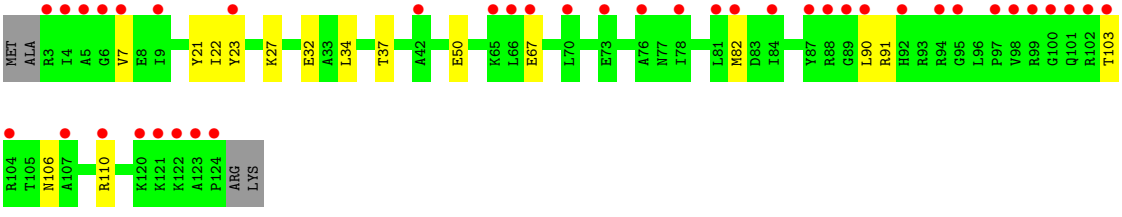


• Molecule 44: 30S ribosomal protein S13

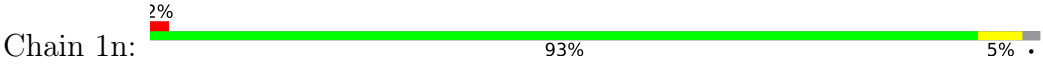


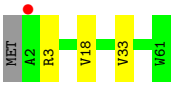
• Molecule 44: 30S ribosomal protein S13





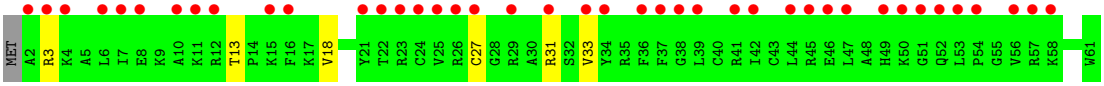
• Molecule 45: 30S ribosomal protein S14 type Z





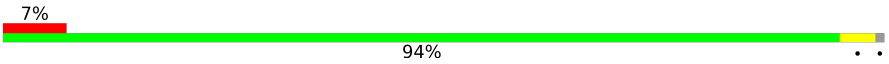
• Molecule 45: 30S ribosomal protein S14 type Z

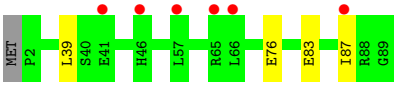
Chain 2n:



• Molecule 46: 30S ribosomal protein S15

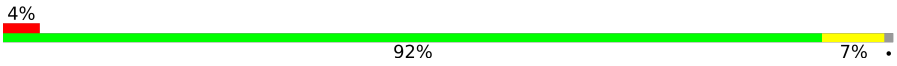
Chain 1o:

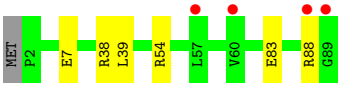




• Molecule 46: 30S ribosomal protein S15

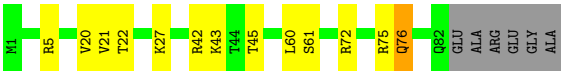
Chain 2o:





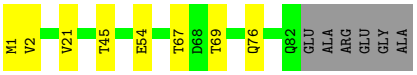
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



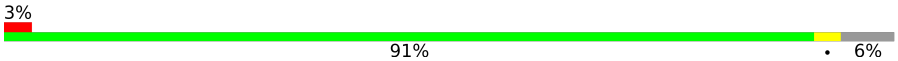
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



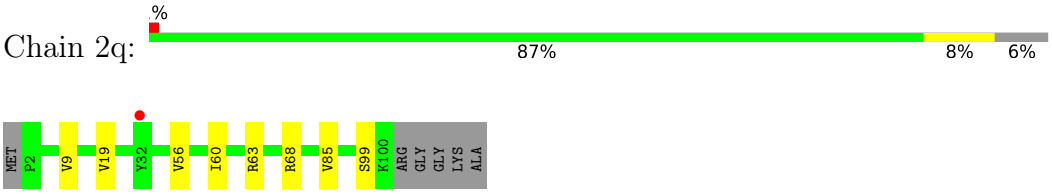
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



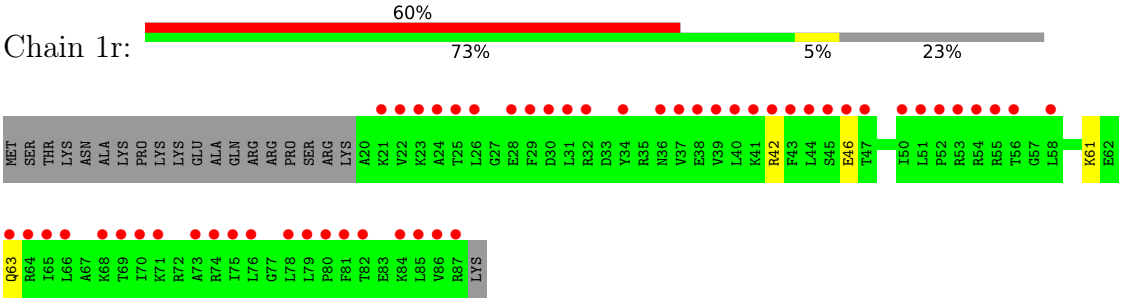
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



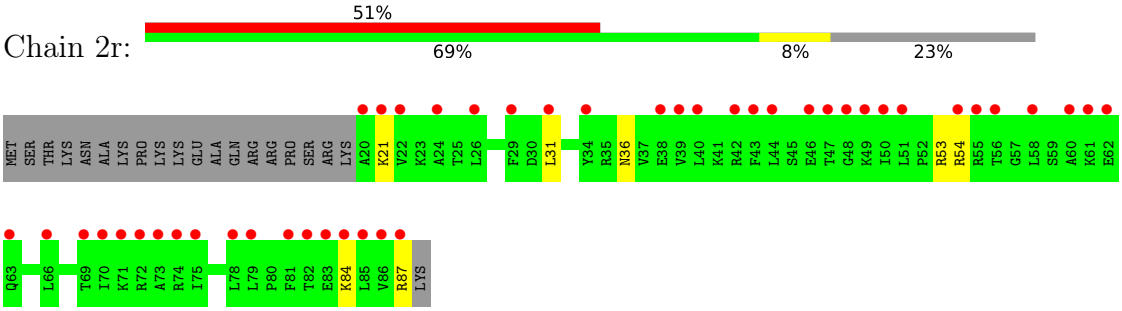
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



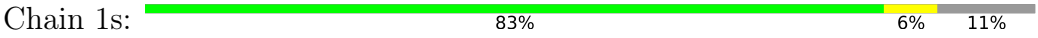
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



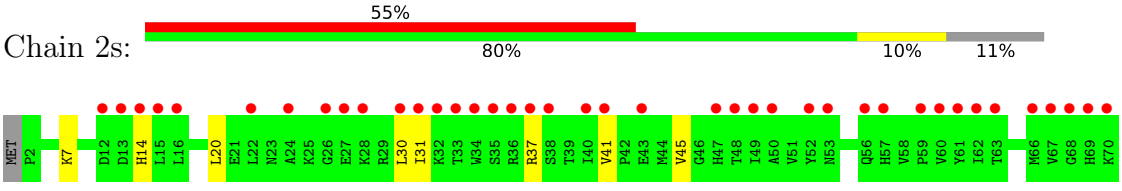
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



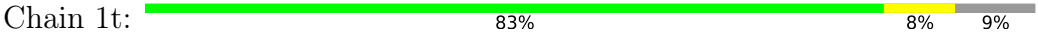
• Molecule 50: 30S ribosomal protein S19

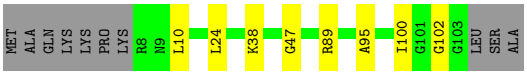
Chain 2s:



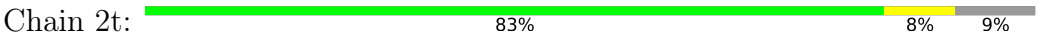
• Molecule 51: 30S ribosomal protein S20

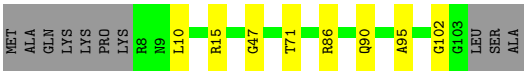
Chain 1t:



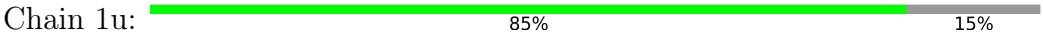


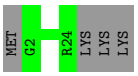
• Molecule 51: 30S ribosomal protein S20



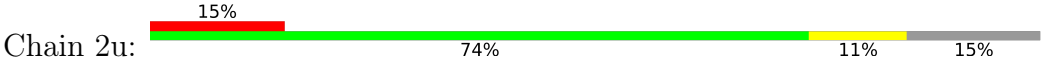


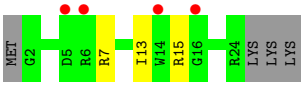
• Molecule 52: 30S ribosomal protein Thx





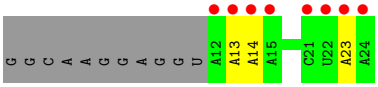
• Molecule 52: 30S ribosomal protein Thx



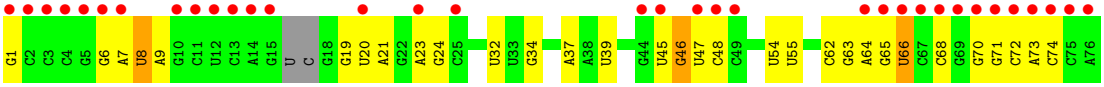


• Molecule 53: MF-mRNA

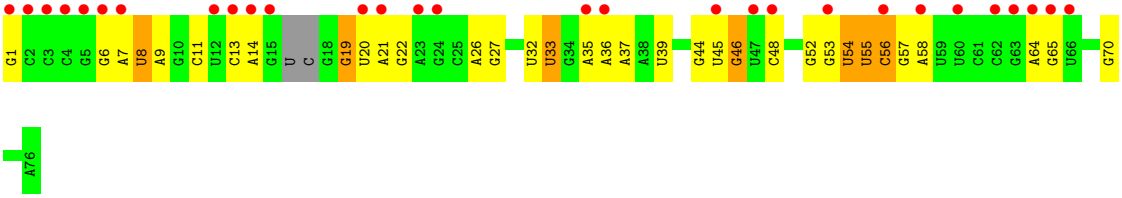
• Molecule 53: MF-mRNA



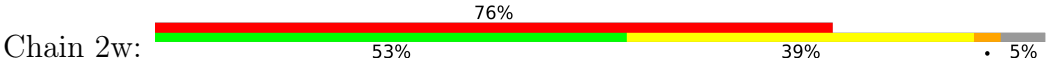
• Molecule 54: A-site and E-site Deacylated tRNAphe

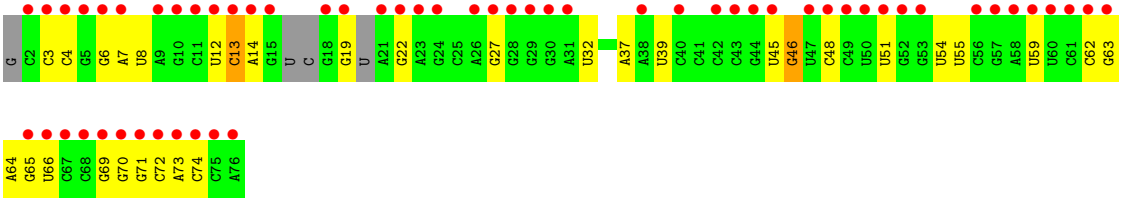


• Molecule 54: A-site and E-site Deacylated tRNAphe

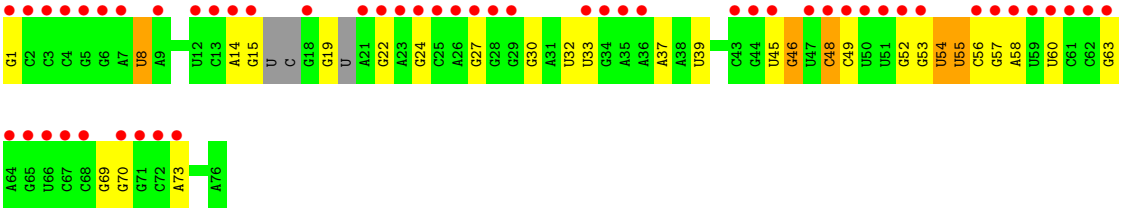


• Molecule 54: A-site and E-site Deacylated tRNAphe

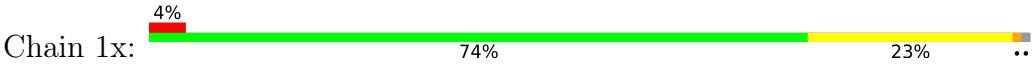


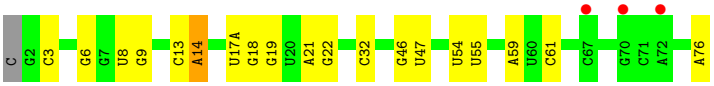


• Molecule 54: A-site and E-site Deacylated tRNAphe

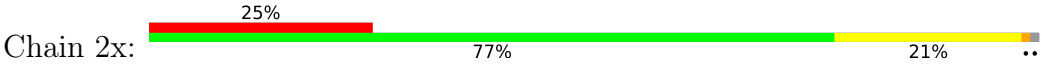


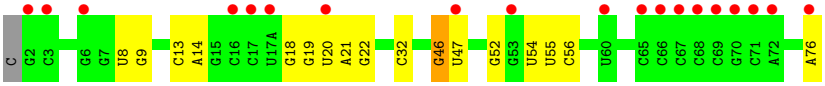
• Molecule 55: P-site Deacylated tRNAmet





• Molecule 55: P-site Deacylated tRNAmet





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.73Å 449.08Å 621.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.84 – 2.75 181.73 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (121.84-2.75) 98.9 (181.73-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.213 , 0.261 0.211 , 0.260	Depositor DCC
R_{free} test set	74514 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	59.1	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	300806	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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: UR3, G7M, OMU, MG, PSU, MA6, OMG, OMC, MIA, M2G, 4OC, 5MC, Y7K, 4SU, SF4, 2MA, 5MU, 0TD, 2MG, ZN, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.53	0/69011	0.96	67/107720 (0.1%)
1	2A	0.38	0/67295	0.84	12/105042 (0.0%)
2	1B	0.45	1/2882 (0.0%)	0.85	0/4494
2	2B	0.41	1/2879 (0.0%)	0.85	1/4487 (0.0%)
3	1D	0.35	0/2186	0.55	0/2944
3	2D	0.31	0/2186	0.51	0/2944
4	1E	0.35	0/1592	0.55	0/2149
4	2E	0.30	0/1592	0.52	0/2149
5	1F	0.35	0/1618	0.54	0/2191
5	2F	0.30	0/1614	0.49	0/2186
6	1G	0.30	0/1448	0.48	0/1957
6	2G	0.30	0/1453	0.49	0/1963
7	1H	0.32	0/1356	0.50	0/1834
7	2H	0.28	0/1356	0.45	0/1834
8	1I	0.29	0/1112	0.48	0/1514
8	2I	0.28	0/1079	0.50	0/1475
9	1N	0.33	0/1144	0.50	0/1543
9	2N	0.30	0/1144	0.45	0/1543
10	1O	0.37	0/943	0.56	0/1269
10	2O	0.31	0/943	0.53	0/1269
11	1P	0.33	0/1152	0.58	0/1533
11	2P	0.30	0/1152	0.52	0/1533
12	1Q	0.36	0/1143	0.53	0/1527
12	2Q	0.30	0/1143	0.49	0/1527
13	1R	0.33	0/982	0.54	0/1312
13	2R	0.27	0/982	0.49	0/1312
14	1S	0.31	0/883	0.53	0/1176
14	2S	0.30	0/880	0.50	0/1172
15	1T	0.33	0/1105	0.52	0/1477
15	2T	0.28	0/1097	0.48	0/1468
16	1U	0.37	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.29	0/977	0.42	0/1301
17	1V	0.35	0/782	0.57	0/1049
17	2V	0.29	0/782	0.52	0/1049
18	1W	0.36	0/897	0.53	0/1205
18	2W	0.29	0/897	0.47	0/1205
19	1X	0.35	0/764	0.55	0/1025
19	2X	0.30	0/764	0.49	0/1025
20	1Y	0.34	0/819	0.55	0/1095
20	2Y	0.31	0/819	0.50	0/1095
21	1Z	0.31	0/1267	0.51	0/1717
21	2Z	0.31	0/1299	0.50	0/1763
22	10	0.36	0/662	0.53	0/881
22	20	0.30	0/662	0.48	0/881
23	11	0.34	0/762	0.50	0/1014
23	21	0.30	0/762	0.50	0/1014
24	12	0.31	0/590	0.43	0/781
24	22	0.27	0/590	0.38	0/781
25	13	0.33	0/474	0.50	0/635
25	23	0.29	0/469	0.45	0/630
26	14	0.32	0/565	0.53	0/761
26	24	0.30	0/545	0.48	0/737
27	15	0.34	0/469	0.54	0/635
27	25	0.34	0/469	0.48	0/635
28	16	0.36	0/460	0.53	0/613
28	26	0.30	0/456	0.48	0/608
29	17	0.35	0/426	0.53	0/561
29	27	0.29	0/426	0.51	0/561
30	18	0.32	0/525	0.54	0/691
30	28	0.28	0/525	0.48	0/691
31	19	0.33	0/310	0.52	0/407
31	29	0.29	0/310	0.51	0/407
32	1a	0.37	0/35795	0.86	15/55864 (0.0%)
32	2a	0.36	3/35886 (0.0%)	0.88	40/56005 (0.1%)
33	1b	0.30	0/1881	0.48	0/2542
33	2b	0.31	0/1860	0.55	0/2518
34	1c	0.29	0/1572	0.47	0/2126
34	2c	0.31	0/1566	0.50	0/2119
35	1d	0.29	0/1685	0.46	0/2262
35	2d	0.28	0/1704	0.44	0/2284
36	1e	0.30	0/1145	0.50	0/1543
36	2e	0.30	0/1149	0.50	0/1548
37	1f	0.30	0/823	0.52	1/1115 (0.1%)
37	2f	0.30	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.28	0/1250	0.42	0/1679
38	2g	0.29	0/1254	0.43	0/1683
39	1h	0.29	0/1108	0.48	0/1494
39	2h	0.27	0/1108	0.45	0/1494
40	1i	0.30	0/1002	0.49	0/1346
40	2i	0.32	0/997	0.50	0/1343
41	1j	0.27	0/722	0.48	0/982
41	2j	0.30	0/727	0.52	0/988
42	1k	0.28	0/844	0.48	0/1145
42	2k	0.29	0/848	0.47	0/1149
43	1l	0.31	0/937	0.51	0/1260
43	2l	0.28	0/937	0.47	0/1260
44	1m	0.30	0/969	0.48	0/1302
44	2m	0.29	0/961	0.48	0/1291
45	1n	0.30	0/501	0.46	0/664
45	2n	0.30	0/501	0.47	0/664
46	1o	0.29	0/739	0.44	0/985
46	2o	0.26	0/739	0.44	0/985
47	1p	0.30	0/697	0.52	0/939
47	2p	0.27	0/693	0.50	0/935
48	1q	0.28	0/836	0.48	0/1117
48	2q	0.29	0/836	0.50	0/1117
49	1r	0.29	0/560	0.50	0/746
49	2r	0.28	0/560	0.49	0/746
50	1s	0.27	0/667	0.51	0/900
50	2s	0.33	0/661	0.59	1/893 (0.1%)
51	1t	0.27	0/730	0.43	0/965
51	2t	0.27	0/729	0.43	0/965
52	1u	0.27	0/203	0.47	0/266
52	2u	0.28	0/203	0.49	0/266
53	1v	0.41	0/310	0.86	0/480
53	2v	0.47	0/310	0.86	0/480
54	1w	0.50	1/1606 (0.1%)	1.01	1/2497 (0.0%)
54	1y	0.54	1/1606 (0.1%)	1.14	14/2497 (0.6%)
54	2w	0.47	0/1556	1.01	3/2418 (0.1%)
54	2y	0.51	1/1583 (0.1%)	1.02	2/2459 (0.1%)
55	1x	0.51	0/1725	1.04	9/2689 (0.3%)
55	2x	0.46	0/1725	1.01	6/2689 (0.2%)
All	All	0.40	8/316688 (0.0%)	0.81	172/474125 (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
33	1b	0	1
40	2i	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	1	G	OP3-P	-10.37	1.48	1.61
54	1w	1	G	OP3-P	-10.33	1.48	1.61
2	1B	1	U	OP3-P	-10.24	1.48	1.61
2	2B	1	U	OP3-P	-10.17	1.49	1.61
54	2y	1	G	OP3-P	-10.04	1.49	1.61
32	2a	1272	G	N1-C2	-8.50	1.30	1.37
32	2a	1272	G	C6-N1	-7.05	1.34	1.39
32	2a	1263	C	N3-C4	-6.48	1.29	1.33

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1263	C	N1-C2-O2	25.88	134.43	118.90
32	2a	1272	G	N3-C2-N2	20.32	134.12	119.90
32	2a	1272	G	C5-C6-O6	19.59	140.35	128.60
32	2a	1272	G	N1-C2-N2	-16.67	101.20	116.20
32	2a	1263	C	N3-C2-O2	-14.70	111.61	121.90
32	2a	1272	G	C6-N1-C2	13.79	133.38	125.10
32	2a	1263	C	C2-N3-C4	13.02	126.41	119.90
54	1y	56	C	N1-C2-O2	12.43	126.36	118.90
32	2a	1272	G	C5-C6-N1	-11.67	105.67	111.50
32	2a	1272	G	N1-C6-O6	-10.01	113.90	119.90
32	2a	1263	C	C5-C6-N1	9.55	125.78	121.00
1	1A	240	G	C5-C6-O6	-9.49	122.90	128.60
32	2a	1263	C	N3-C4-N4	-9.26	111.52	118.00
54	1y	56	C	N3-C2-O2	-9.05	115.56	121.90
32	2a	1263	C	C2-N1-C1'	9.01	128.71	118.80
55	2x	14	A	C5-N7-C8	9.00	108.40	103.90
55	2x	14	A	C4-C5-C6	8.77	121.38	117.00
1	1A	1075	C	N1-C2-O2	8.57	124.04	118.90
1	1A	1063	G	C5-C6-O6	8.30	133.58	128.60
1	1A	512	G	O4'-C1'-N9	8.25	114.80	108.20
32	2a	1263	C	C5-C4-N4	8.22	125.95	120.20
32	2a	1263	C	C4-C5-C6	-8.18	113.31	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	56	C	C2-N1-C1'	8.08	127.69	118.80
1	1A	801	G	O5'-P-OP2	-8.05	98.45	105.70
1	1A	1075	C	C2-N3-C4	7.91	123.86	119.90
2	2B	80	U	O4'-C1'-N1	7.90	114.52	108.20
55	1x	14	A	C5-N7-C8	7.81	107.81	103.90
55	1x	14	A	C4-C5-C6	7.63	120.82	117.00
1	1A	975	C	N1-C2-O2	-7.56	114.37	118.90
32	2a	1263	C	N1-C2-N3	-7.52	113.94	119.20
1	1A	2682	U	O5'-P-OP2	-7.50	98.94	105.70
54	1y	19	G	N3-C4-N9	7.50	130.50	126.00
1	1A	226	G	O4'-C1'-N9	7.46	114.17	108.20
32	1a	1025	U	N1-C2-O2	7.44	128.01	122.80
54	1y	56	C	C6-N1-C2	-7.40	117.34	120.30
32	2a	1272	G	C2-N3-C4	-7.33	108.24	111.90
32	2a	1029	C	N1-C2-O2	7.30	123.28	118.90
1	1A	2554	U	O5'-P-OP1	-7.25	99.18	105.70
1	1A	793	A	O5'-P-OP2	-7.22	99.20	105.70
54	1y	19	G	N9-C4-C5	-7.11	102.56	105.40
1	1A	2006	C	O5'-P-OP1	-7.09	99.32	105.70
54	1y	56	C	C5-C6-N1	7.07	124.53	121.00
1	1A	240	G	N1-C6-O6	6.93	124.06	119.90
1	1A	1614	A	O5'-P-OP1	-6.88	99.51	105.70
1	1A	2167	U	C2-N1-C1'	6.87	125.94	117.70
1	1A	383	U	C2-N1-C1'	-6.87	109.46	117.70
1	1A	1080	C	C2-N3-C4	6.79	123.29	119.90
32	2a	1272	G	C8-N9-C1'	-6.63	118.38	127.00
54	1y	33	U	C2-N1-C1'	6.63	125.65	117.70
1	1A	1080	C	N1-C2-O2	6.61	122.87	118.90
32	2a	754	C	C2-N1-C1'	6.61	126.07	118.80
32	2a	1272	G	C4-N9-C1'	6.50	134.95	126.50
1	1A	12	U	C2-N1-C1'	6.38	125.36	117.70
32	2a	841	U	C5-C6-N1	6.32	125.86	122.70
1	1A	2023	G	O5'-P-OP1	-6.30	100.03	105.70
32	2a	1263	C	C6-N1-C1'	-6.28	113.26	120.80
32	2a	1263	C	C6-N1-C2	-6.25	117.80	120.30
55	2x	14	A	C5-C6-N1	-6.19	114.60	117.70
32	1a	1034	G	C6-N1-C2	6.18	128.81	125.10
55	1x	14	A	C5-C6-N1	-6.17	114.62	117.70
1	1A	31	C	O5'-P-OP1	-6.11	100.20	105.70
37	1f	19	LEU	CA-CB-CG	6.10	129.34	115.30
1	1A	2629	A	P-O3'-C3'	6.09	127.00	119.70
54	1y	56	C	C2-N3-C4	6.08	122.94	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1313	U	C2-N1-C1'	6.06	124.98	117.70
1	1A	450	G	N1-C6-O6	-6.06	116.27	119.90
54	2y	22	G	N1-C6-O6	6.04	123.53	119.90
32	1a	266	G	P-O3'-C3'	6.03	126.94	119.70
32	2a	998	G	C5-C6-O6	6.00	132.20	128.60
1	2A	787	U	O5'-P-OP1	-6.00	100.30	105.70
32	1a	1030(B)	C	C2-N1-C1'	5.98	125.38	118.80
54	1y	19	G	C4-C5-N7	5.95	113.18	110.80
1	1A	1058	G	C6-N1-C2	5.92	128.65	125.10
1	1A	568	U	C5-C4-O4	-5.90	122.36	125.90
1	1A	195	A	C5-N7-C8	5.89	106.85	103.90
54	1y	19	G	C6-C5-N7	-5.89	126.87	130.40
1	1A	1313	U	C2-N1-C1'	5.87	124.75	117.70
32	2a	1225	A	C5-C6-N6	5.87	128.40	123.70
1	1A	2129	C	N1-C2-O2	5.86	122.42	118.90
54	1y	19	G	C8-N9-C1'	-5.86	119.38	127.00
1	1A	975	C	C2-N1-C1'	-5.85	112.37	118.80
55	2x	46	G	C6-N1-C2	-5.84	121.60	125.10
1	1A	847	U	C2-N1-C1'	5.83	124.70	117.70
1	1A	1063	G	N3-C2-N2	5.83	123.98	119.90
1	1A	2430	A	C2-N3-C4	5.80	113.50	110.60
1	2A	2168	G	C4-N9-C1'	5.80	134.03	126.50
32	2a	687	A	P-O3'-C3'	5.78	126.64	119.70
1	1A	240	G	C4-C5-N7	5.75	113.10	110.80
1	1A	2347	C	N1-C2-O2	5.75	122.35	118.90
1	1A	1776	G	O5'-P-OP2	-5.75	100.53	105.70
1	1A	195	A	N7-C8-N9	-5.74	110.93	113.80
1	1A	1075	C	C5-C4-N4	5.73	124.21	120.20
32	2a	754	C	N1-C2-O2	5.72	122.33	118.90
1	1A	1992	G	P-O3'-C3'	5.71	126.55	119.70
1	1A	240	G	N9-C4-C5	-5.70	103.12	105.40
54	2w	13	C	OP1-P-O3'	5.70	117.74	105.20
1	1A	1174	A	P-O3'-C3'	5.68	126.51	119.70
32	1a	299	G	C5-C6-O6	-5.67	125.20	128.60
1	1A	383	U	O4'-C1'-N1	5.67	112.73	108.20
1	2A	1992	G	P-O3'-C3'	5.65	126.48	119.70
1	1A	1385	G	O4'-C1'-N9	5.65	112.72	108.20
55	1x	22	G	N1-C6-O6	-5.64	116.52	119.90
32	2a	955	U	C2-N3-C4	5.60	130.36	127.00
32	1a	90	U	C2-N1-C1'	5.58	124.40	117.70
32	2a	1029	C	N3-C2-O2	-5.56	118.00	121.90
1	1A	240	G	N3-C4-N9	5.56	129.34	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	19	G	C4-N9-C1'	5.55	133.72	126.50
32	2a	1150	U	C5-C4-O4	5.55	129.23	125.90
55	2x	46	G	N3-C2-N2	-5.52	116.03	119.90
1	1A	1176	G	OP1-P-O3'	5.51	117.33	105.20
32	1a	267	C	O5'-P-OP1	-5.50	100.75	105.70
1	1A	240	G	C6-C5-N7	-5.48	127.11	130.40
1	2A	383	U	O4'-C1'-N1	5.47	112.58	108.20
1	2A	2689	U	P-O3'-C3'	5.46	126.25	119.70
1	1A	1063	G	C6-N1-C2	5.45	128.37	125.10
54	1y	19	G	N3-C2-N2	5.45	123.71	119.90
32	2a	1026	G	C4-N9-C1'	5.42	133.55	126.50
32	1a	1029	C	C2-N3-C4	5.41	122.60	119.90
32	2a	266	G	P-O3'-C3'	5.40	126.18	119.70
1	1A	1174	A	OP1-P-O3'	5.38	117.02	105.20
1	1A	2167	U	N1-C2-O2	5.37	126.56	122.80
1	1A	2848	G	O4'-C1'-N9	5.32	112.46	108.20
32	2a	1201	A	P-O3'-C3'	5.32	126.09	119.70
1	1A	1063	G	N1-C6-O6	-5.31	116.71	119.90
1	1A	1086	A	N1-C6-N6	-5.31	115.42	118.60
1	2A	1653	G	P-O3'-C3'	5.30	126.06	119.70
1	1A	821	A	O5'-P-OP2	-5.30	100.93	105.70
32	1a	1036	G	N1-C6-O6	-5.29	116.73	119.90
1	2A	1204	A	O4'-C1'-N9	5.27	112.42	108.20
32	2a	266	G	N3-C4-C5	-5.27	125.97	128.60
1	1A	1058	G	C5-C6-O6	5.26	131.76	128.60
1	1A	1306	C	O5'-P-OP2	-5.26	100.97	105.70
55	1x	22	G	C6-C5-N7	5.25	133.55	130.40
32	2a	1065	U	P-O3'-C3'	5.23	125.98	119.70
1	1A	2055	C	OP1-P-O3'	5.22	116.68	105.20
55	1x	22	G	N3-C4-N9	-5.21	122.87	126.00
1	1A	372	G	O4'-C1'-N9	5.21	112.36	108.20
1	1A	383	U	C6-N1-C1'	5.20	128.48	121.20
54	2w	63	G	C5-C6-O6	5.20	131.72	128.60
1	2A	512	G	O4'-C1'-N9	5.18	112.35	108.20
1	1A	2873	A	O4'-C1'-N9	5.16	112.33	108.20
55	1x	22	G	C8-N9-C1'	5.15	133.70	127.00
1	2A	2140	C	N1-C2-O2	5.14	121.99	118.90
54	1w	66	U	C5-C4-O4	-5.14	122.82	125.90
32	2a	955	U	C5-C4-O4	5.14	128.98	125.90
32	1a	90	U	N3-C2-O2	-5.13	118.61	122.20
55	1x	46	G	C6-N1-C2	-5.12	122.03	125.10
54	2y	48	C	N1-C2-O2	-5.11	115.83	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	987	G	O5'-P-OP2	5.10	116.82	110.70
55	1x	14	A	C4-C5-N7	-5.09	108.15	110.70
32	2a	1067	A	P-O3'-C3'	5.09	125.80	119.70
1	1A	2005	A	OP1-P-O3'	5.08	116.38	105.20
1	1A	975	C	C6-N1-C1'	5.07	126.89	120.80
32	1a	90	U	N1-C2-O2	5.07	126.34	122.80
32	2a	1026	G	C8-N9-C1'	-5.07	120.42	127.00
1	1A	748	G	O4'-C1'-N9	5.06	112.25	108.20
32	2a	748	C	P-O3'-C3'	5.06	125.78	119.70
32	1a	1030(B)	C	N1-C2-O2	5.06	121.94	118.90
1	2A	847	U	C2-N1-C1'	5.06	123.77	117.70
1	1A	2167	U	N3-C2-O2	-5.05	118.66	122.20
1	1A	774	A	C8-N9-C4	-5.04	103.78	105.80
54	2w	13	C	P-O3'-C3'	5.04	125.75	119.70
32	1a	266	G	N3-C4-C5	-5.04	126.08	128.60
50	2s	30	LEU	CA-CB-CG	5.04	126.90	115.30
55	2x	14	A	C8-N9-C1'	-5.03	118.64	127.70
32	2a	1026	G	N3-C4-N9	5.03	129.02	126.00
1	1A	548	A	P-O3'-C3'	5.03	125.73	119.70
32	1a	687	A	P-O3'-C3'	5.03	125.73	119.70
1	1A	2609	U	C2-N1-C1'	-5.02	111.68	117.70
32	1a	748	C	P-O3'-C3'	5.02	125.72	119.70
1	1A	1131	G	O4'-C1'-N9	5.01	112.20	108.20
1	2A	205	G	C8-N9-C4	5.00	108.40	106.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	123	ALA	Peptide
40	2i	38	GLN	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%)	256 (94%)	17 (6%)	0	100 100
3	2D	273/276 (99%)	252 (92%)	21 (8%)	0	100 100
4	1E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	29 47
4	2E	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	15 27
5	1F	200/210 (95%)	195 (98%)	4 (2%)	1 (0%)	29 47
5	2F	200/210 (95%)	190 (95%)	7 (4%)	3 (2%)	10 18
6	1G	179/182 (98%)	166 (93%)	11 (6%)	2 (1%)	14 25
6	2G	179/182 (98%)	156 (87%)	18 (10%)	5 (3%)	5 7
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	25 42
7	2H	172/180 (96%)	155 (90%)	16 (9%)	1 (1%)	25 42
8	1I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	22 39
8	2I	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	11 19
9	1N	138/140 (99%)	130 (94%)	8 (6%)	0	100 100
9	2N	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	22 39
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100 100
10	2O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19 34
11	1P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	11 19
11	2P	147/150 (98%)	127 (86%)	17 (12%)	3 (2%)	7 13
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100 100
12	2Q	139/141 (99%)	125 (90%)	13 (9%)	1 (1%)	22 39
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100 100
13	2R	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	17 31
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100 100
14	2S	108/112 (96%)	93 (86%)	11 (10%)	4 (4%)	3 4
15	1T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	19 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	2T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	19 34
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
16	2U	114/118 (97%)	108 (95%)	6 (5%)	0	100 100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15 27
17	2V	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	7 13
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
19	1X	93/96 (97%)	89 (96%)	2 (2%)	2 (2%)	6 11
19	2X	93/96 (97%)	86 (92%)	7 (8%)	0	100 100
20	1Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	8 14
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100 100
21	1Z	148/206 (72%)	132 (89%)	15 (10%)	1 (1%)	22 39
21	2Z	156/206 (76%)	123 (79%)	28 (18%)	5 (3%)	4 6
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
22	20	81/85 (95%)	74 (91%)	7 (9%)	0	100 100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14 25
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14 25
24	12	68/72 (94%)	66 (97%)	1 (2%)	1 (2%)	10 18
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
26	14	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1 0
26	24	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1 0
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
33	1b	229/256 (90%)	190 (83%)	33 (14%)	6 (3%)	5 8
33	2b	229/256 (90%)	183 (80%)	44 (19%)	2 (1%)	17 31
34	1c	204/239 (85%)	185 (91%)	17 (8%)	2 (1%)	15 27
34	2c	204/239 (85%)	170 (83%)	30 (15%)	4 (2%)	7 13
35	1d	206/209 (99%)	187 (91%)	18 (9%)	1 (0%)	29 47
35	2d	206/209 (99%)	180 (87%)	26 (13%)	0	100 100
36	1e	146/162 (90%)	129 (88%)	15 (10%)	2 (1%)	11 19
36	2e	146/162 (90%)	127 (87%)	13 (9%)	6 (4%)	3 3
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100 100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100 100
38	1g	153/156 (98%)	144 (94%)	9 (6%)	0	100 100
38	2g	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	12 21
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100 100
39	2h	135/138 (98%)	121 (90%)	13 (10%)	1 (1%)	22 39
40	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	19 34
40	2i	125/128 (98%)	108 (86%)	17 (14%)	0	100 100
41	1j	95/105 (90%)	76 (80%)	14 (15%)	5 (5%)	2 2
41	2j	94/105 (90%)	72 (77%)	18 (19%)	4 (4%)	2 3
42	1k	112/129 (87%)	105 (94%)	5 (4%)	2 (2%)	8 15
42	2k	112/129 (87%)	96 (86%)	14 (12%)	2 (2%)	8 15
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100 100
43	2l	119/132 (90%)	109 (92%)	10 (8%)	0	100 100
44	1m	121/126 (96%)	111 (92%)	8 (7%)	2 (2%)	9 16
44	2m	120/126 (95%)	97 (81%)	19 (16%)	4 (3%)	4 5
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100 100
45	2n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9 16
46	1o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13 23
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100 100
47	1p	80/88 (91%)	72 (90%)	6 (8%)	2 (2%)	5 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100 100
48	1q	97/105 (92%)	86 (89%)	11 (11%)	0	100 100
48	2q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	15 27
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100 100
49	2r	66/88 (75%)	56 (85%)	9 (14%)	1 (2%)	10 18
50	1s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	13 23
50	2s	81/93 (87%)	58 (72%)	23 (28%)	0	100 100
51	1t	94/106 (89%)	85 (90%)	5 (5%)	4 (4%)	2 3
51	2t	94/106 (89%)	85 (90%)	5 (5%)	4 (4%)	2 3
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100 100
All	All	11368/12128 (94%)	10346 (91%)	901 (8%)	121 (1%)	14 25

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
21	1Z	53	ILE
26	14	49	PHE
26	14	62	ARG
33	1b	125	PRO
33	1b	126	GLU
40	1i	54	ASP
44	1m	67	GLU
44	1m	106	ASN
5	2F	130	ALA
8	2I	10	GLU
11	2P	36	LYS
17	2V	79	VAL
33	2b	17	PHE
38	2g	55	GLY
38	2g	80	VAL
44	2m	67	GLU
48	2q	68	ARG
6	1G	43	LEU
6	1G	47	LYS
15	1T	37	GLY
19	1X	93	GLU

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Mol	Chain	Res	Type
20	1Y	54	LYS
23	11	3	LYS
26	14	47	GLN
34	1c	66	VAL
36	1e	85	GLY
41	1j	30	SER
41	1j	75	ILE
42	1k	77	MET
6	2G	42	GLY
6	2G	47	LYS
6	2G	51	ARG
6	2G	84	LYS
8	2I	40	THR
10	2O	5	GLN
12	2Q	24	GLY
14	2S	96	GLY
21	2Z	52	SER
21	2Z	144	LEU
21	2Z	163	LEU
34	2c	91	LEU
34	2c	95	THR
36	2e	85	GLY
39	2h	68	ARG
41	2j	75	ILE
41	2j	79	ARG
24	12	69	ARG
26	14	45	GLY
35	1d	179	GLU
41	1j	77	PRO
41	1j	79	ARG
47	1p	76	GLN
51	1t	102	GLY
4	2E	52	LEU
5	2F	166	ALA
6	2G	43	LEU
14	2S	84	GLN
23	21	3	LYS
33	2b	20	GLU
34	2c	100	ALA
34	2c	181	ASN
41	2j	56	HIS
42	2k	106	LYS

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Mol	Chain	Res	Type
44	2m	23	TYR
49	2r	36	ASN
51	2t	95	ALA
4	1E	52	LEU
8	1I	104	GLN
26	14	18	CYS
34	1c	107	GLN
51	1t	95	ALA
5	2F	18	ARG
7	2H	126	PRO
9	2N	2	LYS
11	2P	45	LEU
13	2R	2	ARG
14	2S	20	ARG
21	2Z	157	LEU
26	24	46	GLN
42	2k	49	GLY
45	2n	27	CYS
11	1P	29	LYS
17	1V	79	VAL
19	1X	2	LYS
33	1b	8	LYS
33	1b	124	SER
33	1b	231	GLU
41	1j	78	ASN
47	1p	75	ARG
51	1t	47	GLY
51	1t	100	ILE
4	2E	113	PHE
15	2T	55	ASN
21	2Z	146	ILE
26	24	11	PRO
26	24	47	GLN
26	24	49	PHE
36	2e	77	PRO
44	2m	21	TYR
51	2t	10	LEU
51	2t	47	GLY
11	1P	93	GLY
33	1b	165	VAL
36	1e	70	PRO
26	24	50	VAL

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Mol	Chain	Res	Type
36	2e	63	ARG
51	2t	102	GLY
36	2e	69	VAL
7	1H	55	PRO
20	1Y	103	GLY
11	2P	44	GLY
42	1k	105	VAL
44	2m	7	VAL
46	1o	87	ILE
14	2S	35	ILE
36	2e	96	PRO
41	2j	41	PRO
50	1s	72	GLY
36	2e	22	GLY
17	2V	50	PRO

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%)	206 (96%)	9 (4%)	30 49
3	2D	215/218 (99%)	203 (94%)	12 (6%)	21 36
4	1E	164/166 (99%)	158 (96%)	6 (4%)	34 54
4	2E	164/166 (99%)	159 (97%)	5 (3%)	41 61
5	1F	160/166 (96%)	146 (91%)	14 (9%)	10 17
5	2F	159/166 (96%)	142 (89%)	17 (11%)	6 11
6	1G	143/156 (92%)	134 (94%)	9 (6%)	18 31
6	2G	143/156 (92%)	120 (84%)	23 (16%)	2 3
7	1H	144/148 (97%)	133 (92%)	11 (8%)	13 23
7	2H	144/148 (97%)	131 (91%)	13 (9%)	9 16
8	1I	113/124 (91%)	98 (87%)	15 (13%)	4 6
8	2I	105/124 (85%)	90 (86%)	15 (14%)	3 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	1N	118/119 (99%)	110 (93%)	8 (7%)	16 28
9	2N	118/119 (99%)	107 (91%)	11 (9%)	9 15
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41 61
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31 51
11	1P	115/116 (99%)	105 (91%)	10 (9%)	10 18
11	2P	115/116 (99%)	108 (94%)	7 (6%)	18 33
12	1Q	111/111 (100%)	107 (96%)	4 (4%)	35 55
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9 16
13	1R	101/101 (100%)	97 (96%)	4 (4%)	31 51
13	2R	101/101 (100%)	97 (96%)	4 (4%)	31 51
14	1S	86/88 (98%)	80 (93%)	6 (7%)	15 26
14	2S	85/88 (97%)	73 (86%)	12 (14%)	3 4
15	1T	115/127 (91%)	109 (95%)	6 (5%)	23 39
15	2T	113/127 (89%)	107 (95%)	6 (5%)	22 38
16	1U	93/94 (99%)	87 (94%)	6 (6%)	17 30
16	2U	93/94 (99%)	91 (98%)	2 (2%)	52 70
17	1V	80/82 (98%)	76 (95%)	4 (5%)	24 42
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7 13
18	1W	90/92 (98%)	83 (92%)	7 (8%)	12 22
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28 47
19	1X	77/78 (99%)	73 (95%)	4 (5%)	23 39
19	2X	77/78 (99%)	73 (95%)	4 (5%)	23 39
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5 8
20	2Y	85/91 (93%)	75 (88%)	10 (12%)	5 8
21	1Z	135/179 (75%)	120 (89%)	15 (11%)	6 10
21	2Z	137/179 (76%)	123 (90%)	14 (10%)	7 12
22	10	65/67 (97%)	62 (95%)	3 (5%)	27 46
22	20	65/67 (97%)	64 (98%)	1 (2%)	65 78
23	11	80/83 (96%)	73 (91%)	7 (9%)	10 17
23	21	80/83 (96%)	77 (96%)	3 (4%)	33 53
24	12	65/67 (97%)	61 (94%)	4 (6%)	18 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	22	65/67 (97%)	61 (94%)	4 (6%)	18 32
25	13	51/52 (98%)	46 (90%)	5 (10%)	8 13
25	23	50/52 (96%)	48 (96%)	2 (4%)	31 51
26	14	59/63 (94%)	51 (86%)	8 (14%)	3 5
26	24	53/63 (84%)	44 (83%)	9 (17%)	2 3
27	15	50/52 (96%)	48 (96%)	2 (4%)	31 51
27	25	50/52 (96%)	47 (94%)	3 (6%)	19 33
28	16	51/52 (98%)	46 (90%)	5 (10%)	8 13
28	26	50/52 (96%)	42 (84%)	8 (16%)	2 3
29	17	41/42 (98%)	39 (95%)	2 (5%)	25 43
29	27	41/42 (98%)	37 (90%)	4 (10%)	8 13
30	18	54/55 (98%)	53 (98%)	1 (2%)	57 73
30	28	54/55 (98%)	50 (93%)	4 (7%)	13 24
31	19	34/34 (100%)	34 (100%)	0	100 100
31	29	34/34 (100%)	33 (97%)	1 (3%)	42 62
33	1b	192/220 (87%)	173 (90%)	19 (10%)	8 13
33	2b	187/220 (85%)	154 (82%)	33 (18%)	2 3
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6 11
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4 6
35	1d	169/181 (93%)	160 (95%)	9 (5%)	22 38
35	2d	173/181 (96%)	154 (89%)	19 (11%)	6 10
36	1e	113/123 (92%)	102 (90%)	11 (10%)	8 14
36	2e	114/123 (93%)	94 (82%)	20 (18%)	2 3
37	1f	84/90 (93%)	77 (92%)	7 (8%)	11 20
37	2f	85/90 (94%)	83 (98%)	2 (2%)	49 68
38	1g	119/127 (94%)	109 (92%)	10 (8%)	11 19
38	2g	120/127 (94%)	113 (94%)	7 (6%)	20 35
39	1h	114/119 (96%)	112 (98%)	2 (2%)	59 75
39	2h	114/119 (96%)	107 (94%)	7 (6%)	18 33
40	1i	90/99 (91%)	85 (94%)	5 (6%)	21 36
40	2i	89/99 (90%)	73 (82%)	16 (18%)	1 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
41	1j	66/92 (72%)	58 (88%)	8 (12%)	5 8
41	2j	69/92 (75%)	57 (83%)	12 (17%)	2 3
42	1k	82/99 (83%)	75 (92%)	7 (8%)	10 19
42	2k	83/99 (84%)	76 (92%)	7 (8%)	11 19
43	1l	96/108 (89%)	91 (95%)	5 (5%)	23 39
43	2l	96/108 (89%)	91 (95%)	5 (5%)	23 39
44	1m	93/101 (92%)	86 (92%)	7 (8%)	13 23
44	2m	92/101 (91%)	80 (87%)	12 (13%)	4 6
45	1n	49/50 (98%)	46 (94%)	3 (6%)	18 33
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7 12
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33 53
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13 22
47	1p	69/74 (93%)	57 (83%)	12 (17%)	2 3
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5 8
48	1q	94/97 (97%)	91 (97%)	3 (3%)	39 59
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13 24
49	1r	59/77 (77%)	55 (93%)	4 (7%)	16 28
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7 12
50	1s	69/80 (86%)	64 (93%)	5 (7%)	14 25
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5 8
51	1t	70/82 (85%)	66 (94%)	4 (6%)	20 36
51	2t	70/82 (85%)	66 (94%)	4 (6%)	20 36
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	15 (83%)	3 (17%)	2 3
All	All	9303/10064 (92%)	8551 (92%)	752 (8%)	11 21

All (752) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	12	SER
3	1D	54	ARG
3	1D	115	GLN
3	1D	141	VAL

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Mol	Chain	Res	Type
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	273	ARG
4	1E	47	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	113	PHE
4	1E	116	VAL
4	1E	127	ASP
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	127	GLU
5	1F	140	LEU
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	192	LEU
5	1F	205	ARG
6	1G	3	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	91	ARG
6	1G	133	LEU
6	1G	140	ILE
6	1G	148	MET
6	1G	149	VAL
7	1H	3	ARG
7	1H	15	VAL
7	1H	33	LEU
7	1H	45	VAL
7	1H	56	SER
7	1H	84	SER
7	1H	98	LEU
7	1H	116	GLU
7	1H	119	GLU

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Mol	Chain	Res	Type
7	1H	127	GLU
7	1H	132	ARG
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	38	LEU
8	1I	40	THR
8	1I	41	GLU
8	1I	47	LEU
8	1I	61	ARG
8	1I	76	THR
8	1I	87	LYS
8	1I	92	VAL
8	1I	108	THR
8	1I	133	HIS
8	1I	140	LEU
8	1I	142	VAL
9	1N	1	MET
9	1N	8	GLN
9	1N	28	THR
9	1N	48	MET
9	1N	68	GLU
9	1N	104	LYS
9	1N	112	LEU
9	1N	138	LEU
10	1O	28	SER
10	1O	80	ASP
10	1O	89	ASN
11	1P	1	MET
11	1P	4	SER
11	1P	7	ARG
11	1P	42	SER
11	1P	45	LEU
11	1P	95	VAL
11	1P	126	VAL
11	1P	147	LEU
11	1P	148	LEU
11	1P	149	GLU
12	1Q	7	MET
12	1Q	16	ARG
12	1Q	75	THR
12	1Q	109	VAL

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Mol	Chain	Res	Type
13	1R	6	SER
13	1R	36	THR
13	1R	67	LEU
13	1R	100	LEU
14	1S	25	ARG
14	1S	36	TYR
14	1S	49	VAL
14	1S	69	VAL
14	1S	73	LEU
14	1S	110	LEU
15	1T	28	VAL
15	1T	36	GLU
15	1T	49	VAL
15	1T	96	ARG
15	1T	118	ARG
15	1T	128	GLU
16	1U	31	SER
16	1U	74	LEU
16	1U	77	SER
16	1U	78	THR
16	1U	95	LEU
16	1U	100	VAL
17	1V	7	THR
17	1V	73	SER
17	1V	79	VAL
17	1V	85	LYS
18	1W	4	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	63	ASP
18	1W	67	ASP
19	1X	2	LYS
19	1X	35	THR
19	1X	81	VAL
19	1X	88	LYS
20	1Y	1	MET
20	1Y	24	VAL
20	1Y	43	ASN
20	1Y	64	GLU
20	1Y	67	LEU

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Mol	Chain	Res	Type
20	1Y	70	SER
20	1Y	87	LYS
20	1Y	99	CYS
20	1Y	106	LEU
20	1Y	107	ASP
21	1Z	1	MET
21	1Z	28	MET
21	1Z	33	LEU
21	1Z	49	ARG
21	1Z	61	LEU
21	1Z	84	GLU
21	1Z	86	VAL
21	1Z	129	SER
21	1Z	138	GLU
21	1Z	150	LEU
21	1Z	154	ASP
21	1Z	161	VAL
21	1Z	163	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	7	LEU
22	10	49	LYS
22	10	55	ARG
23	11	30	VAL
23	11	35	THR
23	11	38	SER
23	11	56	GLN
23	11	80	LEU
23	11	83	GLU
23	11	91	LYS
24	12	3	LEU
24	12	19	VAL
24	12	28	LYS
24	12	68	ARG
25	13	29	ARG
25	13	35	ARG
25	13	54	VAL
25	13	55	ARG
25	13	60	GLU
26	14	1	MET
26	14	27	THR
26	14	49	PHE

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Mol	Chain	Res	Type
26	14	52	THR
26	14	53	GLU
26	14	63	TYR
26	14	67	TYR
26	14	69	LYS
27	15	6	VAL
27	15	40	LYS
28	16	4	GLU
28	16	5	VAL
28	16	6	ARG
28	16	19	ARG
28	16	44	ARG
29	17	1	MET
29	17	43	THR
30	18	31	HIS
33	1b	12	GLU
33	1b	21	ARG
33	1b	23	ARG
33	1b	24	TRP
33	1b	54	THR
33	1b	83	MET
33	1b	93	VAL
33	1b	94	ASN
33	1b	104	ASN
33	1b	154	LEU
33	1b	160	ASP
33	1b	172	ILE
33	1b	185	ILE
33	1b	196	LEU
33	1b	208	ILE
33	1b	215	LEU
33	1b	223	ILE
33	1b	226	ARG
33	1b	231	GLU
34	1c	3	ASN
34	1c	8	ILE
34	1c	20	SER
34	1c	26	LYS
34	1c	43	LEU
34	1c	66	VAL
34	1c	77	ILE
34	1c	89	GLU

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Mol	Chain	Res	Type
34	1c	104	GLN
34	1c	131	ARG
34	1c	144	SER
34	1c	178	LEU
34	1c	191	THR
34	1c	192	THR
34	1c	207	VAL
35	1d	19	LEU
35	1d	31	CYS
35	1d	135	LEU
35	1d	157	LEU
35	1d	158	ILE
35	1d	177	ASP
35	1d	178	VAL
35	1d	190	ASP
35	1d	194	LEU
36	1e	16	THR
36	1e	19	MET
36	1e	24	ARG
36	1e	27	ARG
36	1e	41	VAL
36	1e	53	LEU
36	1e	64	ARG
36	1e	82	VAL
36	1e	131	ILE
36	1e	147	ASP
36	1e	151	LEU
37	1f	17	SER
37	1f	19	LEU
37	1f	36	ARG
37	1f	55	ASP
37	1f	75	LEU
37	1f	94	GLN
37	1f	98	LEU
38	1g	6	ARG
38	1g	10	ARG
38	1g	12	LEU
38	1g	24	THR
38	1g	50	ILE
38	1g	61	VAL
38	1g	78	ARG
38	1g	79	ARG

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Mol	Chain	Res	Type
38	1g	90	GLU
38	1g	104	LEU
39	1h	39	LEU
39	1h	52	ASP
40	1i	17	VAL
40	1i	23	ASN
40	1i	42	ARG
40	1i	56	LEU
40	1i	128	ARG
41	1j	8	LEU
41	1j	19	SER
41	1j	38	ILE
41	1j	66	ARG
41	1j	67	THR
41	1j	81	THR
41	1j	92	THR
41	1j	95	GLU
42	1k	31	THR
42	1k	33	THR
42	1k	48	ILE
42	1k	87	THR
42	1k	109	VAL
42	1k	114	VAL
42	1k	126	ARG
43	1l	18	VAL
43	1l	54	LYS
43	1l	59	ARG
43	1l	70	ILE
43	1l	123	LYS
44	1m	4	ILE
44	1m	14	ARG
44	1m	43	THR
44	1m	49	THR
44	1m	70	LEU
44	1m	105	THR
44	1m	106	ASN
45	1n	3	ARG
45	1n	18	VAL
45	1n	33	VAL
46	1o	39	LEU
46	1o	76	GLU
46	1o	83	GLU

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Mol	Chain	Res	Type
47	1p	5	ARG
47	1p	20	VAL
47	1p	21	VAL
47	1p	22	THR
47	1p	27	LYS
47	1p	42	ARG
47	1p	43	LYS
47	1p	45	THR
47	1p	60	LEU
47	1p	61	SER
47	1p	72	ARG
47	1p	76	GLN
48	1q	9	VAL
48	1q	19	VAL
48	1q	63	ARG
49	1r	42	ARG
49	1r	46	GLU
49	1r	61	LYS
49	1r	63	GLN
50	1s	5	LEU
50	1s	35	SER
50	1s	38	SER
50	1s	48	THR
50	1s	79	THR
51	1t	10	LEU
51	1t	24	LEU
51	1t	38	LYS
51	1t	89	ARG
3	2D	3	VAL
3	2D	12	SER
3	2D	37	LEU
3	2D	88	ARG
3	2D	113	VAL
3	2D	116	GLN
3	2D	141	VAL
3	2D	162	SER
3	2D	229	VAL
3	2D	242	ARG
3	2D	253	GLN
3	2D	259	THR
4	2E	38	THR
4	2E	73	GLU

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Mol	Chain	Res	Type
4	2E	90	THR
4	2E	116	VAL
4	2E	175	VAL
5	2F	20	LEU
5	2F	33	LEU
5	2F	50	SER
5	2F	53	THR
5	2F	60	SER
5	2F	70	THR
5	2F	74	ARG
5	2F	108	LYS
5	2F	125	LEU
5	2F	126	VAL
5	2F	153	SER
5	2F	157	VAL
5	2F	158	THR
5	2F	160	ASN
5	2F	175	THR
5	2F	192	LEU
5	2F	197	ASP
6	2G	7	LEU
6	2G	8	LYS
6	2G	18	GLU
6	2G	28	VAL
6	2G	31	VAL
6	2G	33	ARG
6	2G	43	LEU
6	2G	45	GLU
6	2G	51	ARG
6	2G	53	LEU
6	2G	60	LEU
6	2G	75	LYS
6	2G	79	ASN
6	2G	88	ILE
6	2G	91	ARG
6	2G	92	VAL
6	2G	130	ASN
6	2G	140	ILE
6	2G	148	MET
6	2G	152	LEU
6	2G	155	MET
6	2G	159	VAL

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Mol	Chain	Res	Type
6	2G	170	ARG
7	2H	3	ARG
7	2H	23	ARG
7	2H	52	VAL
7	2H	57	ASP
7	2H	68	THR
7	2H	71	LEU
7	2H	81	GLU
7	2H	84	SER
7	2H	92	ILE
7	2H	111	HIS
7	2H	122	THR
7	2H	129	THR
7	2H	152	ARG
8	2I	38	LEU
8	2I	47	LEU
8	2I	50	ARG
8	2I	58	LEU
8	2I	66	GLU
8	2I	69	LYS
8	2I	77	LEU
8	2I	82	ARG
8	2I	86	THR
8	2I	96	ASP
8	2I	102	SER
8	2I	117	GLU
8	2I	127	VAL
8	2I	139	GLN
8	2I	144	VAL
9	2N	1	MET
9	2N	15	LEU
9	2N	23	LEU
9	2N	28	THR
9	2N	38	HIS
9	2N	43	THR
9	2N	46	VAL
9	2N	58	ASP
9	2N	60	ILE
9	2N	68	GLU
9	2N	138	LEU
10	2O	38	VAL
10	2O	52	VAL

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Mol	Chain	Res	Type
10	2O	66	LYS
10	2O	69	ILE
11	2P	3	LEU
11	2P	7	ARG
11	2P	45	LEU
11	2P	70	GLN
11	2P	95	VAL
11	2P	135	LEU
11	2P	149	GLU
12	2Q	1	MET
12	2Q	5	ARG
12	2Q	7	MET
12	2Q	10	ARG
12	2Q	12	GLN
12	2Q	14	ARG
12	2Q	75	THR
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	133	ARG
13	2R	6	SER
13	2R	24	GLN
13	2R	100	LEU
13	2R	114	VAL
14	2S	12	PHE
14	2S	20	ARG
14	2S	21	THR
14	2S	36	TYR
14	2S	44	LYS
14	2S	49	VAL
14	2S	53	SER
14	2S	58	LEU
14	2S	71	ARG
14	2S	98	VAL
14	2S	101	LEU
14	2S	107	GLU
15	2T	15	VAL
15	2T	17	THR
15	2T	63	VAL
15	2T	89	VAL
15	2T	96	ARG
15	2T	124	ASP
16	2U	5	LYS

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Mol	Chain	Res	Type
16	2U	95	LEU
17	2V	1	MET
17	2V	7	THR
17	2V	33	VAL
17	2V	52	VAL
17	2V	53	GLU
17	2V	79	VAL
17	2V	95	LEU
17	2V	98	GLU
18	2W	11	ARG
18	2W	15	ARG
18	2W	67	ASP
18	2W	85	VAL
19	2X	2	LYS
19	2X	35	THR
19	2X	57	LEU
19	2X	81	VAL
20	2Y	1	MET
20	2Y	11	ASP
20	2Y	38	ILE
20	2Y	49	VAL
20	2Y	61	ILE
20	2Y	70	SER
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	99	CYS
20	2Y	107	ASP
21	2Z	11	GLU
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	46	LYS
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	76	LEU
21	2Z	123	ASP
21	2Z	129	SER
21	2Z	133	ILE
21	2Z	145	GLU
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	171	ILE
22	20	68	GLU

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Mol	Chain	Res	Type
23	21	26	ARG
23	21	35	THR
23	21	83	GLU
24	22	5	GLU
24	22	19	VAL
24	22	52	ASP
24	22	70	GLN
25	23	6	VAL
25	23	31	LEU
26	24	9	LEU
26	24	24	THR
26	24	27	THR
26	24	34	GLU
26	24	49	PHE
26	24	58	ARG
26	24	59	PHE
26	24	63	TYR
26	24	67	TYR
27	25	33	CYS
27	25	40	LYS
27	25	59	GLU
28	26	6	ARG
28	26	9	LEU
28	26	19	ARG
28	26	20	ASN
28	26	23	THR
28	26	49	HIS
28	26	50	ARG
28	26	52	VAL
29	27	1	MET
29	27	4	THR
29	27	43	THR
29	27	47	ARG
30	28	4	MET
30	28	19	SER
30	28	31	HIS
30	28	34	TRP
31	29	28	GLU
33	2b	8	LYS
33	2b	11	LEU
33	2b	16	HIS
33	2b	24	TRP

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Mol	Chain	Res	Type
33	2b	33	TYR
33	2b	45	GLN
33	2b	47	THR
33	2b	56	ARG
33	2b	58	ILE
33	2b	68	ILE
33	2b	71	VAL
33	2b	76	GLN
33	2b	83	MET
33	2b	93	VAL
33	2b	94	ASN
33	2b	101	MET
33	2b	107	THR
33	2b	109	SER
33	2b	115	LEU
33	2b	118	LEU
33	2b	127	ILE
33	2b	140	HIS
33	2b	141	GLU
33	2b	149	LEU
33	2b	160	ASP
33	2b	164	VAL
33	2b	175	ARG
33	2b	180	LEU
33	2b	189	ASP
33	2b	210	SER
33	2b	217	ARG
33	2b	223	ILE
33	2b	230	VAL
34	2c	4	LYS
34	2c	22	TRP
34	2c	28	GLN
34	2c	46	GLU
34	2c	49	SER
34	2c	56	ASP
34	2c	58	GLU
34	2c	68	VAL
34	2c	69	HIS
34	2c	77	ILE
34	2c	111	LEU
34	2c	128	PHE
34	2c	132	ARG

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Mol	Chain	Res	Type
34	2c	140	ARG
34	2c	190	ARG
34	2c	191	THR
34	2c	192	THR
34	2c	193	TYR
35	2d	8	VAL
35	2d	12	CYS
35	2d	17	VAL
35	2d	42	GLN
35	2d	47	ARG
35	2d	50	ARG
35	2d	59	ARG
35	2d	71	SER
35	2d	83	SER
35	2d	94	LEU
35	2d	96	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	157	LEU
35	2d	158	ILE
35	2d	168	ARG
35	2d	201	GLN
36	2e	13	ILE
36	2e	18	ARG
36	2e	25	ARG
36	2e	27	ARG
36	2e	38	GLN
36	2e	41	VAL
36	2e	47	LYS
36	2e	50	GLU
36	2e	51	VAL
36	2e	60	TYR
36	2e	72	GLN
36	2e	78	HIS
36	2e	81	GLU
36	2e	84	PHE
36	2e	100	VAL
36	2e	115	VAL
36	2e	136	MET
36	2e	141	GLN

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Mol	Chain	Res	Type
36	2e	144	THR
36	2e	149	GLU
37	2f	36	ARG
37	2f	69	GLU
38	2g	51	GLN
38	2g	57	GLU
38	2g	75	VAL
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	155	ARG
39	2h	3	THR
39	2h	23	SER
39	2h	52	ASP
39	2h	54	ASP
39	2h	107	LEU
39	2h	112	LEU
39	2h	122	ARG
40	2i	20	ARG
40	2i	41	VAL
40	2i	50	LEU
40	2i	54	ASP
40	2i	64	THR
40	2i	65	VAL
40	2i	66	ARG
40	2i	75	ASP
40	2i	89	ASN
40	2i	102	LEU
40	2i	107	ARG
40	2i	108	VAL
40	2i	113	LYS
40	2i	114	TYR
40	2i	120	ARG
40	2i	125	TYR
41	2j	8	LEU
41	2j	9	ARG
41	2j	29	ARG
41	2j	30	SER
41	2j	38	ILE
41	2j	67	THR
41	2j	72	VAL
41	2j	74	ILE

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Mol	Chain	Res	Type
41	2j	81	THR
41	2j	89	ASP
41	2j	95	GLU
41	2j	97	GLU
42	2k	14	VAL
42	2k	24	SER
42	2k	33	THR
42	2k	48	ILE
42	2k	81	ASP
42	2k	96	ARG
42	2k	117	ASN
43	2l	36	VAL
43	2l	38	THR
43	2l	39	VAL
43	2l	40	VAL
43	2l	59	ARG
44	2m	22	ILE
44	2m	27	LYS
44	2m	32	GLU
44	2m	34	LEU
44	2m	37	THR
44	2m	50	GLU
44	2m	82	MET
44	2m	90	LEU
44	2m	91	ARG
44	2m	103	THR
44	2m	106	ASN
44	2m	110	ARG
45	2n	3	ARG
45	2n	13	THR
45	2n	18	VAL
45	2n	31	ARG
45	2n	33	VAL
46	2o	7	GLU
46	2o	38	ARG
46	2o	39	LEU
46	2o	54	ARG
46	2o	83	GLU
46	2o	88	ARG
47	2p	1	MET
47	2p	2	VAL
47	2p	21	VAL

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Mol	Chain	Res	Type
47	2p	45	THR
47	2p	54	GLU
47	2p	67	THR
47	2p	69	THR
47	2p	76	GLN
48	2q	9	VAL
48	2q	19	VAL
48	2q	56	VAL
48	2q	60	ILE
48	2q	63	ARG
48	2q	85	VAL
48	2q	99	SER
49	2r	21	LYS
49	2r	31	LEU
49	2r	53	ARG
49	2r	54	ARG
49	2r	84	LYS
49	2r	87	ARG
50	2s	7	LYS
50	2s	14	HIS
50	2s	20	LEU
50	2s	31	ILE
50	2s	37	ARG
50	2s	41	VAL
50	2s	45	VAL
50	2s	81	ARG
51	2t	15	ARG
51	2t	71	THR
51	2t	86	ARG
51	2t	90	GLN
52	2u	7	ARG
52	2u	13	ILE
52	2u	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	116	GLN
3	1D	164	GLN
4	1E	48	GLN
5	1F	69	HIS
5	1F	203	GLN

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Mol	Chain	Res	Type
6	1G	26	GLN
10	1O	89	ASN
12	1Q	123	HIS
13	1R	91	GLN
15	1T	58	ASN
16	1U	81	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	34	ASN
21	1Z	54	HIS
21	1Z	73	GLN
21	1Z	132	ASN
21	1Z	151	HIS
23	11	56	GLN
25	13	32	GLN
26	14	47	GLN
33	1b	40	HIS
33	1b	94	ASN
33	1b	135	GLN
34	1c	6	HIS
34	1c	69	HIS
34	1c	162	GLN
34	1c	170	GLN
35	1d	43	HIS
35	1d	77	ASN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
36	1e	65	ASN
36	1e	78	HIS
36	1e	141	GLN
37	1f	13	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	153	HIS
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS

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Mol	Chain	Res	Type
40	1i	73	GLN
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
47	1p	76	GLN
49	1r	63	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	56	GLN
50	1s	83	HIS
51	1t	26	ASN
51	1t	90	GLN
3	2D	143	HIS
4	2E	48	GLN
5	2F	69	HIS
5	2F	160	ASN
5	2F	204	ASN
6	2G	130	ASN
6	2G	132	ASN
7	2H	111	HIS
8	2I	133	HIS
9	2N	131	GLN
10	2O	5	GLN
11	2P	70	GLN
12	2Q	12	GLN
12	2Q	123	HIS
14	2S	38	GLN
15	2T	58	ASN
15	2T	123	GLN
16	2U	94	ASN
18	2W	60	ASN
19	2X	31	HIS
21	2Z	32	HIS
21	2Z	55	HIS
21	2Z	73	GLN
21	2Z	151	HIS
22	20	70	GLN
23	21	56	GLN
24	22	70	GLN
26	24	40	HIS
26	24	46	GLN

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Mol	Chain	Res	Type
33	2b	45	GLN
33	2b	135	GLN
33	2b	146	GLN
33	2b	212	GLN
34	2c	98	ASN
34	2c	102	ASN
34	2c	136	GLN
34	2c	162	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	161	ASN
35	2d	201	GLN
36	2e	20	GLN
36	2e	72	GLN
37	2f	64	GLN
37	2f	73	ASN
37	2f	94	GLN
37	2f	100	ASN
38	2g	11	GLN
38	2g	28	ASN
38	2g	37	ASN
38	2g	148	ASN
39	2h	82	HIS
40	2i	3	GLN
40	2i	58	HIS
40	2i	89	ASN
42	2k	38	ASN
42	2k	104	GLN
42	2k	117	ASN
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
46	2o	13	GLN
47	2p	13	HIS
49	2r	63	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	16	HIS
51	2t	45	GLN

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Mol	Chain	Res	Type
51	2t	75	ASN
51	2t	90	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	444 (15%)	29 (1%)
1	2A	2790/2915 (95%)	468 (16%)	19 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	34 (28%)	0
32	1a	1494/1521 (98%)	250 (16%)	0
32	2a	1498/1521 (98%)	308 (20%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	25 (35%)	0
54	1y	71/76 (93%)	30 (42%)	0
54	2w	68/76 (89%)	25 (36%)	0
54	2y	69/76 (90%)	24 (34%)	0
55	1x	75/77 (97%)	13 (17%)	0
55	2x	75/77 (97%)	12 (16%)	0
All	All	9335/9620 (97%)	1644 (17%)	48 (0%)

All (1644) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	55	G
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	78	A
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G

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Mol	Chain	Res	Type
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	250	G
1	1A	269	U
1	1A	271(B)	C
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(R)	G
1	1A	272(B)	G
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	342	G
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	363(F)	A
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	421	U
1	1A	428	A
1	1A	443	A

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Mol	Chain	Res	Type
1	1A	444	C
1	1A	448	U
1	1A	454	A
1	1A	456	C
1	1A	457	A
1	1A	480	A
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	551	G
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	619	G
1	1A	627	A
1	1A	634	C
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	668	G
1	1A	669	G

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Mol	Chain	Res	Type
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	832	G
1	1A	855	G
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	952	G
1	1A	953	A
1	1A	958	U

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Mol	Chain	Res	Type
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1005	C
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1041	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1063	G
1	1A	1067	A
1	1A	1069	A
1	1A	1071	G
1	1A	1072	C
1	1A	1073	A
1	1A	1075	C
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1083	U
1	1A	1085	A
1	1A	1087	G
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1101	U
1	1A	1104	C

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Mol	Chain	Res	Type
1	1A	1108	U
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1117	G
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1218	C
1	1A	1220	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1276	A
1	1A	1300	U
1	1A	1301	A
1	1A	1329	U
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1439	A

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Mol	Chain	Res	Type
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1467	C
1	1A	1472	A
1	1A	1473	G
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1540	U
1	1A	1542	A
1	1A	1545	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1589	C
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A

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Mol	Chain	Res	Type
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1900	A
1	1A	1906	G
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	1983	C
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2030	A
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2101	G
1	1A	2108	C
1	1A	2113	U

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Mol	Chain	Res	Type
1	1A	2114	A
1	1A	2116	G
1	1A	2121	G
1	1A	2122	U
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	2145	C
1	1A	2146	C
1	1A	2147	G
1	1A	2149	G
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2163	C
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G

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Mol	Chain	Res	Type
1	1A	2208	A
1	1A	2218	U
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2268	A
1	1A	2269	A
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2410	G
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2440	C
1	1A	2441	C
1	1A	2448	A
1	1A	2474	C
1	1A	2476	A
1	1A	2490	G
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2525	G
1	1A	2529	G

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Mol	Chain	Res	Type
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2582	G
1	1A	2585	U
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	2733	A
1	1A	2744	G
1	1A	2757	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
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2803	C
1	1A	2820	A
1	1A	2821	A

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Mol	Chain	Res	Type
1	1A	2835	A
1	1A	2836	U
1	1A	2839	G
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	25	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	106	G
2	1B	109	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	65	U
32	1a	73	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	129(A)	G
32	1a	131	C
32	1a	151	A
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	189(H)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A

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Mol	Chain	Res	Type
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	219	C
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	317	G
32	1a	318	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	344	A
32	1a	345	C
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	461	A

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Mol	Chain	Res	Type
32	1a	470	C
32	1a	483	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	639	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	666	G
32	1a	671	G
32	1a	672	U
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	717	C
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	734	G
32	1a	747	C
32	1a	749	C

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Mol	Chain	Res	Type
32	1a	753	A
32	1a	755	G
32	1a	759	A
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	872	A
32	1a	876	G
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	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	983	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1001	A
32	1a	1001(A)	G

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Mol	Chain	Res	Type
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1007	C
32	1a	1009	G
32	1a	1010	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1041	A
32	1a	1042	G
32	1a	1043	C
32	1a	1044	A
32	1a	1046	A
32	1a	1063	C
32	1a	1068	G
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A

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Mol	Chain	Res	Type
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1213	A
32	1a	1227	A
32	1a	1238	A
32	1a	1246	C
32	1a	1250	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	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	1370	G
32	1a	1378	C
32	1a	1394	A
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A

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Mol	Chain	Res	Type
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	9	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	34	G
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	62	C
54	1w	63	G
54	1w	64	A
54	1w	65	G
54	1w	66	U
54	1w	68	C
54	1w	70	G
54	1w	71	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
55	1x	3	C
55	1x	6	G
55	1x	9	G

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Mol	Chain	Res	Type
55	1x	13	C
55	1x	14	A
55	1x	17(A)	U
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	59	A
55	1x	61	C
55	1x	76	A
54	1y	6	G
54	1y	7	A
54	1y	8	4SU
54	1y	9	A
54	1y	11	C
54	1y	13	C
54	1y	14	A
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	22	G
54	1y	26	A
54	1y	27	G
54	1y	33	U
54	1y	35	A
54	1y	36	A
54	1y	44	G
54	1y	45	U
54	1y	46	G7M
54	1y	48	C
54	1y	52	G
54	1y	53	G
54	1y	54	5MU
54	1y	55	PSU
54	1y	56	C
54	1y	57	G
54	1y	58	A
54	1y	64	A
54	1y	65	G
54	1y	70	G
1	2A	8	A
1	2A	15	G

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Mol	Chain	Res	Type
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	266	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A

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Mol	Chain	Res	Type
1	2A	279	C
1	2A	311	A
1	2A	316	C
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	354	G
1	2A	357	A
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	434	U
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	496	G
1	2A	503	A
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	556	G
1	2A	563	G
1	2A	568	U

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Mol	Chain	Res	Type
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	595	C
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	649	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	753	C
1	2A	764	A
1	2A	771	G
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	793	A
1	2A	794	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	847	U
1	2A	857	C

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Mol	Chain	Res	Type
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	875	G
1	2A	877	U
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	907	U
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	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	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	995	C
1	2A	996	A
1	2A	999	U
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1020	A
1	2A	1022	G

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Mol	Chain	Res	Type
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1126	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1169	G
1	2A	1171	G
1	2A	1195	G
1	2A	1204	A
1	2A	1205	U
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1244	G
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
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	1373	A

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Mol	Chain	Res	Type
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1412	A
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1428	C
1	2A	1436	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1506	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1640	C

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Mol	Chain	Res	Type
1	2A	1648	C
1	2A	1653	G
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1896	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

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Mol	Chain	Res	Type
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2035	G
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2063	C
1	2A	2069	G
1	2A	2093	G
1	2A	2106	G
1	2A	2108	C
1	2A	2109	U
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C

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Mol	Chain	Res	Type
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2140	C
1	2A	2143	C
1	2A	2146	C
1	2A	2148	G
1	2A	2150	U
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2181	G
1	2A	2182	G
1	2A	2185	C
1	2A	2189	U
1	2A	2190	G
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A

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Mol	Chain	Res	Type
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2469	A
1	2A	2476	A
1	2A	2490	G
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C

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Mol	Chain	Res	Type
1	2A	2582	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2623	G
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2646	C
1	2A	2654	A
1	2A	2669	G
1	2A	2673	G
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
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	2748	A
1	2A	2751	G
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2769	C
1	2A	2778	A
1	2A	2780	G
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2807	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G

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Mol	Chain	Res	Type
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	20	C
2	2B	24	G
2	2B	25	A
2	2B	30	C
2	2B	33	G
2	2B	34	U
2	2B	35	U
2	2B	41	U
2	2B	42	C
2	2B	45	A
2	2B	51	G
2	2B	53	A
2	2B	58	A
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	89	G
2	2B	91	C
2	2B	105	A
2	2B	106	G
2	2B	110	G
2	2B	112	U
2	2B	116	G
2	2B	120	A
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	31	G

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Mol	Chain	Res	Type
32	2a	32	A
32	2a	39	G
32	2a	41	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	105	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	156	G
32	2a	159	G
32	2a	163	C
32	2a	180	U
32	2a	182	U
32	2a	189	G
32	2a	189(F)	U
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	274	A

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Mol	Chain	Res	Type
32	2a	281	G
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	381	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
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	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A

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Mol	Chain	Res	Type
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	607	A
32	2a	630	G
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	708	C
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	748	C
32	2a	749	C
32	2a	755	G
32	2a	760	G
32	2a	772	U
32	2a	773	G
32	2a	777	A
32	2a	787	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U

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Mol	Chain	Res	Type
32	2a	853	G
32	2a	854	G
32	2a	859	A
32	2a	864	A
32	2a	872	A
32	2a	873	A
32	2a	885	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	978	A
32	2a	979	C
32	2a	984	C
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	996	A
32	2a	997	U
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A

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Mol	Chain	Res	Type
32	2a	1017	G
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1051	C
32	2a	1053	G
32	2a	1054	C
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1109	C
32	2a	1113	C
32	2a	1118	C
32	2a	1122	U
32	2a	1126	U
32	2a	1127	G
32	2a	1128	C
32	2a	1129	C

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Mol	Chain	Res	Type
32	2a	1133	G
32	2a	1134	G
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1172	C
32	2a	1173	G
32	2a	1181	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1195	C
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1202	G
32	2a	1207	2MG
32	2a	1208	C
32	2a	1211	U
32	2a	1213	A
32	2a	1226	C
32	2a	1227	A
32	2a	1228	C
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1246	C
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1262	C
32	2a	1264	C
32	2a	1270	C

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Mol	Chain	Res	Type
32	2a	1272	G
32	2a	1273	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1283	G
32	2a	1285	A
32	2a	1287	A
32	2a	1293	G
32	2a	1294	G
32	2a	1297	C
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1312	G
32	2a	1321	C
32	2a	1322	C
32	2a	1323	G
32	2a	1336	C
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1354	C
32	2a	1358	U
32	2a	1359	C
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1368	G
32	2a	1380	U
32	2a	1398	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1497	G
32	2a	1499	A

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Mol	Chain	Res	Type
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	23	A
54	2w	3	C
54	2w	4	C
54	2w	6	G
54	2w	7	A
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	27	G
54	2w	45	U
54	2w	46	G7M
54	2w	48	C
54	2w	51	U
54	2w	59	U
54	2w	62	C
54	2w	64	A
54	2w	65	G
54	2w	66	U
54	2w	69	G
54	2w	70	G
54	2w	71	G
54	2w	72	C
54	2w	73	A
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	19	G

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Mol	Chain	Res	Type
55	2x	20	U
55	2x	21	A
55	2x	22	G
55	2x	46	G
55	2x	47	U
55	2x	52	G
55	2x	56	C
55	2x	76	A
54	2y	8	4SU
54	2y	14	A
54	2y	15	G
54	2y	19	G
54	2y	24	G
54	2y	27	G
54	2y	30	G
54	2y	33	U
54	2y	45	U
54	2y	46	G7M
54	2y	48	C
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	54	5MU
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	60	U
54	2y	63	G
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	774	A

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Mol	Chain	Res	Type
1	1A	827	U
1	1A	974	G
1	1A	1047	G
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1275	A
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2126	A
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U

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

84 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	$\#\|Z\| > 2$
54	PSU	1y	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
54	4SU	1w	8	54	18,21,22	1.68	5 (27%)	26,30,33	1.90	5 (19%)
32	MA6	1a	1519	32	18,26,27	0.82	0	19,38,41	1.48	2 (10%)
32	MA6	1a	1518	32	18,26,27	0.80	0	19,38,41	1.43	2 (10%)
54	MIA	1w	37	54	24,31,32	2.19	3 (12%)	26,44,47	2.59	9 (34%)
54	PSU	2y	55	54	18,21,22	1.29	2 (11%)	22,30,33	1.81	3 (13%)
32	5MC	2a	1407	32	18,22,23	1.02	2 (11%)	26,32,35	1.20	3 (11%)
55	5MU	1x	54	55	19,22,23	1.41	6 (31%)	28,32,35	2.10	6 (21%)
54	4SU	2y	8	54	18,21,22	1.64	4 (22%)	26,30,33	2.03	4 (15%)
1	OMU	1A	2552	1	19,22,23	1.10	3 (15%)	26,31,34	1.95	5 (19%)
32	5MC	2a	967	32	18,22,23	0.99	2 (11%)	26,32,35	1.14	2 (7%)
54	5MU	1w	54	54	19,22,23	1.41	6 (31%)	28,32,35	1.93	7 (25%)
54	MIA	1y	37	54	18,24,32	1.19	2 (11%)	18,35,47	1.26	2 (11%)
32	M2G	2a	966	32	20,27,28	1.48	3 (15%)	22,40,43	1.02	2 (9%)
54	5MU	1y	54	54	19,22,23	1.46	5 (26%)	28,32,35	1.59	5 (17%)
1	5MU	2A	1939	1,56	19,22,23	1.43	5 (26%)	28,32,35	2.30	6 (21%)
54	PSU	1y	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.76	3 (13%)
55	5MU	2x	54	55	19,22,23	1.39	5 (26%)	28,32,35	2.05	6 (21%)
1	PSU	1A	1917	1	18,21,22	1.39	3 (16%)	22,30,33	1.90	3 (13%)
54	PSU	1w	39	54	18,21,22	1.32	2 (11%)	22,30,33	2.00	4 (18%)
54	5MU	2y	54	54	19,22,23	1.51	4 (21%)	28,32,35	1.93	9 (32%)
1	OMC	1A	1920	1	19,22,23	0.88	0	26,31,34	1.04	1 (3%)
32	PSU	1a	516	32,56	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	2A	2251	1,56,55	18,26,27	0.91	1 (5%)	19,38,41	1.13	3 (15%)
54	G7M	2w	46	54	20,26,27	1.15	1 (5%)	17,39,42	0.90	0
54	PSU	2w	32	54	18,21,22	1.32	2 (11%)	22,30,33	1.83	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	PSU	1w	32	56,54	18,21,22	1.32	2 (11%)	22,30,33	1.67	3 (13%)
43	0TD	1l	92	43	7,9,10	4.79	1 (14%)	6,11,13	4.87	2 (33%)
1	5MU	1A	1915	1	19,22,23	1.40	5 (26%)	28,32,35	2.11	7 (25%)
54	G7M	1y	46	54	20,26,27	1.36	2 (10%)	17,39,42	0.54	0
32	5MC	1a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.16	3 (11%)
54	MIA	2y	37	54	18,24,32	1.20	2 (11%)	18,35,47	1.31	2 (11%)
54	MIA	2w	37	54	20,27,32	1.81	3 (15%)	22,39,47	1.78	7 (31%)
1	OMG	1A	2251	1,56,55	18,26,27	0.97	1 (5%)	19,38,41	1.15	3 (15%)
55	5MC	1x	32	55	18,22,23	1.01	2 (11%)	26,32,35	1.20	2 (7%)
55	4SU	1x	8	55	18,21,22	2.02	5 (27%)	26,30,33	1.43	6 (23%)
1	5MU	2A	1915	1,56	19,22,23	1.43	6 (31%)	28,32,35	2.18	6 (21%)
54	PSU	2y	39	54	18,21,22	1.39	2 (11%)	22,30,33	1.56	2 (9%)
32	4OC	2a	1402	32,56	20,23,24	0.79	0	26,32,35	1.08	3 (11%)
54	PSU	2w	55	54	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.14	2 (12%)
32	5MC	2a	1404	32	18,22,23	0.97	2 (11%)	26,32,35	1.11	2 (7%)
55	PSU	2x	55	55	18,21,22	1.31	2 (11%)	22,30,33	1.95	4 (18%)
32	5MC	1a	967	32	18,22,23	0.95	2 (11%)	26,32,35	1.09	2 (7%)
1	5MC	2A	1962	1,56	18,22,23	0.97	2 (11%)	26,32,35	1.20	2 (7%)
32	M2G	1a	966	32	20,27,28	1.48	3 (15%)	22,40,43	0.92	2 (9%)
32	G7M	2a	527	32,56	20,26,27	1.27	2 (10%)	17,39,42	0.54	0
1	5MC	2A	1942	1	18,22,23	0.97	2 (11%)	26,32,35	1.12	2 (7%)
1	OMU	2A	2552	1,56	19,22,23	1.19	2 (10%)	26,31,34	1.68	5 (19%)
32	5MC	1a	1407	32	18,22,23	0.94	2 (11%)	26,32,35	1.12	3 (11%)
54	4SU	2w	8	54	18,21,22	1.60	5 (27%)	26,30,33	2.01	5 (19%)
55	4SU	2x	8	56,55	18,21,22	1.92	5 (27%)	26,30,33	1.29	3 (11%)
32	UR3	2a	1498	32	19,22,23	1.04	2 (10%)	26,32,35	1.42	1 (3%)
1	PSU	2A	1911	1	18,21,22	1.38	2 (11%)	22,30,33	1.75	3 (13%)
54	PSU	1y	39	54	18,21,22	1.38	2 (11%)	22,30,33	1.82	3 (13%)
1	2MA	1A	2503	1,56	17,25,26	1.00	1 (5%)	17,37,40	1.02	2 (11%)
32	5MC	2a	1400	32	18,22,23	0.95	2 (11%)	26,32,35	1.20	3 (11%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	1A	1911	1	18,21,22	1.40	2 (11%)	22,30,33	1.87	4 (18%)
32	MA6	2a	1519	32	18,26,27	0.78	0	19,38,41	1.45	2 (10%)
32	MA6	2a	1518	32	18,26,27	0.79	0	19,38,41	1.38	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	4OC	1a	1402	32,56	20,23,24	0.74	0	26,32,35	0.91	1 (3%)
54	5MU	2w	54	54	19,22,23	1.42	4 (21%)	28,32,35	1.61	5 (17%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	22,30,33	1.73	4 (18%)
54	4SU	1y	8	54	18,21,22	1.74	6 (33%)	26,30,33	1.71	4 (15%)
1	5MC	1A	1962	1,56	18,22,23	0.95	2 (11%)	26,32,35	1.14	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.33	3 (16%)	22,30,33	1.85	4 (18%)
32	UR3	1a	1498	32	19,22,23	1.08	1 (5%)	26,32,35	1.43	2 (7%)
1	PSU	1A	2605	1,56	18,21,22	1.37	4 (22%)	22,30,33	1.86	4 (18%)
1	2MA	2A	2503	1,56	17,25,26	1.00	1 (5%)	17,37,40	1.03	2 (11%)
55	PSU	1x	55	55	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
54	G7M	2y	46	54	20,26,27	1.41	2 (10%)	17,39,42	0.63	0
54	PSU	2y	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.77	3 (13%)
43	0TD	2l	92	43	7,9,10	4.74	1 (14%)	6,11,13	9.17	1 (16%)
32	G7M	1a	527	32,56	20,26,27	1.28	2 (10%)	17,39,42	0.53	0
54	PSU	2w	39	54	18,21,22	1.45	2 (11%)	22,30,33	1.48	2 (9%)
1	5MU	1A	1939	1,56	19,22,23	1.42	4 (21%)	28,32,35	2.29	6 (21%)
32	2MG	2a	1207	32,56	18,26,27	0.93	1 (5%)	16,38,41	0.98	1 (6%)
1	OMC	2A	1920	1	19,22,23	0.79	0	26,31,34	0.82	0
54	G7M	1w	46	54	20,26,27	1.25	2 (10%)	17,39,42	0.58	0
55	5MC	2x	32	55	18,22,23	0.97	2 (11%)	26,32,35	1.18	3 (11%)
54	PSU	1w	55	54	18,21,22	1.38	2 (11%)	22,30,33	1.83	4 (18%)
1	5MC	1A	1942	1,56	18,22,23	0.94	2 (11%)	26,32,35	1.14	2 (7%)
32	5MC	1a	1404	32	18,22,23	1.01	2 (11%)	26,32,35	1.21	4 (15%)

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
54	PSU	1y	55	54	-	2/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	2/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/9/27/28	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
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
54	5MU	2y	54	54	-	3/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,56,55	-	2/5/27/28	0/3/3/3
54	G7M	2w	46	54	-	1/3/25/26	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	56,54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
54	G7M	1y	46	54	-	3/3/25/26	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	3/3/25/34	0/3/3/3
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
1	OMG	1A	2251	1,56,55	-	0/5/27/28	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1,56	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	1/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	G7M	2a	527	32,56	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	56,55	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	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
1	2MA	1A	2503	1,56	-	2/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	4OC	1a	1402	32,56	-	1/9/29/30	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
1	5MC	1A	1962	1,56	-	2/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
55	PSU	1x	55	55	-	2/7/25/26	0/2/2/2
54	G7M	2y	46	54	-	0/3/25/26	0/3/3/3
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
32	G7M	1a	527	32,56	-	3/3/25/26	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	2/5/27/28	0/3/3/3
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2

All (199) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.33	1.69	1.82
43	2l	92	0TD	CB-SB	-12.26	1.69	1.82
54	1w	37	MIA	C13-C14	7.05	1.52	1.32
54	2w	37	MIA	C2-S10	-6.62	1.70	1.75
54	1w	37	MIA	C2-S10	-6.52	1.70	1.75
32	2a	966	M2G	C2-N3	4.94	1.36	1.30
55	2x	8	4SU	C4-N3	-4.63	1.32	1.37
32	1a	966	M2G	C2-N3	4.59	1.36	1.30
55	1x	8	4SU	C4-N3	-4.57	1.32	1.37
54	2y	46	G7M	C5-C4	4.32	1.47	1.39
54	2y	8	4SU	C4-S4	-4.25	1.60	1.68
54	1y	8	4SU	C4-S4	-4.22	1.60	1.68
54	1w	8	4SU	C4-S4	-4.20	1.60	1.68
54	1y	46	G7M	C5-C4	4.14	1.47	1.39
55	1x	8	4SU	C4-S4	-4.08	1.60	1.68
54	2w	8	4SU	C4-S4	-4.01	1.60	1.68
54	2w	39	PSU	C6-C5	3.89	1.39	1.35
54	1y	39	PSU	C6-C5	3.89	1.39	1.35
54	1w	46	G7M	C5-C4	3.87	1.46	1.39
32	1a	527	G7M	C5-C4	3.86	1.46	1.39
55	2x	8	4SU	C4-S4	-3.84	1.61	1.68
32	2a	527	G7M	C5-C4	3.81	1.46	1.39
54	1w	55	PSU	C6-C5	3.77	1.39	1.35
54	2y	32	PSU	C6-C5	3.72	1.39	1.35
54	2w	55	PSU	C6-C5	3.70	1.39	1.35
54	2y	39	PSU	C6-C5	3.69	1.39	1.35
1	1A	1911	PSU	C6-C5	3.66	1.39	1.35
54	1y	32	PSU	C6-C5	3.65	1.39	1.35
54	1y	55	PSU	C6-C5	3.65	1.39	1.35
55	1x	8	4SU	C2-N3	-3.64	1.31	1.38
54	2w	46	G7M	C5-C4	3.56	1.46	1.39
1	1A	1917	PSU	C6-C5	3.56	1.39	1.35
1	2A	1911	PSU	C6-C5	3.43	1.39	1.35
54	1y	8	4SU	C4-N3	-3.42	1.34	1.37
32	2a	516	PSU	C6-C5	3.41	1.39	1.35
54	2w	32	PSU	C6-C5	3.37	1.39	1.35
32	1a	516	PSU	C6-C5	3.32	1.39	1.35
55	2x	55	PSU	C6-C5	3.32	1.39	1.35
1	2A	1917	PSU	C6-C5	3.28	1.39	1.35
54	2y	54	5MU	C2-N1	3.15	1.43	1.38
1	1A	1939	5MU	C4-N3	-3.12	1.33	1.38
54	1y	54	5MU	C6-C5	3.11	1.39	1.34
54	1w	32	PSU	C6-C5	3.10	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	8	4SU	C5-C4	-3.08	1.38	1.42
1	2A	2605	PSU	C6-C5	3.08	1.38	1.35
55	1x	32	5MC	C6-C5	3.06	1.39	1.34
55	1x	55	PSU	C6-C5	3.02	1.38	1.35
54	1w	8	4SU	C4-N3	-3.01	1.34	1.37
54	1w	39	PSU	C6-C5	3.01	1.38	1.35
54	2y	54	5MU	C6-C5	3.00	1.39	1.34
54	1y	54	5MU	C4-N3	-2.99	1.33	1.38
54	2w	54	5MU	C6-C5	2.97	1.39	1.34
1	2A	1942	5MC	C6-C5	2.93	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.92	1.33	1.38
54	1y	37	MIA	C5-C4	2.92	1.48	1.40
55	2x	54	5MU	C6-C5	2.91	1.39	1.34
55	2x	8	4SU	C5-C4	-2.91	1.38	1.42
54	2y	37	MIA	C5-C4	2.90	1.48	1.40
54	2y	55	PSU	C6-C5	2.90	1.38	1.35
54	2w	39	PSU	C4-N3	-2.89	1.33	1.38
32	1a	966	M2G	C2-N2	2.88	1.40	1.35
55	2x	8	4SU	C2-N3	-2.87	1.32	1.38
55	2x	32	5MC	C6-C5	2.86	1.39	1.34
32	2a	1404	5MC	C6-C5	2.86	1.39	1.34
32	2a	967	5MC	C6-C5	2.86	1.39	1.34
32	1a	1400	5MC	C6-C5	2.85	1.39	1.34
54	2w	8	4SU	C4-N3	-2.84	1.34	1.37
32	2a	1407	5MC	C6-C5	2.79	1.39	1.34
54	2y	8	4SU	C4-N3	-2.77	1.34	1.37
1	2A	1939	5MU	C6-C5	2.76	1.39	1.34
32	2a	966	M2G	C2-N2	2.73	1.40	1.35
1	2A	1939	5MU	C4-N3	-2.73	1.33	1.38
54	1w	54	5MU	C4-N3	-2.73	1.33	1.38
54	2y	37	MIA	C2-N3	2.72	1.36	1.32
1	2A	1911	PSU	C4-N3	-2.71	1.33	1.38
1	1A	1939	5MU	C6-C5	2.71	1.39	1.34
54	1y	37	MIA	C2-N3	2.70	1.36	1.32
54	2w	37	MIA	C5-C4	2.70	1.48	1.40
55	1x	54	5MU	C6-C5	2.69	1.39	1.34
32	1a	967	5MC	C6-C5	2.68	1.39	1.34
54	1w	39	PSU	C4-N3	-2.66	1.33	1.38
55	1x	54	5MU	C4-N3	-2.66	1.33	1.38
1	1A	1915	5MU	C6-C5	2.66	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.66	1.33	1.38
54	1w	32	PSU	C4-N3	-2.65	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1917	PSU	C4-N3	-2.64	1.33	1.38
1	2A	1915	5MU	C6-C5	2.62	1.38	1.34
54	1w	37	MIA	C5-C4	2.61	1.47	1.40
32	1a	1407	5MC	C6-C5	2.61	1.38	1.34
1	1A	1915	5MU	C4-N3	-2.61	1.34	1.38
54	2y	39	PSU	C4-N3	-2.61	1.34	1.38
32	1a	1404	5MC	C6-C5	2.60	1.38	1.34
1	2A	1915	5MU	C4-C5	2.59	1.49	1.44
54	1w	54	5MU	C6-C5	2.59	1.38	1.34
54	2y	54	5MU	C4-C5	2.58	1.49	1.44
32	1a	1404	5MC	C6-N1	-2.58	1.33	1.38
32	1a	966	M2G	C6-N1	-2.57	1.34	1.37
1	2A	1939	5MU	C4-C5	2.56	1.49	1.44
1	1A	1911	PSU	C4-N3	-2.55	1.34	1.38
32	2a	1400	5MC	C6-C5	2.54	1.38	1.34
54	2y	46	G7M	C6-N1	-2.54	1.34	1.37
1	1A	1915	5MU	C2-N1	2.54	1.42	1.38
1	1A	2251	OMG	C6-N1	-2.54	1.34	1.37
32	1a	1498	UR3	C2-N1	2.54	1.42	1.38
1	2A	1962	5MC	C6-C5	2.53	1.38	1.34
1	2A	1917	PSU	C4-N3	-2.53	1.34	1.38
1	1A	1962	5MC	C6-C5	2.52	1.38	1.34
54	1y	39	PSU	C4-N3	-2.52	1.34	1.38
1	1A	2605	PSU	C6-C5	2.52	1.38	1.35
1	1A	1942	5MC	C6-C5	2.51	1.38	1.34
1	2A	1915	5MU	C4-N3	-2.51	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.50	1.34	1.38
54	2y	54	5MU	C4-N3	-2.49	1.34	1.38
54	2y	55	PSU	C4-N3	-2.47	1.34	1.38
32	1a	516	PSU	C4-N3	-2.47	1.34	1.38
54	1w	55	PSU	C4-N3	-2.47	1.34	1.38
54	2w	54	5MU	C4-N3	-2.47	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.46	1.33	1.38
54	1w	54	5MU	C4-C5	2.46	1.48	1.44
55	2x	55	PSU	C4-N3	-2.46	1.34	1.38
1	2A	1915	5MU	C2-N1	2.46	1.42	1.38
55	2x	54	5MU	C4-C5	2.46	1.48	1.44
54	2y	8	4SU	C5-C4	-2.46	1.39	1.42
1	1A	1939	5MU	C6-N1	-2.45	1.33	1.38
54	2w	54	5MU	C2-N1	2.45	1.42	1.38
32	1a	1207	2MG	C6-N1	-2.44	1.34	1.37
1	1A	1942	5MC	C6-N1	-2.44	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	54	5MU	C4-C5	2.43	1.48	1.44
54	1y	32	PSU	C4-N3	-2.43	1.34	1.38
55	2x	54	5MU	C4-N3	-2.43	1.34	1.38
1	1A	2552	OMU	C4-N3	-2.42	1.34	1.38
54	2y	32	PSU	C4-N3	-2.40	1.34	1.38
54	1w	8	4SU	C5-C4	-2.40	1.39	1.42
1	1A	1939	5MU	C2-N3	-2.40	1.33	1.38
54	1y	55	PSU	C4-N3	-2.40	1.34	1.38
54	1y	46	G7M	C6-N1	-2.39	1.34	1.37
1	2A	1939	5MU	C6-N1	-2.39	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.36	1.34	1.38
32	1a	527	G7M	C6-N1	-2.36	1.34	1.37
54	1y	8	4SU	C5-C4	-2.36	1.39	1.42
55	1x	55	PSU	C4-N3	-2.36	1.34	1.38
32	2a	516	PSU	C4-N3	-2.36	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.35	1.34	1.38
54	2w	55	PSU	C4-N3	-2.34	1.34	1.38
32	1a	967	5MC	C6-N1	-2.33	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.32	1.34	1.37
1	1A	2552	OMU	C2-N3	-2.32	1.33	1.38
1	1A	1915	5MU	C4-C5	2.30	1.48	1.44
1	2A	2251	OMG	C6-N1	-2.30	1.34	1.37
55	2x	8	4SU	O2-C2	2.28	1.27	1.23
55	1x	32	5MC	C6-N1	-2.27	1.34	1.38
54	2w	32	PSU	C4-N3	-2.27	1.34	1.38
1	1A	2503	2MA	C2-N3	2.26	1.36	1.31
32	2a	1404	5MC	C6-N1	-2.26	1.34	1.38
32	2a	1498	UR3	C2-N1	2.25	1.41	1.38
1	2A	2605	PSU	C2-N3	-2.24	1.33	1.37
54	2w	54	5MU	C4-C5	2.24	1.48	1.44
54	1y	54	5MU	C2-N1	2.22	1.42	1.38
54	1w	46	G7M	C6-N1	-2.22	1.34	1.37
55	1x	54	5MU	C6-N1	-2.21	1.34	1.38
54	2w	37	MIA	C6-N1	2.21	1.35	1.32
32	2a	527	G7M	C6-N1	-2.21	1.34	1.37
54	1w	54	5MU	C2-N3	-2.21	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.20	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.20	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.19	1.34	1.38
55	2x	54	5MU	C2-N1	2.19	1.42	1.38
32	2a	1498	UR3	C6-C5	2.18	1.40	1.35
32	1a	1407	5MC	C6-N1	-2.17	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	8	4SU	C2-N1	2.17	1.41	1.38
1	1A	2605	PSU	C2-N3	-2.17	1.33	1.37
54	2w	8	4SU	C2-N1	2.13	1.41	1.38
1	2A	1942	5MC	C6-N1	-2.13	1.34	1.38
32	2a	967	5MC	C6-N1	-2.13	1.34	1.38
54	2w	8	4SU	C5-C4	-2.11	1.39	1.42
54	2w	8	4SU	C6-C5	2.11	1.39	1.35
1	2A	2503	2MA	C6-N1	-2.10	1.33	1.38
54	1y	8	4SU	C2-N3	-2.10	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.09	1.34	1.38
54	1y	8	4SU	C2-N1	2.09	1.41	1.38
55	1x	54	5MU	C2-N1	2.09	1.41	1.38
1	1A	2605	PSU	C2-N1	-2.08	1.33	1.36
32	2a	966	M2G	C6-N1	-2.08	1.34	1.37
55	1x	8	4SU	C6-C5	2.07	1.39	1.35
55	1x	54	5MU	C2-N3	-2.06	1.34	1.38
54	2y	8	4SU	C2-N1	2.06	1.41	1.38
54	1w	54	5MU	C6-N1	-2.06	1.34	1.38
1	2A	1915	5MU	C2-N3	-2.05	1.34	1.38
54	1y	8	4SU	C6-C5	2.05	1.39	1.35
54	1y	54	5MU	O2-C2	2.04	1.26	1.23
54	1w	54	5MU	C2-N1	2.04	1.41	1.38
1	2A	2552	OMU	C2-N3	-2.04	1.34	1.38
54	1y	54	5MU	C4-C5	2.03	1.48	1.44
1	1A	1917	PSU	C2-N3	-2.03	1.34	1.37
1	1A	2552	OMU	C6-C5	2.03	1.39	1.35
55	2x	32	5MC	C6-N1	-2.03	1.34	1.38
54	1w	8	4SU	C2-N3	-2.02	1.34	1.38
55	2x	54	5MU	C6-N1	-2.02	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.01	1.34	1.38

All (264) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-22.30	62.09	102.44
43	1l	92	0TD	CSB-SB-CB	-11.46	81.70	102.44
54	1w	37	MIA	C12-C13-C14	-8.54	110.52	127.14
54	1w	39	PSU	N1-C2-N3	6.30	122.27	115.13
54	2w	8	4SU	C4-N3-C2	-6.21	121.31	127.34
1	1A	1917	PSU	N1-C2-N3	6.13	122.08	115.13
55	2x	55	PSU	N1-C2-N3	6.11	122.06	115.13
54	2y	8	4SU	C4-N3-C2	-6.01	121.50	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	55	PSU	N1-C2-N3	5.95	121.87	115.13
1	2A	1917	PSU	N1-C2-N3	5.94	121.86	115.13
55	1x	55	PSU	N1-C2-N3	5.93	121.85	115.13
1	2A	1939	5MU	C4-N3-C2	-5.87	119.75	127.35
1	1A	2605	PSU	N1-C2-N3	5.86	121.77	115.13
32	1a	516	PSU	N1-C2-N3	5.83	121.73	115.13
54	2w	55	PSU	N1-C2-N3	5.82	121.72	115.13
54	1y	39	PSU	N1-C2-N3	5.81	121.72	115.13
32	2a	1498	UR3	C4-N3-C2	-5.78	119.12	124.56
54	2w	32	PSU	N1-C2-N3	5.73	121.62	115.13
1	1A	1939	5MU	C4-N3-C2	-5.68	119.99	127.35
1	1A	1911	PSU	N1-C2-N3	5.65	121.53	115.13
54	1w	8	4SU	C4-N3-C2	-5.62	121.88	127.34
32	1a	1498	UR3	C4-N3-C2	-5.59	119.30	124.56
54	2y	32	PSU	N1-C2-N3	5.58	121.45	115.13
54	1w	55	PSU	N1-C2-N3	5.57	121.44	115.13
1	2A	1915	5MU	C4-N3-C2	-5.55	120.16	127.35
54	1y	32	PSU	N1-C2-N3	5.48	121.34	115.13
1	2A	1911	PSU	N1-C2-N3	5.45	121.31	115.13
32	2a	516	PSU	N1-C2-N3	5.44	121.29	115.13
1	1A	1939	5MU	C5-C4-N3	5.41	119.93	115.31
54	2y	8	4SU	C5-C4-N3	5.40	119.70	114.69
1	2A	2605	PSU	N1-C2-N3	5.40	121.25	115.13
54	2y	55	PSU	N1-C2-N3	5.35	121.19	115.13
1	2A	1939	5MU	C5-C4-N3	5.26	119.80	115.31
55	1x	54	5MU	C4-N3-C2	-5.25	120.55	127.35
1	2A	1915	5MU	C5-C4-N3	5.24	119.78	115.31
54	1w	32	PSU	N1-C2-N3	5.23	121.06	115.13
55	1x	54	5MU	N3-C2-N1	5.22	121.83	114.89
55	2x	54	5MU	N3-C2-N1	5.22	121.82	114.89
1	1A	1915	5MU	C4-N3-C2	-5.16	120.67	127.35
54	1w	8	4SU	C5-C4-N3	5.14	119.46	114.69
55	2x	54	5MU	C4-N3-C2	-5.10	120.75	127.35
1	1A	2552	OMU	C4-N3-C2	-5.08	119.87	126.58
1	1A	1915	5MU	N3-C2-N1	5.06	121.61	114.89
54	2w	8	4SU	C5-C4-N3	5.05	119.38	114.69
32	1a	1519	MA6	N3-C2-N1	-5.01	120.84	128.68
1	2A	1939	5MU	N3-C2-N1	4.97	121.49	114.89
32	1a	1518	MA6	N3-C2-N1	-4.96	120.92	128.68
1	1A	1939	5MU	C5-C6-N1	-4.96	118.23	123.34
1	1A	2552	OMU	N3-C2-N1	4.95	121.46	114.89
54	2y	39	PSU	N1-C2-N3	4.95	120.74	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	8	4SU	C4-N3-C2	-4.93	122.55	127.34
1	1A	1939	5MU	N3-C2-N1	4.87	121.36	114.89
1	2A	1939	5MU	C5-C6-N1	-4.83	118.37	123.34
54	1y	8	4SU	C5-C4-N3	4.79	119.13	114.69
1	2A	1915	5MU	N3-C2-N1	4.78	121.23	114.89
32	2a	1518	MA6	N3-C2-N1	-4.77	121.22	128.68
54	2w	39	PSU	N1-C2-N3	4.67	120.42	115.13
54	1w	54	5MU	C4-N3-C2	-4.66	121.32	127.35
32	2a	1519	MA6	N3-C2-N1	-4.62	121.45	128.68
1	1A	1915	5MU	C5-C4-N3	4.57	119.21	115.31
54	1w	54	5MU	N3-C2-N1	4.57	120.95	114.89
1	1A	1939	5MU	O4-C4-C5	-4.46	119.73	124.90
54	1w	37	MIA	C2-N3-C4	4.44	121.44	115.32
54	2w	37	MIA	C2-N3-C4	4.39	121.37	115.32
54	2y	54	5MU	C4-N3-C2	-4.36	121.70	127.35
1	2A	2552	OMU	C4-N3-C2	-4.33	120.86	126.58
54	2y	54	5MU	N3-C2-N1	4.33	120.63	114.89
54	1w	54	5MU	C5-C4-N3	4.29	118.97	115.31
1	2A	2552	OMU	N3-C2-N1	4.27	120.56	114.89
54	1w	39	PSU	C4-N3-C2	-4.26	120.20	126.34
55	1x	54	5MU	C5-C4-N3	4.25	118.94	115.31
54	2w	8	4SU	N3-C2-N1	4.24	120.51	114.89
55	2x	55	PSU	C4-N3-C2	-4.20	120.28	126.34
54	2y	54	5MU	C5-C4-N3	4.20	118.90	115.31
1	1A	2552	OMU	O2-C2-N1	-4.20	117.21	122.79
54	1w	37	MIA	C15-C14-C13	-4.14	110.68	122.65
1	2A	2605	PSU	C4-N3-C2	-4.13	120.39	126.34
54	1w	37	MIA	C16-C14-C13	-4.11	110.77	122.65
55	1x	32	5MC	C5-C6-N1	-4.04	119.19	123.34
1	2A	1915	5MU	O4-C4-C5	-4.03	120.23	124.90
55	2x	54	5MU	C5-C4-N3	4.02	118.74	115.31
54	2w	55	PSU	C4-N3-C2	-3.99	120.59	126.34
1	2A	1915	5MU	C5-C6-N1	-3.98	119.24	123.34
54	2y	55	PSU	C4-N3-C2	-3.97	120.61	126.34
1	1A	1915	5MU	O4-C4-C5	-3.95	120.33	124.90
54	1y	55	PSU	C4-N3-C2	-3.94	120.67	126.34
1	1A	2605	PSU	C4-N3-C2	-3.91	120.71	126.34
1	2A	1939	5MU	O4-C4-C5	-3.90	120.38	124.90
32	2a	1400	5MC	C5-C6-N1	-3.90	119.33	123.34
55	1x	54	5MU	O4-C4-C5	-3.87	120.41	124.90
55	2x	54	5MU	O4-C4-C5	-3.87	120.42	124.90
1	1A	1911	PSU	C4-N3-C2	-3.84	120.81	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1942	5MC	C5-C6-N1	-3.84	119.39	123.34
1	2A	1917	PSU	C4-N3-C2	-3.84	120.81	126.34
1	1A	2552	OMU	C5-C4-N3	3.81	120.55	114.84
54	1y	39	PSU	C4-N3-C2	-3.80	120.86	126.34
55	1x	55	PSU	O2-C2-N1	-3.80	118.61	122.79
54	1y	54	5MU	C5-C4-N3	3.78	118.54	115.31
1	1A	1917	PSU	C4-N3-C2	-3.77	120.90	126.34
32	1a	516	PSU	C4-N3-C2	-3.75	120.93	126.34
54	2y	8	4SU	N3-C2-N1	3.73	119.84	114.89
54	2w	32	PSU	C4-N3-C2	-3.72	120.98	126.34
55	1x	8	4SU	C6-C5-C4	-3.69	116.75	119.95
55	1x	54	5MU	C5-C6-N1	-3.68	119.55	123.34
32	2a	967	5MC	C5-C6-N1	-3.66	119.58	123.34
32	2a	1404	5MC	C5-C6-N1	-3.65	119.58	123.34
54	2y	8	4SU	C5-C4-S4	-3.63	119.78	124.47
54	1w	39	PSU	O2-C2-N1	-3.63	118.80	122.79
54	1y	54	5MU	N3-C2-N1	3.62	119.69	114.89
54	1w	8	4SU	N3-C2-N1	3.61	119.69	114.89
55	1x	55	PSU	C4-N3-C2	-3.61	121.14	126.34
54	1y	32	PSU	C4-N3-C2	-3.61	121.14	126.34
54	2w	54	5MU	C5-C4-N3	3.59	118.38	115.31
54	2w	54	5MU	N3-C2-N1	3.57	119.62	114.89
32	2a	516	PSU	C4-N3-C2	-3.56	121.21	126.34
54	2y	32	PSU	C4-N3-C2	-3.52	121.26	126.34
54	2w	54	5MU	O4-C4-C5	-3.52	120.82	124.90
54	1y	54	5MU	C4-N3-C2	-3.52	122.80	127.35
1	1A	1962	5MC	C5-C6-N1	-3.51	119.72	123.34
54	2w	54	5MU	C4-N3-C2	-3.51	122.81	127.35
1	2A	1942	5MC	C5-C6-N1	-3.49	119.74	123.34
54	2w	32	PSU	O2-C2-N1	-3.49	118.95	122.79
54	1w	55	PSU	C4-N3-C2	-3.49	121.31	126.34
32	1a	1400	5MC	C5-C6-N1	-3.47	119.77	123.34
54	2w	37	MIA	C5-C6-N1	-3.46	117.94	120.81
1	2A	1911	PSU	C4-N3-C2	-3.45	121.36	126.34
1	2A	1962	5MC	C5-C6-N1	-3.44	119.80	123.34
32	1a	967	5MC	C5-C6-N1	-3.43	119.81	123.34
55	2x	54	5MU	C5-C6-N1	-3.40	119.84	123.34
54	1w	54	5MU	C5-C6-N1	-3.39	119.85	123.34
54	1y	54	5MU	O4-C4-C5	-3.38	120.98	124.90
55	2x	55	PSU	O2-C2-N1	-3.38	119.07	122.79
54	2y	54	5MU	O4-C4-C5	-3.37	121.00	124.90
32	2a	1519	MA6	C4-C5-N7	-3.36	105.89	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	37	MIA	N3-C2-N1	-3.36	123.42	128.68
1	2A	1917	PSU	O2-C2-N1	-3.36	119.09	122.79
54	1w	37	MIA	C5-C6-N1	-3.35	118.03	120.81
54	1y	8	4SU	N3-C2-N1	3.34	119.32	114.89
54	1w	32	PSU	C4-N3-C2	-3.33	121.54	126.34
54	2w	55	PSU	O2-C2-N1	-3.33	119.13	122.79
1	2A	1939	5MU	O2-C2-N1	-3.30	118.40	122.79
55	1x	8	4SU	C5-C4-N3	3.29	117.75	114.69
32	1a	1404	5MC	C5-C6-N1	-3.29	119.95	123.34
54	1y	37	MIA	N3-C2-N1	-3.26	123.58	128.68
54	1y	54	5MU	C5-C6-N1	-3.26	119.99	123.34
1	1A	1911	PSU	O2-C2-N1	-3.25	119.21	122.79
54	2y	55	PSU	O2-C2-N1	-3.23	119.23	122.79
54	1y	55	PSU	O2-C2-N1	-3.18	119.29	122.79
1	2A	2552	OMU	C5-C4-N3	3.16	119.57	114.84
54	1w	55	PSU	O2-C2-N1	-3.15	119.32	122.79
54	1w	37	MIA	C12-N6-C6	-3.15	117.88	122.55
54	1w	54	5MU	O4-C4-C5	-3.15	121.25	124.90
54	2y	54	5MU	C5-C6-N1	-3.15	120.10	123.34
32	1a	516	PSU	O2-C2-N1	-3.12	119.35	122.79
55	2x	8	4SU	C6-C5-C4	-3.12	117.25	119.95
1	2A	2552	OMU	O2-C2-N1	-3.11	118.65	122.79
54	2w	37	MIA	C12-N6-C6	-3.09	120.21	122.87
32	2a	1407	5MC	C5-C6-N1	-3.07	120.18	123.34
32	1a	1519	MA6	C4-C5-N7	-3.03	106.24	109.40
1	1A	1915	5MU	C5-C6-N1	-3.03	120.22	123.34
55	2x	32	5MC	C5-C6-N1	-3.03	120.22	123.34
54	1w	8	4SU	C5-C4-S4	-3.03	120.56	124.47
55	2x	8	4SU	C1'-N1-C2	3.02	123.04	117.57
54	1y	37	MIA	C4-C5-N7	-3.00	106.27	109.40
1	1A	1917	PSU	O2-C2-N1	-3.00	119.49	122.79
54	2y	32	PSU	O2-C2-N1	-2.98	119.50	122.79
54	2w	8	4SU	C5-C4-S4	-2.93	120.69	124.47
32	1a	1407	5MC	C5-C6-N1	-2.91	120.35	123.34
1	1A	2605	PSU	O2-C2-N1	-2.91	119.59	122.79
55	1x	8	4SU	O2-C2-N1	2.89	126.63	122.79
1	2A	1911	PSU	O2-C2-N1	-2.89	119.61	122.79
54	2y	39	PSU	C4-N3-C2	-2.88	122.19	126.34
32	1a	1407	5MC	C5-C4-N3	-2.87	118.58	121.67
55	2x	8	4SU	C5-C4-N3	2.86	117.34	114.69
32	2a	1407	5MC	C5-C4-N3	-2.82	118.63	121.67
55	1x	32	5MC	C5-C4-N3	-2.81	118.64	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	37	MIA	C4-C5-N7	-2.78	106.50	109.40
1	1A	2251	OMG	C5-C6-N1	2.76	118.83	113.95
1	1A	1939	5MU	O2-C2-N1	-2.74	119.15	122.79
32	1a	1207	2MG	C8-N7-C5	2.73	108.20	102.99
54	1w	32	PSU	O2-C2-N1	-2.73	119.78	122.79
55	1x	54	5MU	O2-C2-N1	-2.73	119.16	122.79
32	2a	516	PSU	O2-C2-N1	-2.72	119.79	122.79
32	2a	1518	MA6	C4-C5-N7	-2.71	106.58	109.40
55	2x	54	5MU	O2-C2-N1	-2.70	119.20	122.79
32	1a	1518	MA6	C4-C5-N7	-2.70	106.59	109.40
54	1w	37	MIA	C2-N1-C6	2.65	121.93	117.19
54	2w	54	5MU	C5-C6-N1	-2.65	120.61	123.34
1	1A	2503	2MA	C5-C6-N1	2.64	118.58	114.02
32	1a	1404	5MC	C5-C4-N3	-2.62	118.85	121.67
32	1a	1400	5MC	C5-C4-N3	-2.61	118.86	121.67
1	1A	1962	5MC	C5-C4-N3	-2.60	118.86	121.67
54	1y	32	PSU	O2-C2-N1	-2.60	119.93	122.79
54	2w	37	MIA	C2-N1-C6	2.59	121.83	117.19
32	2a	1407	5MC	O2-C2-N3	-2.59	118.12	122.33
32	1a	1404	5MC	CM5-C5-C6	-2.58	119.40	122.85
1	1A	1920	OMC	O2-C2-N3	-2.58	118.14	122.33
54	2w	37	MIA	C4-C5-N7	-2.58	106.72	109.40
54	2y	54	5MU	C1'-N1-C2	2.55	122.18	117.57
1	2A	2552	OMU	O4-C4-C5	-2.54	120.70	125.16
1	1A	2552	OMU	O4-C4-C5	-2.53	120.71	125.16
1	2A	2503	2MA	C8-N7-C5	2.52	107.79	102.99
1	2A	2503	2MA	C5-C6-N1	2.51	118.34	114.02
1	2A	1942	5MC	C5-C4-N3	-2.48	119.00	121.67
1	2A	1962	5MC	C5-C4-N3	-2.47	119.00	121.67
54	1y	39	PSU	O2-C2-N1	-2.46	120.08	122.79
43	1l	92	0TD	OD2-CG-CB	2.46	118.47	113.15
32	2a	967	5MC	C5-C4-N3	-2.46	119.02	121.67
54	1w	54	5MU	C5M-C5-C4	2.46	121.47	118.77
32	1a	967	5MC	C5-C4-N3	-2.44	119.04	121.67
55	2x	32	5MC	C5-C4-N3	-2.44	119.04	121.67
54	1w	37	MIA	C4-C5-N7	-2.44	106.86	109.40
32	2a	1404	5MC	C5-C4-N3	-2.43	119.05	121.67
32	1a	1207	2MG	CM2-N2-C2	-2.42	118.51	123.86
1	1A	1942	5MC	C5-C4-N3	-2.42	119.07	121.67
1	2A	2251	OMG	C5-C6-N1	2.41	118.21	113.95
55	2x	32	5MC	O2-C2-N3	-2.41	118.41	122.33
1	1A	2503	2MA	C8-N7-C5	2.39	107.55	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	N3-C2-N1	-2.37	122.61	126.98
55	1x	8	4SU	C1'-N1-C2	2.36	121.84	117.57
54	2w	39	PSU	C4-N3-C2	-2.35	122.95	126.34
1	1A	2251	OMG	C8-N7-C5	2.35	107.46	102.99
1	2A	2251	OMG	C8-N7-C5	2.31	107.38	102.99
32	2a	1400	5MC	C5-C4-N3	-2.30	119.20	121.67
1	1A	1911	PSU	C6-C5-C4	-2.28	116.60	118.20
32	2a	1402	4OC	C6-C5-C4	2.28	119.75	116.96
54	2y	54	5MU	O2-C2-N3	-2.27	117.27	121.50
1	2A	1915	5MU	C5M-C5-C4	2.26	121.25	118.77
54	2w	37	MIA	N3-C2-N1	-2.25	122.83	126.98
1	1A	1915	5MU	C5M-C5-C4	2.25	121.24	118.77
55	2x	55	PSU	C5-C6-N1	-2.25	118.74	122.11
32	2a	1400	5MC	CM5-C5-C6	-2.25	119.85	122.85
32	2a	1207	2MG	C8-N7-C5	2.25	107.27	102.99
32	1a	966	M2G	C8-N7-C5	2.24	107.26	102.99
54	1y	8	4SU	C5-C4-S4	-2.23	121.59	124.47
1	2A	2605	PSU	C5-C6-N1	-2.23	118.76	122.11
32	1a	966	M2G	C5-C6-N1	2.23	117.89	113.95
32	2a	1402	4OC	O2-C2-N3	-2.22	118.71	122.33
32	1a	1498	UR3	C1'-N1-C2	2.21	120.72	116.99
32	1a	1402	4OC	C6-C5-C4	2.20	119.65	116.96
54	1w	55	PSU	C6-C5-C4	-2.19	116.67	118.20
54	2y	54	5MU	C1'-N1-C6	-2.19	117.48	121.12
54	1w	54	5MU	O2-C2-N1	-2.17	119.91	122.79
54	1y	55	PSU	O4'-C1'-C2'	2.16	108.19	105.14
32	1a	1407	5MC	CM5-C5-C6	-2.15	119.98	122.85
32	2a	516	PSU	O4'-C1'-C2'	2.13	108.15	105.14
54	2w	8	4SU	O2-C2-N1	-2.13	119.95	122.79
32	1a	1404	5MC	O2-C2-N3	-2.11	118.89	122.33
1	1A	2251	OMG	O6-C6-C5	-2.11	120.25	124.37
54	2w	37	MIA	N6-C6-N1	2.10	121.12	118.50
55	1x	8	4SU	S4-C4-N3	-2.09	118.15	120.21
1	2A	2605	PSU	O2-C2-N1	-2.08	120.50	122.79
32	2a	966	M2G	C8-N7-C5	2.08	106.95	102.99
54	1w	8	4SU	C1'-N1-C2	2.06	121.30	117.57
32	2a	966	M2G	C5-C6-N1	2.06	117.59	113.95
54	2w	32	PSU	O4'-C1'-C2'	2.06	108.04	105.14
55	1x	8	4SU	O2-C2-N3	-2.05	117.69	121.50
54	2y	54	5MU	C5M-C5-C4	2.05	121.02	118.77
1	1A	1915	5MU	O2-C2-N1	-2.03	120.09	122.79
32	1a	1400	5MC	O2-C2-N3	-2.03	119.03	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1402	4OC	CM4-N4-C4	-2.02	118.51	122.45
1	1A	2605	PSU	C5-C6-N1	-2.02	119.08	122.11
54	1w	39	PSU	C5-C6-N1	-2.02	119.09	122.11
1	2A	2251	OMG	O6-C6-C5	-2.01	120.45	124.37

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	527	G7M	C3'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
54	1w	37	MIA	C12-C13-C14-C16
54	1y	8	4SU	O4'-C4'-C5'-O5'
54	1y	46	G7M	C4'-C5'-O5'-P
54	1y	54	5MU	O4'-C4'-C5'-O5'
54	1y	55	PSU	C3'-C4'-C5'-O5'
54	1y	55	PSU	O4'-C4'-C5'-O5'
32	2a	1207	2MG	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
54	2w	37	MIA	N1-C2-S10-C11
54	2w	37	MIA	N3-C2-S10-C11
54	2y	8	4SU	O4'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	2y	54	5MU	C3'-C4'-C5'-O5'
54	2y	54	5MU	O4'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C1'-C5-C6
54	2y	55	PSU	C3'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	54	5MU	C3'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	1y	46	G7M	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	2y	8	4SU	C3'-C4'-C5'-O5'
54	2y	37	MIA	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	1x	55	PSU	O4'-C4'-C5'-O5'
54	2y	37	MIA	C4'-C5'-O5'-P
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
32	2a	527	G7M	C4'-C5'-O5'-P
54	2w	46	G7M	C4'-C5'-O5'-P
54	1y	46	G7M	O4'-C4'-C5'-O5'
54	1w	46	G7M	C4'-C5'-O5'-P
32	1a	1400	5MC	O4'-C4'-C5'-O5'
54	1y	8	4SU	C4'-C5'-O5'-P
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
1	1A	2503	2MA	O4'-C4'-C5'-O5'
55	1x	55	PSU	C3'-C4'-C5'-O5'
1	2A	2251	OMG	C1'-C2'-O2'-CM2
54	2y	54	5MU	C2'-C1'-N1-C2
32	1a	1400	5MC	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	1962	5MC	C2'-C1'-N1-C6
43	1l	92	0TD	CG-CB-SB-CSB
1	1A	2503	2MA	C4'-C5'-O5'-P
1	2A	2251	OMG	C4'-C5'-O5'-P
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	1A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
32	1a	527	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	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 2879 ligands modelled in this entry, 2875 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	Y7K	2a	1841	-	35,36,36	0.85	2 (5%)	39,54,54	1.24	4 (10%)
58	Y7K	1a	1842	-	35,36,36	0.82	1 (2%)	39,54,54	1.38	7 (17%)
59	SF4	1d	501	35	0,12,12	-	-	-		
59	SF4	2d	303	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	Y7K	2a	1841	-	-	4/11/77/77	0/4/4/4
58	Y7K	1a	1842	-	-	3/11/77/77	0/4/4/4
59	SF4	1d	501	35	-	-	0/6/5/5
59	SF4	2d	303	35	-	-	0/6/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2a	1841	Y7K	CAQ-CAL	-2.83	1.51	1.54
58	1a	1842	Y7K	OAP-CAL	2.61	1.44	1.39
58	2a	1841	Y7K	OAP-CAL	2.36	1.43	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	2a	1841	Y7K	CAR-NAM-CAI	-3.74	108.93	114.38
58	1a	1842	Y7K	OAS-CAN-OAJ	-3.71	102.52	107.01
58	1a	1842	Y7K	CAR-NAM-CAI	-3.60	109.15	114.38
58	1a	1842	Y7K	CAQ-CAU-CAV	-3.18	108.82	114.22
58	2a	1841	Y7K	CAU-CAQ-CAL	-3.12	108.16	110.33
58	2a	1841	Y7K	CAQ-CAU-CAV	-2.85	109.37	114.22
58	1a	1842	Y7K	CAU-CAQ-CAL	-2.74	108.42	110.33
58	1a	1842	Y7K	CAZ-NAY-CAX	-2.44	108.41	113.35
58	2a	1841	Y7K	CAB-NAA-CAC	2.42	117.91	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	1a	1842	Y7K	CAB-NAA-CAC	-2.34	110.98	114.38
58	1a	1842	Y7K	CAZ-CBA-CBB	-2.16	108.83	114.32

There are no chirality outliers.

All (7) torsion outliers are listed below:

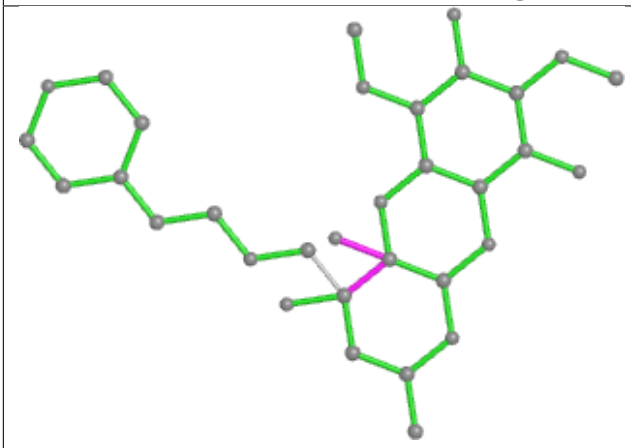
Mol	Chain	Res	Type	Atoms
58	1a	1842	Y7K	NAY-CAZ-CBA-CBB
58	2a	1841	Y7K	NAY-CAZ-CBA-CBB
58	2a	1841	Y7K	CAZ-CBA-CBB-CBC
58	2a	1841	Y7K	CBA-CAZ-NAY-CAX
58	2a	1841	Y7K	CAZ-CBA-CBB-CBG
58	1a	1842	Y7K	CAZ-CBA-CBB-CBC
58	1a	1842	Y7K	CBA-CAZ-NAY-CAX

There are no ring outliers.

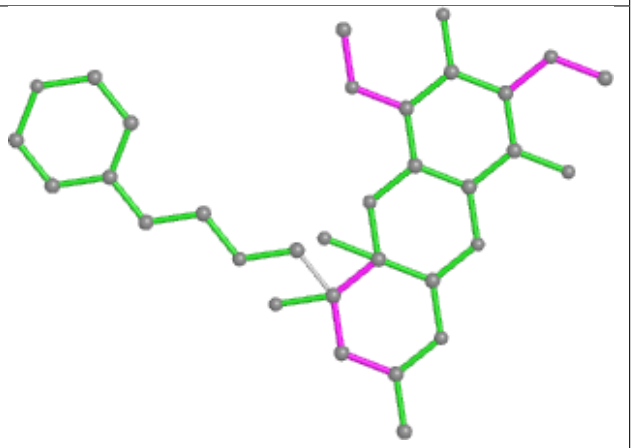
No monomer is involved in short contacts.

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

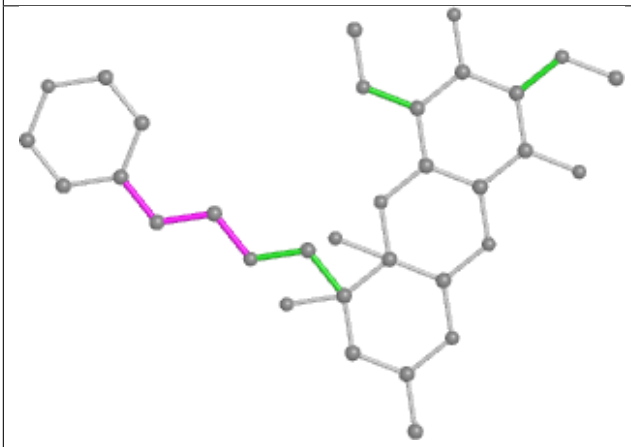
Ligand Y7K 2a 1841



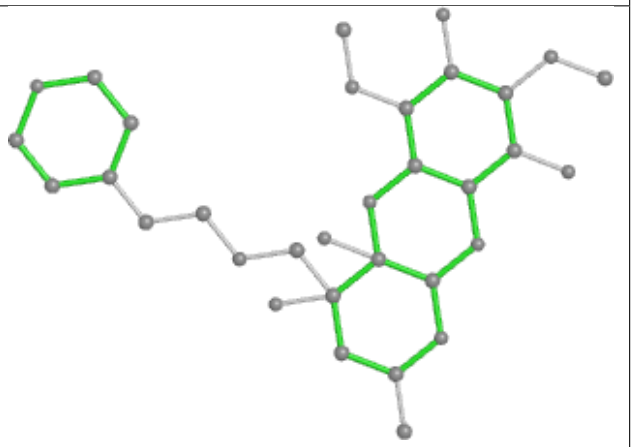
Bond lengths



Bond angles

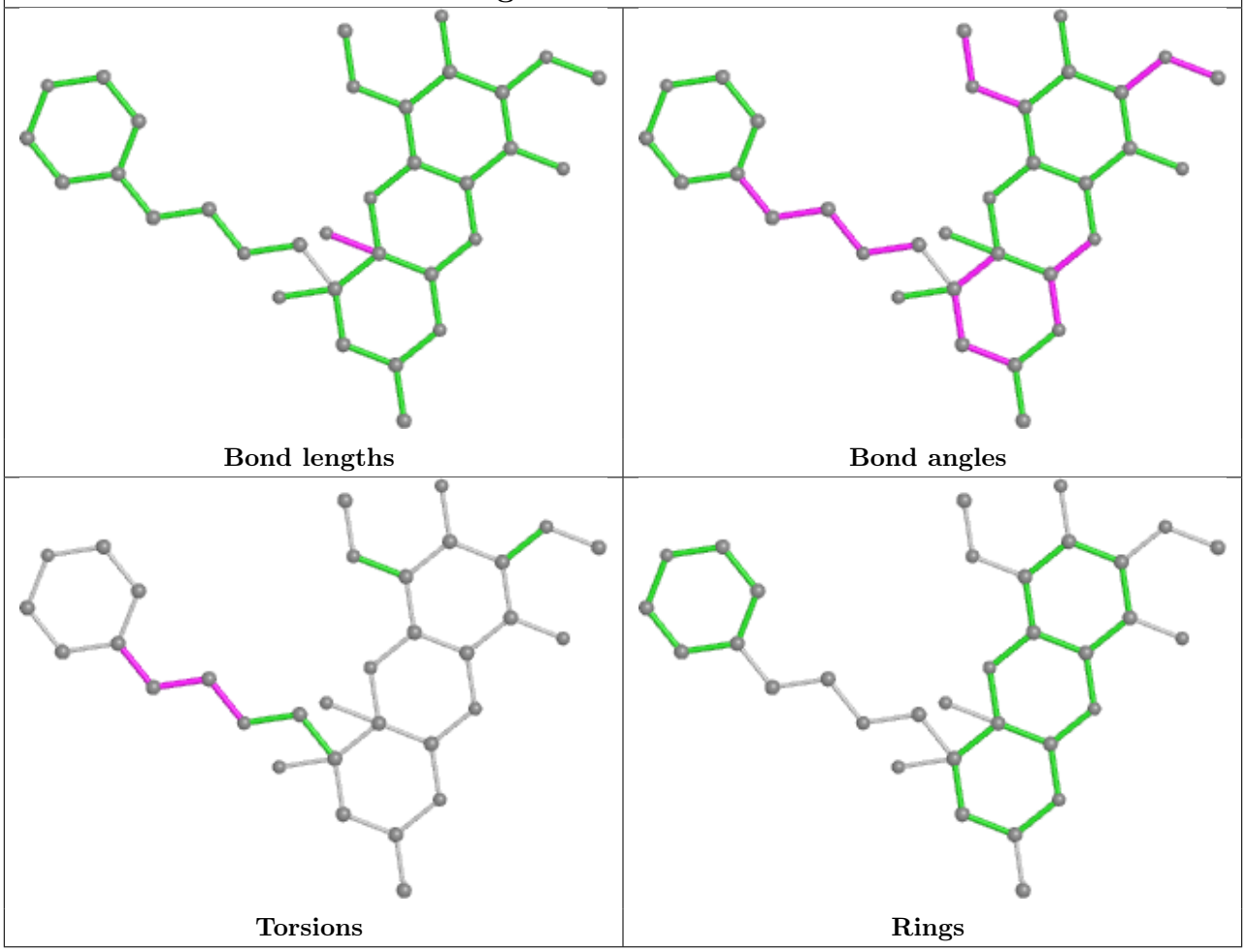


Torsions



Rings

Ligand Y7K 1a 1842



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%)	0.08	73 (2%) 56 65	17, 35, 94, 110	0
1	2A	2789/2915 (95%)	0.22	108 (3%) 39 46	33, 60, 95, 109	0
2	1B	120/121 (99%)	-0.29	0 100 100	26, 48, 60, 87	0
2	2B	120/121 (99%)	-0.57	0 100 100	65, 87, 96, 98	0
3	1D	275/276 (99%)	0.66	9 (3%) 46 54	21, 36, 51, 80	0
3	2D	275/276 (99%)	0.85	21 (7%) 13 16	32, 52, 66, 85	0
4	1E	204/206 (99%)	0.48	2 (0%) 82 87	19, 38, 59, 74	0
4	2E	204/206 (99%)	0.48	10 (4%) 29 36	36, 61, 73, 85	0
5	1F	202/210 (96%)	0.19	2 (0%) 82 87	20, 40, 67, 86	0
5	2F	202/210 (96%)	0.68	14 (6%) 16 20	38, 70, 83, 88	0
6	1G	181/182 (99%)	-0.06	0 100 100	40, 59, 72, 90	0
6	2G	181/182 (99%)	1.16	45 (24%) 0 0	74, 85, 90, 96	0
7	1H	174/180 (96%)	0.24	3 (1%) 70 78	39, 53, 66, 70	0
7	2H	174/180 (96%)	2.57	107 (61%) 0 0	70, 86, 93, 98	0
8	1I	146/148 (98%)	0.21	5 (3%) 45 53	45, 73, 83, 86	0
8	2I	146/148 (98%)	1.80	60 (41%) 0 0	56, 75, 85, 88	0
9	1N	140/140 (100%)	0.36	0 100 100	25, 37, 60, 73	0
9	2N	140/140 (100%)	1.95	61 (43%) 0 0	49, 66, 79, 88	0
10	1O	122/122 (100%)	0.76	8 (6%) 18 21	24, 39, 57, 65	0
10	2O	122/122 (100%)	0.54	8 (6%) 18 21	48, 61, 72, 78	0
11	1P	149/150 (99%)	0.39	4 (2%) 54 63	17, 42, 68, 75	0
11	2P	149/150 (99%)	2.40	85 (57%) 0 0	37, 70, 85, 88	0
12	1Q	141/141 (100%)	0.18	0 100 100	27, 39, 57, 73	0
12	2Q	141/141 (100%)	1.72	51 (36%) 0 0	47, 70, 80, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.03	0 100 100	25, 33, 50, 60	0
13	2R	118/118 (100%)	0.14	0 100 100	43, 54, 64, 73	0
14	1S	110/112 (98%)	-0.01	0 100 100	37, 48, 60, 65	0
14	2S	110/112 (98%)	0.29	4 (3%) 42 51	69, 80, 86, 90	0
15	1T	131/146 (89%)	0.19	2 (1%) 73 81	33, 43, 66, 75	0
15	2T	131/146 (89%)	0.02	1 (0%) 86 90	52, 64, 78, 85	0
16	1U	116/118 (98%)	0.15	0 100 100	20, 30, 46, 61	0
16	2U	116/118 (98%)	1.56	35 (30%) 0 0	45, 63, 78, 85	0
17	1V	101/101 (100%)	0.13	0 100 100	22, 38, 58, 70	0
17	2V	101/101 (100%)	2.21	54 (53%) 0 0	46, 74, 84, 87	0
18	1W	112/113 (99%)	0.11	0 100 100	23, 32, 47, 76	0
18	2W	112/113 (99%)	0.20	1 (0%) 84 89	39, 51, 67, 90	0
19	1X	95/96 (98%)	0.24	0 100 100	23, 38, 59, 75	0
19	2X	95/96 (98%)	0.17	0 100 100	45, 62, 76, 79	0
20	1Y	107/110 (97%)	-0.02	0 100 100	36, 49, 69, 77	0
20	2Y	107/110 (97%)	0.12	0 100 100	62, 74, 82, 88	0
21	1Z	154/206 (74%)	0.03	0 100 100	38, 63, 82, 93	0
21	2Z	160/206 (77%)	1.25	41 (25%) 0 0	71, 84, 92, 97	0
22	10	83/85 (97%)	0.57	7 (8%) 11 13	28, 37, 60, 77	0
22	20	83/85 (97%)	1.69	22 (26%) 0 0	45, 68, 78, 83	0
23	11	97/98 (98%)	0.54	4 (4%) 37 44	24, 42, 69, 74	0
23	21	97/98 (98%)	1.13	20 (20%) 1 1	40, 58, 78, 84	0
24	12	70/72 (97%)	0.23	0 100 100	34, 47, 60, 74	0
24	22	70/72 (97%)	-0.11	0 100 100	59, 73, 80, 82	0
25	13	59/60 (98%)	0.22	1 (1%) 70 78	23, 34, 58, 80	0
25	23	59/60 (98%)	3.08	45 (76%) 0 0	55, 67, 79, 88	0
26	14	69/71 (97%)	-0.35	0 100 100	48, 73, 88, 92	0
26	24	69/71 (97%)	0.45	9 (13%) 3 4	79, 90, 95, 101	0
27	15	59/60 (98%)	0.19	1 (1%) 70 78	19, 32, 47, 62	0
27	25	59/60 (98%)	0.05	0 100 100	40, 52, 66, 81	0
28	16	53/54 (98%)	0.57	1 (1%) 66 75	30, 42, 56, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	1.70	19 (35%) 0 0	54, 64, 71, 75	0
29	17	48/49 (97%)	0.32	1 (2%) 63 72	21, 27, 55, 63	0
29	27	48/49 (97%)	0.35	1 (2%) 63 72	32, 43, 63, 78	0
30	18	64/65 (98%)	0.28	0 100 100	26, 33, 43, 55	0
30	28	64/65 (98%)	2.29	37 (57%) 0 0	48, 58, 67, 75	0
31	19	37/37 (100%)	0.45	0 100 100	29, 40, 59, 63	0
31	29	37/37 (100%)	2.01	16 (43%) 0 0	62, 71, 80, 85	0
32	1a	1488/1521 (97%)	-0.27	28 (1%) 66 75	37, 67, 93, 110	0
32	2a	1491/1521 (98%)	-0.10	47 (3%) 47 56	53, 81, 99, 109	0
33	1b	231/256 (90%)	1.35	63 (27%) 0 0	66, 81, 89, 94	0
33	2b	231/256 (90%)	3.26	161 (69%) 0 0	75, 88, 94, 96	0
34	1c	206/239 (86%)	1.20	46 (22%) 0 0	62, 72, 84, 89	0
34	2c	206/239 (86%)	3.38	156 (75%) 0 0	76, 87, 92, 95	0
35	1d	208/209 (99%)	1.97	94 (45%) 0 0	58, 71, 80, 83	0
35	2d	208/209 (99%)	1.50	60 (28%) 0 0	63, 74, 82, 89	0
36	1e	148/162 (91%)	1.05	18 (12%) 4 4	54, 65, 74, 90	0
36	2e	148/162 (91%)	1.37	40 (27%) 0 0	68, 79, 85, 90	0
37	1f	100/101 (99%)	1.87	44 (44%) 0 0	53, 66, 76, 78	0
37	2f	100/101 (99%)	1.81	40 (40%) 0 0	61, 72, 79, 83	0
38	1g	155/156 (99%)	0.45	15 (9%) 7 8	53, 70, 87, 96	0
38	2g	155/156 (99%)	1.68	46 (29%) 0 0	68, 80, 89, 98	0
39	1h	137/138 (99%)	0.58	8 (5%) 23 28	54, 67, 74, 79	0
39	2h	137/138 (99%)	0.58	11 (8%) 12 15	71, 80, 85, 90	0
40	1i	127/128 (99%)	-0.15	0 100 100	54, 75, 84, 88	0
40	2i	127/128 (99%)	0.43	8 (6%) 20 24	75, 86, 93, 97	0
41	1j	97/105 (92%)	0.56	9 (9%) 8 10	60, 78, 87, 90	0
41	2j	96/105 (91%)	1.02	22 (22%) 0 0	78, 88, 93, 96	0
42	1k	114/129 (88%)	2.61	71 (62%) 0 0	45, 66, 77, 83	0
42	2k	114/129 (88%)	2.15	54 (47%) 0 0	59, 74, 82, 85	0
43	1l	121/132 (91%)	1.59	37 (30%) 0 0	45, 55, 67, 76	0
43	2l	121/132 (91%)	1.30	26 (21%) 0 0	60, 72, 80, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	-0.37	1 (0%) 86 90	57, 69, 78, 82	0
44	2m	122/126 (96%)	1.46	40 (32%) 0 0	75, 87, 92, 94	0
45	1n	60/61 (98%)	0.09	1 (1%) 70 78	59, 67, 73, 75	0
45	2n	60/61 (98%)	2.90	41 (68%) 0 0	81, 88, 93, 98	0
46	1o	88/89 (98%)	0.66	6 (6%) 17 20	51, 66, 75, 79	0
46	2o	88/89 (98%)	0.43	4 (4%) 33 39	66, 75, 83, 86	0
47	1p	82/88 (93%)	-0.36	0 100 100	55, 69, 78, 87	0
47	2p	82/88 (93%)	-0.11	0 100 100	61, 71, 81, 89	0
48	1q	99/105 (94%)	0.09	3 (3%) 50 59	56, 68, 78, 80	0
48	2q	99/105 (94%)	0.23	1 (1%) 82 87	65, 75, 85, 88	0
49	1r	68/88 (77%)	3.44	53 (77%) 0 0	56, 66, 77, 80	0
49	2r	68/88 (77%)	2.89	45 (66%) 0 0	63, 73, 82, 85	0
50	1s	83/93 (89%)	-0.50	0 100 100	62, 72, 80, 87	0
50	2s	83/93 (89%)	2.64	51 (61%) 0 0	82, 91, 97, 101	0
51	1t	96/106 (90%)	-0.29	0 100 100	60, 69, 81, 88	0
51	2t	96/106 (90%)	0.09	0 100 100	62, 73, 83, 85	0
52	1u	23/27 (85%)	-0.28	0 100 100	60, 67, 73, 76	0
52	2u	23/27 (85%)	1.27	4 (17%) 1 1	79, 83, 88, 89	0
53	1v	13/24 (54%)	1.47	4 (30%) 0 0	48, 62, 93, 100	0
53	2v	13/24 (54%)	2.44	8 (61%) 0 0	74, 89, 100, 104	0
54	1w	67/76 (88%)	2.60	34 (50%) 0 0	55, 91, 102, 107	0
54	1y	67/76 (88%)	1.75	29 (43%) 0 0	37, 95, 102, 106	0
54	2w	65/76 (85%)	5.09	58 (89%) 0 0	77, 101, 107, 109	0
54	2y	66/76 (86%)	3.26	53 (80%) 0 0	57, 101, 105, 106	0
55	1x	72/77 (93%)	0.13	3 (4%) 36 43	39, 68, 85, 93	0
55	2x	72/77 (93%)	1.17	19 (26%) 0 0	58, 85, 94, 104	0
All	All	20873/21748 (95%)	0.57	2560 (12%) 4 4	17, 65, 92, 110	0

All (2560) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
54	2w	71	G	13.4
54	1w	71	G	13.0

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Mol	Chain	Res	Type	RSRZ
33	2b	165	VAL	12.7
38	2g	82	GLY	12.5
54	2w	72	C	12.4
54	2w	73	A	11.0
54	2w	4	C	10.9
54	2w	70	G	10.9
45	2n	2	ALA	10.8
22	10	6	GLY	10.8
22	20	7	LEU	10.4
34	2c	124	ILE	10.2
38	2g	80	VAL	10.0
44	2m	123	ALA	9.9
38	2g	83	ALA	9.7
33	2b	152	PHE	9.6
54	1w	70	G	9.5
34	2c	197	GLY	9.3
33	2b	187	LEU	9.2
44	2m	124	PRO	9.2
22	10	7	LEU	9.1
33	2b	214	ILE	9.0
33	2b	163	PHE	9.0
54	2w	13	C	9.0
54	2w	3	C	8.9
54	2w	2	C	8.9
35	1d	23	GLY	8.6
45	2n	25	VAL	8.4
50	2s	80	TYR	8.4
49	2r	85	LEU	8.3
54	1w	72	C	8.2
23	21	2	SER	7.9
34	2c	71	ALA	7.9
1	2A	2802	G	7.9
54	2w	44	G	7.9
54	2w	76	A	7.8
37	1f	46	ARG	7.8
38	2g	154	TYR	7.8
7	2H	115	VAL	7.7
33	2b	118	LEU	7.7
34	2c	153	VAL	7.7
33	2b	70	PHE	7.7
49	1r	22	VAL	7.6
33	2b	101	MET	7.6

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Mol	Chain	Res	Type	RSRZ
1	2A	2897	U	7.6
33	2b	93	VAL	7.6
33	2b	161	ALA	7.5
38	2g	156	TRP	7.5
49	1r	79	LEU	7.4
38	1g	80	VAL	7.4
54	1w	3	C	7.4
21	2Z	144	LEU	7.4
1	1A	2152	G	7.3
35	1d	157	LEU	7.2
54	2w	45	U	7.2
54	2w	14	A	7.2
42	1k	14	VAL	7.2
25	23	29	ARG	7.2
49	2r	87	ARG	7.2
49	2r	46	GLU	7.1
12	2Q	104	PHE	7.1
38	2g	81	GLY	7.1
33	2b	92	TYR	7.1
6	2G	48	GLU	7.1
17	2V	94	LEU	7.1
1	2A	2896	C	7.1
38	2g	85	TYR	7.1
1	2A	652(B)	A	7.1
49	1r	24	ALA	7.1
45	2n	39	LEU	6.9
54	2w	56	C	6.9
53	2v	24	A	6.9
33	2b	148	TYR	6.9
34	2c	52	LEU	6.9
54	2w	75	C	6.9
38	1g	156	TRP	6.8
54	1w	20	U	6.8
16	2U	88	ILE	6.8
34	2c	188	LEU	6.8
33	2b	112	VAL	6.8
54	2y	52	G	6.8
22	20	5	LYS	6.8
34	2c	189	ALA	6.8
34	2c	14	ILE	6.7
49	1r	85	LEU	6.7
42	1k	13	GLN	6.7

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Mol	Chain	Res	Type	RSRZ
35	1d	101	LEU	6.7
38	1g	85	TYR	6.7
54	2w	6	G	6.7
33	2b	188	ALA	6.6
54	2y	36	A	6.6
1	2A	883	G	6.6
49	2r	84	LYS	6.6
50	2s	52	TYR	6.6
54	2y	65	G	6.6
34	2c	204	LEU	6.6
54	2y	53	G	6.6
34	2c	182	ILE	6.6
33	2b	98	LEU	6.6
33	2b	115	LEU	6.6
9	2N	8	GLN	6.5
33	2b	69	LEU	6.5
38	1g	154	TYR	6.5
50	2s	82	GLY	6.5
34	2c	187	ALA	6.5
54	1w	44	G	6.5
9	2N	9	VAL	6.5
33	2b	232	PRO	6.4
11	2P	123	LEU	6.4
49	1r	78	LEU	6.4
35	2d	168	ARG	6.4
54	2y	63	G	6.4
45	2n	53	LEU	6.4
38	2g	78	ARG	6.4
8	2I	107	VAL	6.3
7	2H	103	LEU	6.3
34	2c	134	ILE	6.3
54	2w	7	A	6.3
49	1r	87	ARG	6.3
11	2P	79	ARG	6.3
25	23	26	LEU	6.3
54	1w	10	G	6.3
50	2s	84	GLY	6.3
9	2N	140	VAL	6.3
36	2e	12	LEU	6.3
28	26	54	ILE	6.3
44	2m	102	ARG	6.2
54	2w	50	U	6.2

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Mol	Chain	Res	Type	RSRZ
45	2n	34	TYR	6.2
35	1d	2	GLY	6.2
8	2I	85	GLU	6.2
34	2c	109	PRO	6.2
37	2f	48	LEU	6.1
22	20	2	ALA	6.1
33	2b	67	THR	6.1
25	23	60	GLU	6.1
45	2n	11	LYS	6.1
34	2c	160	ALA	6.1
53	1v	12	A	6.1
34	2c	57	ILE	6.1
33	2b	97	TRP	6.1
6	2G	41	GLN	6.0
34	2c	51	GLY	6.0
54	2y	64	A	6.0
1	1A	2132	U	6.0
37	1f	48	LEU	6.0
34	2c	184	TYR	6.0
1	1A	2138	C	6.0
3	2D	276	LYS	6.0
33	2b	197	VAL	6.0
33	2b	211	ILE	6.0
44	2m	90	LEU	6.0
33	2b	181	PHE	6.0
34	2c	6	HIS	6.0
31	29	37	GLY	6.0
34	2c	171	GLY	6.0
1	2A	2132	U	6.0
34	2c	198	VAL	5.9
35	2d	185	PHE	5.9
45	2n	6	LEU	5.9
1	2A	2154	G	5.9
54	1w	69	G	5.9
35	1d	70	ILE	5.9
9	2N	61	ARG	5.9
30	28	16	ILE	5.9
49	1r	40	LEU	5.9
54	2w	10	G	5.8
33	2b	215	LEU	5.8
35	1d	11	LEU	5.8
34	2c	142	MET	5.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2793	G	5.8
7	2H	145	ALA	5.8
35	1d	21	LEU	5.8
33	2b	63	MET	5.8
6	2G	136	ARG	5.8
50	2s	76	PRO	5.8
42	2k	109	VAL	5.8
35	1d	158	ILE	5.7
49	1r	29	PHE	5.7
1	1A	2151	G	5.7
1	2A	2133	G	5.7
33	2b	90	MET	5.7
49	2r	49	LYS	5.7
17	2V	5	VAL	5.7
6	2G	157	ILE	5.7
41	2j	47	PHE	5.7
38	1g	153	HIS	5.6
17	2V	64	HIS	5.6
1	1A	885	C	5.6
49	1r	31	LEU	5.6
33	2b	184	VAL	5.6
54	2w	23	A	5.6
7	2H	35	VAL	5.6
17	2V	12	TYR	5.6
44	2m	70	LEU	5.6
55	2x	20	U	5.6
34	2c	55	VAL	5.6
54	2w	5	G	5.6
33	2b	96	ARG	5.6
34	2c	186	PHE	5.6
54	1w	73	A	5.6
54	2w	15	G	5.6
54	2w	28	G	5.6
54	1y	20	U	5.6
6	2G	152	LEU	5.6
41	2j	55	LYS	5.5
11	2P	148	LEU	5.5
33	2b	155	LEU	5.5
35	1d	111	ALA	5.5
54	1y	36	A	5.5
49	2r	26	LEU	5.5
54	2w	47	U	5.5

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Mol	Chain	Res	Type	RSRZ
1	1A	2108	C	5.5
54	2w	49	C	5.5
3	1D	276	LYS	5.5
17	2V	42	GLY	5.5
1	2A	2155	G	5.5
50	2s	49	ILE	5.5
26	24	54	GLY	5.5
33	2b	71	VAL	5.5
17	2V	20	LEU	5.5
33	2b	113	HIS	5.5
34	2c	115	LEU	5.5
42	1k	83	ILE	5.5
54	2w	69	G	5.4
55	2x	70	G	5.4
1	2A	885	C	5.4
34	2c	72	LYS	5.4
49	1r	54	ARG	5.4
33	2b	223	ILE	5.4
30	28	15	LYS	5.4
54	2w	21	A	5.4
33	2b	164	VAL	5.4
43	2l	64	TYR	5.4
7	2H	72	ILE	5.4
38	2g	79	ARG	5.4
43	2l	39	VAL	5.4
35	2d	184	LYS	5.4
7	2H	159	GLU	5.4
49	2r	43	PHE	5.4
33	2b	228	GLY	5.4
34	2c	158	GLY	5.4
1	2A	2128	C	5.4
54	2w	67	C	5.4
25	23	24	LYS	5.4
49	1r	25	THR	5.3
34	2c	146	ALA	5.3
8	2I	122	GLU	5.3
33	2b	220	ASP	5.3
23	21	28	GLY	5.3
32	2a	1030(B)	C	5.3
22	20	4	LYS	5.3
25	23	25	ALA	5.3
1	2A	2801(A)	A	5.3

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Mol	Chain	Res	Type	RSRZ
50	2s	31	ILE	5.3
50	2s	63	THR	5.3
33	2b	145	LEU	5.3
34	2c	126	ARG	5.3
49	2r	34	TYR	5.3
53	2v	13	A	5.3
7	2H	113	VAL	5.3
1	2A	652(C)	G	5.3
54	2w	22	G	5.3
35	2d	37	PRO	5.3
34	2c	80	GLY	5.3
54	2w	31	A	5.2
11	2P	149	GLU	5.2
33	2b	233	SER	5.2
49	1r	38	GLU	5.2
7	2H	48	GLY	5.2
33	2b	122	PHE	5.2
54	2w	74	C	5.2
37	2f	89	MET	5.2
54	2y	47	U	5.2
33	2b	99	GLY	5.2
1	2A	6	A	5.2
1	2A	2794	C	5.2
34	2c	8	ILE	5.2
42	1k	91	ARG	5.2
54	2y	5	G	5.2
1	2A	229	A	5.2
34	2c	65	ALA	5.2
54	2w	19	G	5.2
44	2m	94	ARG	5.2
49	1r	42	ARG	5.2
35	1d	5	ILE	5.2
38	2g	84	ASN	5.1
25	23	30	ARG	5.1
6	2G	88	ILE	5.1
32	1a	345	C	5.1
34	2c	77	ILE	5.1
33	2b	201	ILE	5.1
34	2c	87	LEU	5.1
42	1k	81	ASP	5.1
1	1A	2131	G	5.1
1	2A	2131	G	5.1

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Mol	Chain	Res	Type	RSRZ
54	2w	18	G	5.1
12	2Q	2	LEU	5.1
38	1g	79	ARG	5.1
43	1l	61	THR	5.1
9	2N	44	PRO	5.1
34	2c	167	TRP	5.1
33	2b	116	GLU	5.1
54	1w	4	C	5.1
1	1A	2145	C	5.1
11	2P	91	PHE	5.0
50	2s	79	THR	5.0
33	2b	200	ILE	5.0
33	1b	21	ARG	5.0
25	23	28	LEU	5.0
7	2H	37	VAL	5.0
42	1k	19	ALA	5.0
45	2n	10	ALA	5.0
1	1A	2146	C	5.0
7	2H	175	LYS	5.0
49	1r	26	LEU	5.0
54	2w	24	G	5.0
36	1e	10	MET	5.0
44	2m	122	LYS	5.0
34	2c	53	ALA	5.0
1	2A	652(T)	C	5.0
7	2H	121	ILE	5.0
38	2g	155	ARG	5.0
54	2y	6	G	5.0
34	2c	185	GLY	4.9
28	26	11	LEU	4.9
34	2c	191	THR	4.9
38	2g	147	ALA	4.9
36	2e	109	ILE	4.9
50	2s	36	ARG	4.9
1	1A	2174	C	4.9
8	2I	12	LEU	4.9
42	2k	25	TYR	4.9
34	2c	200	ALA	4.9
7	2H	24	VAL	4.9
22	20	8	GLY	4.9
34	2c	194	GLY	4.9
54	1w	1	G	4.9

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Mol	Chain	Res	Type	RSRZ
49	1r	23	LYS	4.9
52	2u	16	GLY	4.9
49	1r	39	VAL	4.9
17	2V	1	MET	4.9
49	2r	83	GLU	4.9
54	2y	45	U	4.9
38	2g	77	SER	4.9
7	2H	114	VAL	4.9
1	1A	2109	U	4.9
44	2m	121	LYS	4.9
44	2m	88	ARG	4.9
6	2G	86	MET	4.9
7	2H	94	TYR	4.9
11	2P	95	VAL	4.9
16	2U	79	PHE	4.9
49	2r	86	VAL	4.9
9	2N	116	LEU	4.9
34	2c	19	GLU	4.9
38	1g	84	ASN	4.9
33	2b	81	VAL	4.8
33	2b	227	GLY	4.8
33	2b	37	ASN	4.8
34	2c	47	LEU	4.8
34	2c	78	GLY	4.8
37	1f	61	LEU	4.8
34	2c	147	LYS	4.8
33	2b	108	ILE	4.8
11	2P	144	GLU	4.8
33	2b	207	ALA	4.8
42	2k	60	ALA	4.8
1	1A	1096	A	4.8
33	2b	111	ARG	4.8
33	2b	146	GLN	4.8
1	1A	2141	G	4.8
34	2c	105	GLU	4.8
44	2m	4	ILE	4.8
33	2b	121	LEU	4.8
1	1A	2142	C	4.8
11	2P	125	VAL	4.7
33	2b	142	LEU	4.7
37	2f	45	LEU	4.7
43	1l	64	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
54	2w	66	U	4.7
32	1a	1030(B)	C	4.7
33	2b	153	ARG	4.7
44	2m	6	GLY	4.7
1	1A	2133	G	4.7
17	2V	14	VAL	4.7
31	29	15	LYS	4.7
45	2n	50	LYS	4.7
33	2b	210	SER	4.7
34	2c	206	GLU	4.7
6	2G	72	ARG	4.7
34	2c	172	ARG	4.7
33	2b	91	PRO	4.7
34	2c	180	ALA	4.7
35	2d	27	TYR	4.7
49	1r	47	THR	4.7
44	2m	66	LEU	4.7
11	2P	116	GLY	4.7
42	2k	108	ILE	4.7
8	2I	74	ASN	4.7
36	2e	10	MET	4.7
33	2b	72	GLY	4.7
50	2s	14	HIS	4.6
38	1g	82	GLY	4.6
7	2H	20	ALA	4.6
42	2k	13	GLN	4.6
21	2Z	155	LEU	4.6
32	1a	1030(A)	G	4.6
33	2b	89	GLY	4.6
12	2Q	37	LEU	4.6
42	2k	91	ARG	4.6
34	2c	44	GLU	4.6
42	1k	75	TYR	4.6
44	2m	23	TYR	4.6
33	2b	216	SER	4.6
1	1A	2158	A	4.6
35	1d	115	ARG	4.6
36	2e	33	VAL	4.6
42	2k	96	ARG	4.6
1	2A	2803	C	4.6
8	2I	86	THR	4.6
33	2b	177	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
33	2b	114	ARG	4.6
34	2c	127	ARG	4.6
16	2U	90	VAL	4.6
54	1w	14	A	4.6
1	2A	884	C	4.6
34	2c	4	LYS	4.6
7	2H	36	PRO	4.6
42	2k	59	TYR	4.6
7	2H	107	VAL	4.6
16	2U	80	ILE	4.5
38	1g	155	ARG	4.5
44	2m	97	PRO	4.5
35	1d	110	PHE	4.5
49	2r	66	LEU	4.5
53	2v	12	A	4.5
6	2G	49	ASP	4.5
25	23	21	ALA	4.5
54	2w	65	G	4.5
34	2c	48	TYR	4.5
35	1d	122	ARG	4.5
53	1v	24	A	4.5
34	2c	199	LYS	4.5
42	2k	90	GLY	4.5
9	2N	10	GLU	4.5
11	2P	122	PRO	4.5
42	1k	95	ILE	4.5
49	1r	46	GLU	4.5
43	2l	32	PHE	4.5
49	2r	42	ARG	4.5
45	2n	47	LEU	4.5
35	2d	166	LYS	4.5
6	2G	146	TYR	4.5
42	1k	84	VAL	4.5
50	2s	41	VAL	4.5
32	2a	1220	G	4.5
33	2b	95	GLN	4.5
1	1A	1095	A	4.5
7	2H	23	ARG	4.5
33	2b	17	PHE	4.5
37	2f	55	ASP	4.5
42	1k	108	ILE	4.5
1	1A	2129	C	4.5

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Mol	Chain	Res	Type	RSRZ
32	2a	1030	C	4.5
42	1k	15	ALA	4.5
54	1w	13	C	4.5
34	2c	107	GLN	4.5
35	2d	160	GLN	4.5
31	29	16	VAL	4.5
42	2k	114	VAL	4.5
34	2c	202	ILE	4.5
54	2w	48	C	4.5
34	1c	87	LEU	4.4
34	2c	91	LEU	4.4
37	1f	52	ILE	4.4
34	2c	183	ASP	4.4
32	2a	1034	G	4.4
25	23	12	PRO	4.4
33	2b	88	ALA	4.4
38	1g	81	GLY	4.4
32	2a	1532	U	4.4
34	2c	7	PRO	4.4
1	2A	2174	C	4.4
22	10	5	LYS	4.4
54	1w	68	C	4.4
54	2y	72	C	4.4
35	2d	161	ASN	4.4
49	2r	51	LEU	4.4
54	1y	14	A	4.4
34	2c	66	VAL	4.4
50	2s	35	SER	4.4
39	2h	71	GLY	4.4
50	2s	50	ALA	4.4
1	1A	2154	G	4.4
42	1k	18	ARG	4.4
21	2Z	50	GLN	4.4
11	2P	78	PRO	4.4
34	1c	193	TYR	4.4
8	2I	11	ASN	4.4
30	28	61	LEU	4.4
54	1w	6	G	4.4
42	1k	117	ASN	4.4
33	2b	158	LEU	4.4
34	2c	33	LEU	4.4
35	2d	35	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
50	2s	30	LEU	4.4
54	2w	58	A	4.4
49	2r	62	GLU	4.4
34	1c	78	GLY	4.3
1	1A	2140	C	4.3
34	2c	70	VAL	4.3
33	1b	215	LEU	4.3
12	2Q	1	MET	4.3
17	2V	38	LEU	4.3
30	28	29	LYS	4.3
16	2U	62	ILE	4.3
54	2y	34	G	4.3
25	23	54	VAL	4.3
17	2V	93	GLU	4.3
54	2y	4	C	4.3
35	1d	3	ARG	4.3
34	2c	13	GLY	4.3
54	2y	51	U	4.3
6	2G	149	VAL	4.3
21	2Z	139	VAL	4.3
54	1w	15	G	4.3
38	2g	151	TYR	4.3
33	2b	78	GLN	4.3
34	2c	79	ARG	4.3
35	2d	49	ARG	4.3
11	2P	110	TYR	4.3
34	2c	100	ALA	4.3
11	2P	109	GLY	4.3
28	26	7	ILE	4.3
33	1b	214	ILE	4.3
35	2d	169	LYS	4.3
33	2b	160	ASP	4.3
1	1A	2128	C	4.3
32	1a	848	C	4.3
54	1w	25	C	4.3
52	2u	6	ARG	4.3
37	2f	59	TYR	4.3
1	2A	652(U)	G	4.3
53	1v	13	A	4.3
8	2I	1	MET	4.3
54	2w	68	C	4.3
11	2P	93	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
11	2P	127	ALA	4.3
35	2d	183	GLY	4.3
42	1k	87	THR	4.3
33	2b	109	SER	4.3
34	2c	69	HIS	4.2
34	2c	190	ARG	4.2
25	23	53	LEU	4.2
1	2A	1170	G	4.2
26	24	51	ASP	4.2
33	2b	120	ALA	4.2
34	2c	50	ALA	4.2
36	1e	6	PHE	4.2
49	2r	47	THR	4.2
7	2H	21	PRO	4.2
9	2N	23	LEU	4.2
35	1d	10	ARG	4.2
36	2e	64	ARG	4.2
50	2s	83	HIS	4.2
7	2H	49	VAL	4.2
34	2c	149	ALA	4.2
54	2w	12	U	4.2
34	2c	104	GLN	4.2
8	2I	137	PRO	4.2
34	2c	145	GLY	4.2
35	2d	165	MET	4.2
34	2c	21	ARG	4.2
38	2g	4	ARG	4.2
45	2n	29	ARG	4.2
1	1A	2897	U	4.2
50	2s	40	ILE	4.2
3	2D	275	LYS	4.2
8	2I	72	LEU	4.2
34	2c	81	GLY	4.2
54	1y	64	A	4.2
7	2H	17	VAL	4.2
49	2r	55	ARG	4.2
34	2c	203	PHE	4.2
35	2d	164	ALA	4.2
38	2g	139	GLU	4.2
1	1A	1064	C	4.2
3	1D	275	LYS	4.2
11	2P	114	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
25	23	27	GLY	4.2
33	1b	33	TYR	4.2
37	1f	98	LEU	4.2
33	2b	94	ASN	4.2
34	2c	108	ASN	4.2
54	1w	11	C	4.2
34	2c	159	GLY	4.1
6	2G	135	LEU	4.1
17	2V	95	LEU	4.1
21	2Z	138	GLU	4.1
34	2c	178	LEU	4.1
1	1A	2130	U	4.1
21	2Z	174	VAL	4.1
34	2c	173	VAL	4.1
36	2e	63	ARG	4.1
1	1A	2107	C	4.1
34	2c	43	LEU	4.1
49	1r	52	PRO	4.1
42	1k	82	VAL	4.1
34	2c	113	ALA	4.1
43	2l	51	ALA	4.1
35	1d	22	LYS	4.1
6	2G	90	LEU	4.1
16	2U	117	GLN	4.1
37	2f	7	ASN	4.1
7	2H	52	VAL	4.1
32	2a	1001	A	4.1
1	2A	2127	G	4.1
43	1l	59	ARG	4.1
54	2y	1	G	4.1
32	1a	841	U	4.1
32	2a	1257	U	4.1
11	2P	83	VAL	4.1
22	20	9	SER	4.1
34	2c	140	ARG	4.1
28	26	5	VAL	4.1
33	2b	105	PHE	4.1
33	2b	62	ALA	4.1
54	2y	62	C	4.1
1	1A	2150	U	4.1
22	10	3	HIS	4.1
34	2c	143	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
5	2F	207	GLY	4.1
23	21	29	GLY	4.1
23	21	30	VAL	4.1
45	2n	51	GLY	4.1
11	2P	141	ALA	4.1
36	2e	13	ILE	4.1
42	1k	21	ILE	4.1
33	2b	77	ALA	4.1
21	2Z	149	SER	4.0
35	1d	105	VAL	4.0
54	2y	58	A	4.0
1	2A	1026	U	4.0
35	1d	112	VAL	4.0
43	2l	55	VAL	4.0
7	2H	101	ARG	4.0
54	2y	23	A	4.0
34	1c	72	LYS	4.0
7	2H	151	ILE	4.0
49	2r	50	ILE	4.0
33	2b	79	ASP	4.0
38	1g	78	ARG	4.0
8	2I	29	TYR	4.0
38	2g	152	ALA	4.0
54	2w	9	A	4.0
9	2N	51	PHE	4.0
1	2A	888	C	4.0
54	1y	47	U	4.0
15	1T	38	ASN	4.0
17	2V	92	THR	4.0
42	2k	110	ASP	4.0
1	2A	1847	A	4.0
32	1a	344	A	4.0
37	1f	97	PHE	4.0
54	2w	43	C	4.0
25	23	17	LYS	4.0
30	28	21	LYS	4.0
33	2b	144	ARG	4.0
44	2m	120	LYS	4.0
25	23	59	VAL	4.0
33	2b	135	GLN	4.0
53	2v	14	A	4.0
11	2P	147	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
25	23	9	VAL	4.0
34	2c	120	VAL	4.0
1	2A	896	A	3.9
33	2b	76	GLN	3.9
34	2c	170	GLN	3.9
37	2f	46	ARG	3.9
33	1b	213	LEU	3.9
7	2H	124	GLU	3.9
42	2k	35	PRO	3.9
49	2r	54	ARG	3.9
54	2y	48	C	3.9
34	2c	17	ASP	3.9
54	2w	57	G	3.9
3	2D	271	ILE	3.9
11	2P	75	ILE	3.9
42	2k	29	ILE	3.9
7	2H	76	VAL	3.9
8	2I	18	VAL	3.9
44	2m	98	VAL	3.9
6	2G	137	GLU	3.9
50	2s	70	LYS	3.9
34	2c	201	TYR	3.9
34	2c	40	ARG	3.9
8	2I	63	ALA	3.9
11	2P	119	GLU	3.9
35	1d	102	ASP	3.9
11	2P	88	LEU	3.9
32	2a	1044	A	3.9
34	2c	37	GLN	3.9
42	1k	77	MET	3.9
54	2y	61	C	3.9
7	2H	148	ILE	3.9
54	2y	57	G	3.9
49	1r	43	PHE	3.9
42	2k	14	VAL	3.9
30	28	60	LEU	3.9
33	2b	221	LEU	3.9
49	1r	51	LEU	3.9
42	2k	18	ARG	3.9
7	2H	164	TYR	3.9
33	2b	131	PRO	3.9
1	2A	2146	C	3.9

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Mol	Chain	Res	Type	RSRZ
54	2w	11	C	3.9
33	2b	162	ILE	3.9
42	1k	64	ALA	3.9
7	2H	71	LEU	3.9
11	2P	105	LEU	3.9
35	1d	168	ARG	3.9
35	2d	120	LEU	3.9
38	2g	149	ARG	3.9
49	1r	82	THR	3.9
22	10	8	GLY	3.9
35	1d	4	TYR	3.9
35	2d	167	GLY	3.9
42	1k	20	TYR	3.9
54	2y	2	C	3.9
7	2H	19	VAL	3.8
34	2c	101	LEU	3.8
45	2n	56	VAL	3.8
32	1a	1030(C)	G	3.8
54	1y	53	G	3.8
54	2w	27	G	3.8
6	2G	39	ILE	3.8
44	2m	104	ARG	3.8
33	2b	225	ALA	3.8
42	1k	66	LEU	3.8
42	1k	107	SER	3.8
50	2s	71	LEU	3.8
11	2P	92	GLU	3.8
11	2P	94	GLU	3.8
32	1a	1027	C	3.8
25	23	2	PRO	3.8
33	2b	48	MET	3.8
1	1A	2159	G	3.8
32	2a	1001(A)	G	3.8
37	2f	8	ILE	3.8
33	2b	149	LEU	3.8
34	2c	196	LEU	3.8
35	1d	170	VAL	3.8
37	2f	9	VAL	3.8
34	2c	10	PHE	3.8
34	1c	65	ALA	3.8
11	2P	101	VAL	3.8
11	2P	106	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
12	2Q	79	LEU	3.8
25	23	6	VAL	3.8
34	2c	15	THR	3.8
33	2b	157	ARG	3.8
50	2s	66	MET	3.8
32	2a	999	C	3.8
45	2n	37	PHE	3.8
54	1w	45	U	3.8
7	2H	89	ILE	3.8
8	2I	3	VAL	3.8
8	2I	19	VAL	3.8
33	2b	57	PHE	3.8
33	2b	68	ILE	3.8
34	2c	175	LEU	3.8
36	2e	89	ILE	3.8
11	2P	77	ARG	3.8
43	1l	65	GLU	3.8
9	2N	1	MET	3.8
33	1b	37	ASN	3.8
34	1c	128	PHE	3.8
37	1f	50	TYR	3.8
42	1k	25	TYR	3.8
36	2e	31	LEU	3.8
42	2k	89	ALA	3.8
49	2r	24	ALA	3.8
49	2r	48	GLY	3.8
49	2r	79	LEU	3.8
25	23	47	VAL	3.8
33	2b	136	VAL	3.8
42	1k	47	VAL	3.8
37	1f	83	ASP	3.8
38	2g	140	ASP	3.8
3	2D	273	ARG	3.7
42	2k	50	TYR	3.7
12	2Q	66	ILE	3.7
16	2U	98	LEU	3.7
31	29	26	ILE	3.7
35	1d	120	LEU	3.7
49	1r	76	LEU	3.7
37	1f	55	ASP	3.7
49	2r	22	VAL	3.7
30	28	25	MET	3.7

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Mol	Chain	Res	Type	RSRZ
8	2I	109	ILE	3.7
11	2P	124	LYS	3.7
34	2c	157	ILE	3.7
7	2H	141	VAL	3.7
1	2A	1168	G	3.7
21	2Z	170	THR	3.7
1	1A	1094	U	3.7
1	1A	2139	C	3.7
55	1x	67	C	3.7
1	1A	2173	A	3.7
34	2c	155	GLY	3.7
54	1y	21	A	3.7
54	2y	21	A	3.7
11	2P	100	LEU	3.7
50	2s	53	ASN	3.7
34	2c	174	PRO	3.7
12	2Q	91	GLU	3.7
54	1w	12	U	3.7
32	2a	1036	G	3.7
54	1y	5	G	3.7
54	1y	48	C	3.7
21	2Z	140	ASP	3.7
39	2h	83	ILE	3.7
6	2G	47	LYS	3.7
9	2N	43	THR	3.7
49	1r	55	ARG	3.7
50	2s	32	LYS	3.7
6	2G	133	LEU	3.7
34	2c	136	GLN	3.7
7	2H	86	GLU	3.7
25	23	43	ILE	3.7
33	2b	80	ILE	3.7
11	2P	65	ARG	3.7
35	2d	47	ARG	3.7
50	2s	59	PRO	3.7
33	2b	83	MET	3.7
35	1d	165	MET	3.7
11	2P	62	LEU	3.7
35	1d	24	GLU	3.7
1	2A	2145	C	3.7
54	1w	67	C	3.7
35	2d	112	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2156	G	3.7
34	1c	109	PRO	3.7
35	2d	23	GLY	3.7
7	2H	33	LEU	3.7
33	2b	140	HIS	3.7
35	1d	154	ASN	3.7
37	1f	49	ALA	3.7
37	1f	8	ILE	3.7
43	2l	70	ILE	3.7
54	2y	25	C	3.7
11	2P	39	LYS	3.7
54	2y	44	G	3.7
16	2U	60	LEU	3.6
17	2V	39	LEU	3.6
11	2P	140	ALA	3.6
31	29	24	TYR	3.6
43	1l	91	LYS	3.6
42	2k	57	THR	3.6
54	1y	56	C	3.6
8	2I	140	LEU	3.6
33	1b	28	PHE	3.6
41	2j	54	PHE	3.6
43	1l	60	LEU	3.6
54	1w	76	A	3.6
11	1P	149	GLU	3.6
11	2P	68	GLN	3.6
35	1d	179	GLU	3.6
45	2n	16	PHE	3.6
21	2Z	147	GLY	3.6
33	2b	66	GLY	3.6
12	2Q	109	VAL	3.6
17	2V	4	ILE	3.6
33	2b	222	ILE	3.6
41	2j	50	ILE	3.6
42	1k	111	ASP	3.6
30	28	62	LEU	3.6
33	2b	138	LEU	3.6
38	2g	99	LEU	3.6
42	1k	98	LEU	3.6
49	1r	44	LEU	3.6
34	2c	181	ASN	3.6
42	1k	69	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
54	1w	2	C	3.6
6	2G	70	VAL	3.6
11	2P	126	VAL	3.6
49	1r	50	ILE	3.6
1	1A	2125	G	3.6
54	2w	59	U	3.6
36	2e	8	GLU	3.6
34	2c	205	GLY	3.6
1	2A	645	C	3.6
1	2A	652(D)	C	3.6
6	2G	84	LYS	3.6
30	28	59	LYS	3.6
37	1f	54	LYS	3.6
37	2f	92	LYS	3.6
16	2U	105	VAL	3.6
32	1a	1030	C	3.6
49	1r	75	ILE	3.6
42	1k	28	THR	3.6
42	1k	92	GLU	3.6
22	20	69	PHE	3.6
50	2s	16	LEU	3.6
54	2y	33	U	3.6
11	2P	107	LYS	3.6
22	20	11	ARG	3.6
34	2c	114	PRO	3.6
34	2c	162	GLN	3.6
4	1E	1	MET	3.6
34	2c	128	PHE	3.6
9	2N	12	ARG	3.6
25	23	35	ARG	3.6
33	2b	147	LYS	3.6
34	2c	54	ARG	3.6
7	2H	102	ALA	3.6
1	2A	2894	G	3.6
7	2H	84	SER	3.6
34	2c	49	SER	3.6
54	1y	23	A	3.6
30	28	17	THR	3.6
11	2P	45	LEU	3.6
11	2P	85	LEU	3.6
44	2m	100	GLY	3.6
33	1b	188	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
33	2b	166	ASP	3.5
33	2b	218	ALA	3.5
42	2k	19	ALA	3.5
54	2y	60	U	3.5
42	1k	78	GLN	3.5
1	1A	2155	G	3.5
1	2A	1169	G	3.5
35	1d	118	ARG	3.5
35	2d	19	LEU	3.5
35	2d	157	LEU	3.5
6	2G	155	MET	3.5
54	1y	13	C	3.5
54	2w	42	C	3.5
37	1f	99	ALA	3.5
33	2b	150	SER	3.5
9	2N	5	VAL	3.5
16	2U	110	VAL	3.5
35	1d	160	GLN	3.5
42	1k	29	ILE	3.5
49	1r	56	THR	3.5
17	2V	62	LEU	3.5
35	1d	20	TYR	3.5
1	2A	2157	G	3.5
32	2a	1030(A)	G	3.5
11	2P	111	ARG	3.5
34	2c	207	VAL	3.5
37	1f	90	VAL	3.5
28	26	20	ASN	3.5
41	2j	61	GLU	3.5
1	1A	2162	G	3.5
23	21	26	ARG	3.5
1	2A	2188	C	3.5
54	1y	3	C	3.5
34	1c	39	ILE	3.5
45	2n	42	ILE	3.5
33	2b	139	LYS	3.5
7	2H	123	PHE	3.5
11	2P	35	HIS	3.5
11	2P	51	PHE	3.5
33	2b	123	ALA	3.5
25	23	49	LYS	3.5
9	2N	46	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
26	24	50	VAL	3.5
42	1k	109	VAL	3.5
1	2A	882	G	3.5
32	1a	162	A	3.5
34	2c	192	THR	3.5
17	2V	35	LEU	3.5
54	2y	13	C	3.5
54	2y	12	U	3.5
12	2Q	12	GLN	3.5
16	2U	106	PHE	3.5
8	2I	117	GLU	3.5
34	2c	12	LEU	3.5
42	2k	36	ASP	3.5
45	2n	52	GLN	3.5
1	1A	1065	U	3.5
1	1A	2178	C	3.5
32	2a	1092	A	3.5
33	1b	70	PHE	3.5
33	2b	130	ARG	3.5
34	2c	85	ARG	3.5
54	2w	29	G	3.5
54	2y	24	G	3.5
33	1b	77	ALA	3.5
25	23	58	VAL	3.5
33	2b	229	VAL	3.5
8	2I	4	ILE	3.5
42	2k	111	ASP	3.5
10	1O	91	LEU	3.5
34	1c	126	ARG	3.5
49	2r	44	LEU	3.5
6	2G	141	PHE	3.4
41	2j	63	PHE	3.4
32	2a	1000	U	3.4
33	2b	34	ALA	3.4
33	1b	189	ASP	3.4
37	2f	88	VAL	3.4
36	2e	43	LEU	3.4
49	1r	66	LEU	3.4
43	2l	56	ALA	3.4
55	2x	47	U	3.4
1	1A	2143	C	3.4
1	2A	2138	C	3.4

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Mol	Chain	Res	Type	RSRZ
1	2A	2170	A	3.4
55	2x	69	C	3.4
4	1E	87	GLU	3.4
32	2a	1026	G	3.4
32	2a	1033	G	3.4
33	1b	15	VAL	3.4
37	1f	95	GLU	3.4
8	2I	88	ILE	3.4
23	21	22	GLY	3.4
44	2m	92	HIS	3.4
41	2j	59	SER	3.4
42	1k	68	ALA	3.4
12	2Q	10	ARG	3.4
32	2a	1219	U	3.4
35	1d	209	ARG	3.4
35	1d	166	LYS	3.4
38	2g	86	GLN	3.4
30	28	64	TYR	3.4
34	1c	201	TYR	3.4
35	1d	66	ARG	3.4
35	1d	138	TYR	3.4
49	1r	28	GLU	3.4
17	2V	16	PRO	3.4
37	2f	61	LEU	3.4
33	2b	185	ILE	3.4
42	2k	83	ILE	3.4
45	2n	36	PHE	3.4
9	2N	42	TRP	3.4
35	1d	156	GLU	3.4
1	2A	1183	G	3.4
43	2l	69	TYR	3.4
7	2H	55	PRO	3.4
33	1b	194	PRO	3.4
12	2Q	63	LYS	3.4
17	2V	74	LYS	3.4
25	23	7	LYS	3.4
8	2I	92	VAL	3.4
22	20	63	VAL	3.4
33	2b	154	LEU	3.4
35	1d	135	LEU	3.4
35	2d	148	VAL	3.4
42	1k	57	THR	3.4

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Mol	Chain	Res	Type	RSRZ
42	1k	96	ARG	3.4
42	2k	107	SER	3.4
45	2n	46	GLU	3.4
1	2A	886	C	3.4
7	2H	74	ASN	3.4
7	2H	96	ALA	3.4
33	1b	48	MET	3.4
1	1A	2153	G	3.4
17	2V	18	LEU	3.4
55	2x	2	G	3.4
21	2Z	143	GLY	3.4
43	1l	63	GLY	3.4
7	2H	132	ARG	3.4
12	2Q	64	ILE	3.4
36	1e	109	ILE	3.4
42	1k	42	TRP	3.4
34	2c	168	ALA	3.4
36	2e	9	LYS	3.4
1	1A	1509	C	3.4
5	2F	7	TYR	3.4
33	2b	102	LEU	3.4
33	2b	117	GLU	3.4
6	2G	102	PHE	3.3
12	2Q	65	PHE	3.3
42	1k	97	ALA	3.3
1	1A	2161	C	3.3
44	2m	101	GLN	3.3
50	2s	26	GLY	3.3
25	23	37	LEU	3.3
48	1q	98	LEU	3.3
16	2U	63	VAL	3.3
34	2c	103	VAL	3.3
42	1k	80	VAL	3.3
42	2k	51	LYS	3.3
49	2r	56	THR	3.3
30	28	41	ILE	3.3
28	26	42	TRP	3.3
53	2v	22	U	3.3
9	2N	40	PRO	3.3
34	2c	132	ARG	3.3
42	2k	93	GLN	3.3
16	2U	109	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
35	2d	108	LEU	3.3
38	1g	151	TYR	3.3
6	2G	92	VAL	3.3
7	2H	125	VAL	3.3
17	2V	22	VAL	3.3
37	1f	9	VAL	3.3
49	1r	86	VAL	3.3
43	1l	85	ILE	3.3
1	2A	2173	A	3.3
11	2P	129	ALA	3.3
54	2w	26	A	3.3
31	29	13	LYS	3.3
34	2c	150	LYS	3.3
35	1d	132	ARG	3.3
43	1l	28	LYS	3.3
43	2l	88	GLY	3.3
49	1r	41	LYS	3.3
7	2H	144	VAL	3.3
17	2V	15	GLU	3.3
49	1r	71	LYS	3.3
7	2H	22	GLY	3.3
37	2f	21	LEU	3.3
7	2H	32	GLU	3.3
35	1d	163	GLU	3.3
42	1k	16	SER	3.3
44	2m	103	THR	3.3
45	2n	8	GLU	3.3
37	1f	92	LYS	3.3
6	2G	73	ALA	3.3
12	2Q	86	GLY	3.3
17	2V	48	GLY	3.3
16	2U	104	GLN	3.3
33	1b	222	ILE	3.3
33	2b	127	ILE	3.3
44	2m	78	ILE	3.3
33	1b	227	GLY	3.3
35	1d	180	GLY	3.3
34	1c	100	ALA	3.3
43	1l	62	SER	3.3
33	2b	203	GLY	3.3
44	2m	95	GLY	3.3
54	2y	35	A	3.3

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Mol	Chain	Res	Type	RSRZ
38	2g	150	ALA	3.3
49	1r	73	ALA	3.3
9	2N	87	LEU	3.3
54	2w	52	G	3.3
54	2y	22	G	3.3
54	2y	70	G	3.3
12	2Q	5	ARG	3.3
10	1O	52	VAL	3.2
42	2k	117	ASN	3.2
55	2x	67	C	3.2
36	1e	60	TYR	3.2
37	2f	6	VAL	3.2
49	1r	21	LYS	3.2
35	1d	19	LEU	3.2
7	2H	2	SER	3.2
7	2H	82	GLY	3.2
17	2V	101	GLY	3.2
32	2a	998	G	3.2
36	2e	55	VAL	3.2
54	2y	56	C	3.2
55	2x	16	C	3.2
35	1d	35	ARG	3.2
9	2N	112	LEU	3.2
11	2P	145	PRO	3.2
21	2Z	24	LEU	3.2
34	2c	73	PRO	3.2
54	2y	73	A	3.2
7	2H	34	GLU	3.2
17	2V	72	VAL	3.2
37	2f	90	VAL	3.2
42	1k	116	HIS	3.2
44	2m	67	GLU	3.2
50	2s	60	VAL	3.2
40	2i	114	TYR	3.2
34	2c	56	ASP	3.2
54	2y	50	U	3.2
7	2H	105	LEU	3.2
37	1f	10	LEU	3.2
35	1d	167	GLY	3.2
37	2f	40	VAL	3.2
33	2b	226	ARG	3.2
1	2A	2189	U	3.2

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Mol	Chain	Res	Type	RSRZ
54	2w	61	C	3.2
50	2s	34	TRP	3.2
42	2k	30	VAL	3.2
42	2k	71	LYS	3.2
34	2c	39	ILE	3.2
50	2s	62	ILE	3.2
11	2P	120	ALA	3.2
38	2g	22	LEU	3.2
35	1d	16	GLY	3.2
55	2x	68	C	3.2
1	1A	2160	G	3.2
11	2P	64	LYS	3.2
7	2H	43	VAL	3.2
34	2c	106	VAL	3.2
38	2g	75	VAL	3.2
8	2I	25	TYR	3.2
9	2N	91	LEU	3.2
11	2P	118	GLY	3.2
30	28	2	PRO	3.2
12	2Q	103	MET	3.2
17	2V	21	ARG	3.2
42	1k	30	VAL	3.2
49	1r	69	THR	3.2
54	1w	49	C	3.2
32	2a	1224	G	3.2
9	2N	72	TYR	3.2
37	2f	4	TYR	3.2
41	1j	98	ILE	3.2
44	2m	5	ALA	3.2
7	2H	78	GLY	3.2
8	2I	5	LEU	3.2
35	2d	194	LEU	3.2
35	2d	175	SER	3.2
37	1f	58	GLY	3.2
34	2c	179	ARG	3.2
35	2d	33	MET	3.1
1	2A	9	U	3.1
54	1y	45	U	3.1
54	2y	7	A	3.1
7	2H	133	VAL	3.1
33	2b	55	PHE	3.1
34	1c	68	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
35	1d	61	LYS	3.1
49	2r	71	LYS	3.1
8	2I	47	LEU	3.1
16	2U	101	ARG	3.1
33	1b	233	SER	3.1
43	1l	89	ARG	3.1
25	23	34	GLU	3.1
22	20	45	PHE	3.1
49	2r	82	THR	3.1
8	1I	109	ILE	3.1
42	2k	21	ILE	3.1
25	23	23	LEU	3.1
33	2b	213	LEU	3.1
9	2N	11	PRO	3.1
33	1b	232	PRO	3.1
33	2b	183	PRO	3.1
35	1d	29	PRO	3.1
50	2s	47	HIS	3.1
27	15	60	VAL	3.1
34	2c	64	VAL	3.1
43	1l	122	THR	3.1
11	2P	15	ARG	3.1
34	2c	139	GLN	3.1
7	2H	83	TYR	3.1
17	2V	91	TYR	3.1
21	2Z	145	GLU	3.1
35	1d	176	LEU	3.1
44	1m	124	PRO	3.1
7	2H	138	LYS	3.1
32	1a	1028	C	3.1
33	2b	133	LYS	3.1
37	2f	86	ARG	3.1
35	2d	34	GLU	3.1
35	2d	179	GLU	3.1
54	1w	5	G	3.1
9	2N	60	ILE	3.1
34	2c	133	ALA	3.1
37	1f	100	ASN	3.1
42	2k	115	PRO	3.1
43	1l	98	TYR	3.1
1	1A	2896	C	3.1
11	2P	38	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
7	2H	88	LEU	3.1
33	2b	51	LEU	3.1
1	2A	881	G	3.1
23	21	68	PRO	3.1
8	2I	130	TYR	3.1
32	2a	204	U	3.1
54	2w	60	U	3.1
7	2H	47	GLU	3.1
37	1f	57	GLN	3.1
49	1r	53	ARG	3.1
42	2k	31	THR	3.1
17	2V	52	VAL	3.1
21	2Z	161	VAL	3.1
54	2y	49	C	3.1
3	2D	182	LEU	3.1
25	23	42	ALA	3.1
34	1c	189	ALA	3.1
34	2c	60	ALA	3.1
6	2G	140	ILE	3.1
34	2c	5	ILE	3.1
33	2b	74	LYS	3.1
54	2w	30	G	3.1
42	1k	90	GLY	3.1
38	2g	91	VAL	3.1
11	2P	135	LEU	3.1
16	2U	74	LEU	3.1
34	2c	129	ALA	3.1
35	2d	188	LEU	3.1
8	2I	138	ILE	3.1
10	2O	19	ILE	3.1
35	1d	38	TYR	3.0
42	1k	50	TYR	3.0
35	1d	69	GLY	3.0
42	2k	49	GLY	3.0
33	1b	101	MET	3.0
11	2P	146	VAL	3.0
34	2c	138	VAL	3.0
34	2c	135	LYS	3.0
35	1d	117	ALA	3.0
43	1l	41	ARG	3.0
45	2n	57	ARG	3.0
16	2U	71	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
33	1b	39	ILE	3.0
34	1c	77	ILE	3.0
54	2w	38	A	3.0
22	20	3	HIS	3.0
11	2P	1	MET	3.0
22	10	4	LYS	3.0
34	2c	116	VAL	3.0
33	2b	143	GLU	3.0
33	2b	224	GLN	3.0
49	2r	40	LEU	3.0
34	2c	84	ILE	3.0
41	1j	23	ILE	3.0
16	2U	72	HIS	3.0
38	2g	144	MET	3.0
7	2H	131	VAL	3.0
30	28	34	TRP	3.0
35	1d	97	LEU	3.0
35	1d	162	LEU	3.0
10	2O	41	ALA	3.0
1	2A	2125	G	3.0
11	2P	76	LYS	3.0
29	17	48	LYS	3.0
1	2A	2175	C	3.0
11	1P	136	GLU	3.0
37	2f	47	ARG	3.0
42	1k	125	PHE	3.0
6	2G	138	GLN	3.0
17	2V	7	THR	3.0
34	2c	68	VAL	3.0
11	2P	99	LEU	3.0
32	1a	1531	A	3.0
32	2a	1035	A	3.0
35	2d	186	LEU	3.0
35	1d	164	ALA	3.0
6	2G	142	PRO	3.0
7	2H	29	PRO	3.0
8	2I	51	ILE	3.0
12	2Q	85	LYS	3.0
45	2n	7	ILE	3.0
8	2I	133	HIS	3.0
34	1c	105	GLU	3.0
37	1f	94	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
42	1k	59	TYR	3.0
49	1r	34	TYR	3.0
1	2A	2153	G	3.0
7	2H	80	SER	3.0
54	1y	63	G	3.0
7	2H	67	LEU	3.0
10	2O	10	VAL	3.0
32	2a	1002	G	3.0
21	2Z	76	LEU	3.0
7	2H	166	GLY	3.0
9	2N	113	GLY	3.0
55	2x	72	A	3.0
35	1d	126	ILE	3.0
33	2b	209	ARG	3.0
6	2G	80	PHE	3.0
11	2P	58	THR	3.0
12	2Q	87	LYS	3.0
5	2F	193	VAL	3.0
6	2G	3	LEU	3.0
11	2P	115	LEU	3.0
14	2S	110	LEU	3.0
35	1d	17	VAL	3.0
25	23	51	ALA	3.0
32	1a	840	C	3.0
33	1b	66	GLY	3.0
33	2b	38	GLY	3.0
34	1c	206	GLU	3.0
50	2s	24	ALA	3.0
12	2Q	6	ARG	3.0
1	2A	2169	A	3.0
17	2V	26	ASP	3.0
30	28	48	PHE	3.0
50	2s	28	LYS	3.0
33	2b	31	TYR	3.0
9	2N	62	VAL	3.0
12	2Q	81	VAL	3.0
16	2U	83	LEU	3.0
33	1b	81	VAL	3.0
33	1b	126	GLU	3.0
49	2r	31	LEU	3.0
6	2G	151	ALA	3.0
7	2H	165	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
38	1g	83	ALA	3.0
31	29	17	ILE	2.9
44	2m	84	ILE	2.9
49	1r	70	ILE	2.9
33	1b	165	VAL	2.9
34	1c	81	GLY	2.9
35	2d	21	LEU	2.9
35	2d	176	LEU	2.9
34	2c	59	ARG	2.9
42	2k	126	ARG	2.9
49	2r	39	VAL	2.9
7	2H	128	PRO	2.9
21	2Z	121	HIS	2.9
33	1b	19	HIS	2.9
33	2b	41	ILE	2.9
35	1d	125	HIS	2.9
1	1A	2175	C	2.9
33	2b	205	ASP	2.9
22	20	68	GLU	2.9
37	2f	60	PHE	2.9
4	2E	49	LEU	2.9
11	2P	102	ARG	2.9
11	2P	142	GLY	2.9
32	1a	1034	G	2.9
28	26	10	LEU	2.9
40	2i	115	GLY	2.9
35	1d	30	LYS	2.9
35	2d	198	VAL	2.9
25	23	22	ALA	2.9
33	2b	85	ALA	2.9
38	2g	153	HIS	2.9
52	2u	5	ASP	2.9
25	23	10	LYS	2.9
28	26	28	ARG	2.9
33	2b	64	ARG	2.9
34	2c	16	ARG	2.9
42	2k	86	GLY	2.9
54	1y	4	C	2.9
11	2P	112	LEU	2.9
35	1d	202	LEU	2.9
35	2d	162	LEU	2.9
42	2k	63	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
35	2d	170	VAL	2.9
36	2e	67	VAL	2.9
17	2V	50	PRO	2.9
54	1y	1	G	2.9
41	2j	62	HIS	2.9
12	2Q	60	ARG	2.9
49	1r	63	GLN	2.9
33	2b	107	THR	2.9
1	1A	2137	C	2.9
17	2V	33	VAL	2.9
35	1d	181	MET	2.9
31	29	5	ALA	2.9
42	2k	42	TRP	2.9
9	2N	130	HIS	2.9
42	2k	95	ILE	2.9
45	2n	12	ARG	2.9
54	1y	6	G	2.9
33	1b	78	GLN	2.9
37	2f	58	GLY	2.9
54	1w	7	A	2.9
8	2I	75	LEU	2.9
9	2N	14	VAL	2.9
25	23	56	VAL	2.9
54	2y	66	U	2.9
9	2N	13	TRP	2.9
11	2P	137	LYS	2.9
42	1k	115	PRO	2.9
54	2y	3	C	2.9
55	2x	3	C	2.9
8	2I	33	ARG	2.9
49	1r	32	ARG	2.9
21	2Z	153	SER	2.9
34	1c	202	ILE	2.9
1	1A	1068	G	2.9
37	2f	75	LEU	2.9
54	2y	18	G	2.9
45	2n	22	THR	2.9
53	2v	23	A	2.9
7	2H	50	VAL	2.9
12	2Q	136	ALA	2.9
50	2s	69	HIS	2.9
21	2Z	137	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
36	2e	11	ILE	2.9
30	28	26	LYS	2.9
25	23	31	LEU	2.9
11	2P	97	PRO	2.9
35	1d	7	PRO	2.9
43	1l	26	ALA	2.9
54	1w	65	G	2.9
54	1y	35	A	2.8
54	1y	60	U	2.8
33	1b	133	LYS	2.8
42	1k	32	ILE	2.8
49	1r	68	LYS	2.8
11	2P	50	ARG	2.8
12	2Q	59	ARG	2.8
6	2G	50	ALA	2.8
12	2Q	121	ALA	2.8
16	2U	47	TYR	2.8
9	2N	84	LYS	2.8
42	1k	76	GLY	2.8
49	2r	61	LYS	2.8
1	1A	2181	G	2.8
16	2U	77	SER	2.8
21	2Z	146	ILE	2.8
28	26	34	LEU	2.8
30	28	30	ARG	2.8
7	2H	129	THR	2.8
54	2w	40	C	2.8
11	2P	52	GLU	2.8
16	2U	85	LYS	2.8
16	2U	96	ALA	2.8
1	1A	2144	U	2.8
28	16	54	ILE	2.8
35	2d	146	ILE	2.8
1	1A	2157	G	2.8
1	2A	2308	G	2.8
8	2I	35	LEU	2.8
32	2a	1531	A	2.8
17	2V	19	LYS	2.8
11	2P	143	GLY	2.8
35	1d	106	TYR	2.8
37	1f	4	TYR	2.8
31	29	19	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
33	2b	212	GLN	2.8
34	2c	152	ILE	2.8
42	2k	48	ILE	2.8
49	2r	81	PHE	2.8
45	2n	44	LEU	2.8
37	1f	84	ASN	2.8
1	2A	2141	G	2.8
17	2V	63	GLY	2.8
33	2b	230	VAL	2.8
35	2d	121	VAL	2.8
1	2A	897	C	2.8
35	2d	20	TYR	2.8
40	2i	125	TYR	2.8
55	2x	17	C	2.8
4	2E	195	LEU	2.8
8	2I	20	ASP	2.8
9	2N	127	ASP	2.8
12	2Q	34	LEU	2.8
16	2U	95	LEU	2.8
17	2V	25	LEU	2.8
42	1k	110	ASP	2.8
36	2e	114	GLY	2.8
5	2F	183	VAL	2.8
30	28	63	PRO	2.8
49	1r	80	PRO	2.8
21	2Z	156	LYS	2.8
23	21	21	ARG	2.8
33	1b	226	ARG	2.8
44	2m	110	ARG	2.8
1	2A	10	G	2.8
1	2A	2152	G	2.8
32	1a	1035	A	2.8
32	2a	1202	G	2.8
23	21	27	GLU	2.8
36	2e	133	TYR	2.8
54	1w	23	A	2.8
50	2s	43	GLU	2.8
1	1A	884	C	2.8
7	2H	162	ILE	2.8
8	2I	77	LEU	2.8
35	2d	110	PHE	2.8
37	1f	21	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
8	2I	108	THR	2.8
34	2c	41	GLY	2.8
50	2s	48	THR	2.8
9	2N	59	LYS	2.8
45	2n	15	LYS	2.8
30	28	14	VAL	2.8
42	2k	80	VAL	2.8
46	1o	65	ARG	2.8
12	2Q	48	GLU	2.8
16	2U	89	GLU	2.8
50	2s	12	ASP	2.8
1	2A	2191	G	2.8
5	2F	186	ILE	2.8
55	2x	65	C	2.8
50	2s	33	THR	2.8
42	2k	82	VAL	2.7
43	2l	68	ALA	2.7
32	1a	723	U	2.7
54	1w	66	U	2.7
7	1H	105	LEU	2.7
37	1f	60	PHE	2.7
41	2j	96	ILE	2.7
12	2Q	38	GLU	2.7
54	2y	28	G	2.7
7	2H	99	VAL	2.7
8	2I	37	VAL	2.7
17	2V	3	ALA	2.7
17	2V	37	VAL	2.7
33	2b	124	SER	2.7
45	2n	33	VAL	2.7
54	1y	12	U	2.7
54	2y	59	U	2.7
9	2N	26	LEU	2.7
34	2c	30	ARG	2.7
50	2s	22	LEU	2.7
52	2u	14	TRP	2.7
30	28	65	GLU	2.7
33	2b	231	GLU	2.7
34	1c	57	ILE	2.7
42	1k	99	GLN	2.7
3	2D	2	ALA	2.7
31	29	25	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2112	G	2.7
11	2P	87	ASP	2.7
42	1k	126	ARG	2.7
33	1b	148	TYR	2.7
46	1o	57	LEU	2.7
48	2q	32	TYR	2.7
49	1r	58	LEU	2.7
49	1r	64	ARG	2.7
35	2d	106	TYR	2.7
10	1O	47	ILE	2.7
33	1b	127	ILE	2.7
42	2k	32	ILE	2.7
31	29	8	LYS	2.7
34	1c	15	THR	2.7
35	1d	104	VAL	2.7
41	1j	72	VAL	2.7
10	1O	49	ARG	2.7
30	28	40	GLU	2.7
33	2b	137	ARG	2.7
34	2c	82	GLU	2.7
38	2g	119	ARG	2.7
41	1j	25	GLU	2.7
43	2l	59	ARG	2.7
45	2n	23	ARG	2.7
1	2A	2792	G	2.7
5	2F	32	LEU	2.7
34	1c	101	LEU	2.7
33	2b	42	ILE	2.7
12	2Q	75	THR	2.7
7	2H	56	SER	2.7
35	1d	8	VAL	2.7
3	2D	181	GLU	2.7
33	2b	35	GLU	2.7
17	2V	17	GLY	2.7
42	1k	17	GLY	2.7
16	2U	69	CYS	2.7
34	2c	118	GLN	2.7
38	2g	148	ASN	2.7
33	1b	163	PHE	2.7
36	2e	45	PHE	2.7
54	1y	2	C	2.7
32	1a	160	A	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2113	U	2.7
32	2a	723	U	2.7
1	1A	2147	G	2.7
1	2A	2100	G	2.7
3	1D	2	ALA	2.7
21	2Z	122	ARG	2.7
43	1l	68	ALA	2.7
39	2h	129	VAL	2.7
3	2D	180	GLY	2.7
6	2G	75	LYS	2.7
43	2l	28	LYS	2.7
21	2Z	44	PHE	2.7
37	2f	79	LEU	2.7
49	1r	36	ASN	2.7
35	2d	38	TYR	2.7
39	1h	58	TYR	2.7
7	2H	51	ARG	2.7
31	29	9	ARG	2.7
35	2d	159	ARG	2.7
36	2e	135	THR	2.7
32	2a	1102	A	2.7
11	2P	108	LYS	2.7
42	1k	113	PRO	2.7
49	2r	21	LYS	2.7
11	2P	71	VAL	2.7
34	1c	103	VAL	2.7
40	2i	124	GLN	2.7
8	1I	35	LEU	2.7
28	26	24	GLU	2.7
37	1f	59	TYR	2.7
7	2H	122	THR	2.7
9	2N	83	LYS	2.7
11	2P	96	THR	2.7
40	2i	127	LYS	2.7
43	1l	112	ASP	2.7
50	2s	13	ASP	2.7
7	2H	12	PRO	2.6
41	1j	20	ALA	2.6
45	1n	2	ALA	2.6
54	1w	75	C	2.6
21	2Z	39	VAL	2.6
3	2D	147	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
8	2I	44	LEU	2.6
41	2j	88	LEU	2.6
17	2V	83	ARG	2.6
25	23	20	LYS	2.6
35	1d	65	ARG	2.6
50	2s	81	ARG	2.6
11	2P	37	GLY	2.6
17	2V	49	THR	2.6
34	2c	74	GLY	2.6
49	1r	37	VAL	2.6
1	2A	2129	C	2.6
43	1l	23	LYS	2.6
43	1l	77	LEU	2.6
8	2I	82	ARG	2.6
28	26	50	ARG	2.6
54	2y	26	A	2.6
1	2A	2190	G	2.6
9	2N	85	ILE	2.6
30	28	19	SER	2.6
18	2W	112	GLY	2.6
33	1b	190	THR	2.6
37	2f	50	TYR	2.6
41	2j	6	ILE	2.6
7	2H	18	GLU	2.6
12	2Q	96	VAL	2.6
21	2Z	126	VAL	2.6
38	2g	135	VAL	2.6
5	2F	12	LEU	2.6
33	1b	187	LEU	2.6
35	1d	78	LEU	2.6
38	2g	76	ARG	2.6
41	1j	90	LEU	2.6
12	2Q	33	GLY	2.6
34	1c	8	ILE	2.6
34	1c	124	ILE	2.6
34	2c	2	GLY	2.6
36	1e	88	LYS	2.6
6	2G	115	ARG	2.6
7	2H	95	ARG	2.6
32	1a	1002	G	2.6
34	2c	156	ARG	2.6
43	1l	96	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
49	1r	74	ARG	2.6
54	1y	24	G	2.6
7	2H	98	LEU	2.6
35	1d	33	MET	2.6
43	1l	27	LEU	2.6
41	1j	89	ASP	2.6
50	2s	56	GLN	2.6
1	2A	652(V)	C	2.6
50	2s	72	GLY	2.6
7	2H	136	ILE	2.6
16	2U	108	GLU	2.6
33	1b	200	ILE	2.6
34	2c	22	TRP	2.6
1	2A	652(A)	A	2.6
53	2v	15	A	2.6
33	1b	71	VAL	2.6
36	2e	32	VAL	2.6
45	2n	27	CYS	2.6
8	2I	9	LEU	2.6
33	2b	180	LEU	2.6
37	1f	16	GLN	2.6
42	1k	62	GLN	2.6
32	1a	1026	G	2.6
32	2a	80	G	2.6
36	2e	6	PHE	2.6
54	2w	53	G	2.6
55	2x	17(A)	U	2.6
3	2D	270	ILE	2.6
30	28	46	ARG	2.6
34	1c	134	ILE	2.6
16	2U	68	ALA	2.6
34	1c	180	ALA	2.6
43	1l	43	VAL	2.6
1	2A	1182	A	2.6
6	2G	182	LYS	2.6
34	1c	115	LEU	2.6
38	2g	89	MET	2.6
43	1l	124	LYS	2.6
26	24	49	PHE	2.6
22	20	55	ARG	2.6
25	23	16	PRO	2.6
40	2i	90	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
42	1k	35	PRO	2.6
15	2T	131	ALA	2.6
35	1d	62	GLN	2.6
12	2Q	97	VAL	2.6
37	1f	6	VAL	2.6
37	1f	85	VAL	2.6
17	2V	60	GLU	2.6
4	2E	51	PHE	2.6
35	1d	6	GLY	2.6
1	2A	2602	A	2.6
32	2a	1225	A	2.6
49	2r	63	GLN	2.5
1	1A	2112	G	2.5
32	2a	1108	G	2.5
36	2e	60	TYR	2.5
4	2E	196	VAL	2.5
33	1b	229	VAL	2.5
35	1d	174	LEU	2.5
36	1e	69	VAL	2.5
37	1f	43	LEU	2.5
7	2H	100	GLY	2.5
43	1l	29	GLY	2.5
42	2k	16	SER	2.5
12	2Q	76	LYS	2.5
33	1b	75	LYS	2.5
16	2U	65	ILE	2.5
34	1c	14	ILE	2.5
38	2g	120	ILE	2.5
9	2N	4	TYR	2.5
12	2Q	93	TYR	2.5
44	2m	87	TYR	2.5
8	1I	72	LEU	2.5
8	2I	6	LEU	2.5
12	2Q	106	VAL	2.5
34	1c	55	VAL	2.5
39	1h	93	VAL	2.5
41	2j	49	VAL	2.5
1	2A	7	G	2.5
33	2b	23	ARG	2.5
9	2N	48	MET	2.5
12	2Q	80	GLU	2.5
44	2m	73	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
23	21	34	THR	2.5
33	2b	202	PRO	2.5
45	2n	54	PRO	2.5
28	26	2	ALA	2.5
36	1e	86	ALA	2.5
42	1k	89	ALA	2.5
7	2H	31	GLY	2.5
9	2N	33	LEU	2.5
11	2P	80	TYR	2.5
37	1f	86	ARG	2.5
40	2i	53	VAL	2.5
44	2m	7	VAL	2.5
12	2Q	3	MET	2.5
25	23	11	SER	2.5
35	1d	185	PHE	2.5
25	23	57	GLU	2.5
33	1b	128	GLU	2.5
43	1l	79	GLU	2.5
1	2A	845	G	2.5
53	2v	21	C	2.5
34	1c	67	THR	2.5
37	1f	51	PRO	2.5
42	1k	48	ILE	2.5
45	2n	49	HIS	2.5
34	2c	119	ARG	2.5
35	1d	139	ARG	2.5
8	2I	101	LEU	2.5
9	2N	15	LEU	2.5
33	1b	180	LEU	2.5
36	1e	55	VAL	2.5
37	2f	37	VAL	2.5
46	2o	60	VAL	2.5
1	2A	2310	A	2.5
35	2d	98	GLU	2.5
7	2H	85	LYS	2.5
8	2I	121	LYS	2.5
7	2H	65	HIS	2.5
30	28	7	HIS	2.5
42	1k	86	GLY	2.5
44	2m	9	ILE	2.5
48	1q	36	ILE	2.5
8	2I	123	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
17	2V	40	LEU	2.5
23	1l	98	LEU	2.5
33	1b	95	GLN	2.5
33	1b	149	LEU	2.5
33	2b	196	LEU	2.5
35	2d	196	LEU	2.5
36	2e	123	LEU	2.5
43	2l	27	LEU	2.5
49	2r	58	LEU	2.5
7	2H	119	GLU	2.5
15	1T	34	VAL	2.5
34	2c	130	VAL	2.5
43	1l	18	VAL	2.5
7	2H	38	SER	2.5
37	2f	97	PHE	2.5
49	1r	81	PHE	2.5
4	2E	1	MET	2.5
44	2m	82	MET	2.5
7	2H	13	LYS	2.5
42	2k	85	ARG	2.5
5	1F	14	PRO	2.5
30	28	58	ILE	2.5
33	2b	13	ALA	2.5
38	2g	7	ALA	2.5
49	2r	70	ILE	2.5
11	2P	70	GLN	2.5
26	24	57	GLU	2.5
8	2I	21	VAL	2.5
1	2A	2192	G	2.5
9	2N	2	LYS	2.5
9	2N	118	LYS	2.5
12	2Q	32	TYR	2.5
31	29	2	LYS	2.5
54	1y	15	G	2.5
3	1D	200	ASP	2.5
12	2Q	82	ARG	2.5
37	1f	56	PRO	2.5
21	2Z	172	ALA	2.5
38	2g	113	GLU	2.5
44	2m	76	ALA	2.5
46	1o	46	HIS	2.5
21	2Z	102	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
28	26	9	LEU	2.5
33	2b	235	SER	2.5
43	2l	18	VAL	2.5
33	2b	28	PHE	2.5
34	1c	48	TYR	2.5
38	2g	32	ARG	2.5
41	2j	66	ARG	2.5
54	1y	62	C	2.5
1	2A	652(E)	G	2.5
1	1A	1175	U	2.4
11	2P	53	GLY	2.4
12	2Q	113	GLN	2.4
34	2c	148	GLY	2.4
11	2P	6	LEU	2.4
35	1d	196	LEU	2.4
12	2Q	41	TRP	2.4
44	2m	99	ARG	2.4
49	2r	29	PHE	2.4
6	2G	89	GLY	2.4
32	2a	91	C	2.4
32	2a	1018	C	2.4
41	2j	10	GLY	2.4
43	2l	47	LYS	2.4
55	2x	66	C	2.4
1	2A	2160	G	2.4
8	2I	36	ALA	2.4
16	2U	67	ALA	2.4
34	1c	152	ILE	2.4
34	2c	111	LEU	2.4
38	2g	42	ILE	2.4
41	2j	65	LEU	2.4
33	1b	230	VAL	2.4
38	2g	141	VAL	2.4
11	2P	130	PHE	2.4
33	1b	160	ASP	2.4
37	2f	83	ASP	2.4
23	21	23	LYS	2.4
32	2a	412	A	2.4
35	1d	40	PRO	2.4
1	1A	888	C	2.4
11	2P	128	HIS	2.4
22	10	2	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
42	1k	41	THR	2.4
44	2m	42	ALA	2.4
5	1F	17	ARG	2.4
6	2G	62	LEU	2.4
33	2b	58	ILE	2.4
36	1e	118	ILE	2.4
46	2o	88	ARG	2.4
11	2P	54	GLY	2.4
33	2b	100	GLY	2.4
10	1O	112	MET	2.4
1	1A	2135	A	2.4
43	1l	125	PRO	2.4
35	2d	48	ALA	2.4
49	2r	74	ARG	2.4
4	2E	87	GLU	2.4
7	2H	7	LEU	2.4
12	2Q	114	ALA	2.4
21	2Z	125	LEU	2.4
25	23	8	LEU	2.4
50	2s	15	LEU	2.4
1	2A	2139	C	2.4
33	1b	68	ILE	2.4
35	2d	18	LYS	2.4
54	1w	74	C	2.4
1	2A	2099	U	2.4
55	2x	60	U	2.4
6	2G	37	VAL	2.4
9	2N	41	ASP	2.4
10	2O	58	VAL	2.4
35	1d	161	ASN	2.4
1	1A	2149	G	2.4
33	1b	31	TYR	2.4
33	2b	236	TYR	2.4
36	1e	133	TYR	2.4
3	1D	176	ARG	2.4
33	2b	87	ARG	2.4
11	1P	105	LEU	2.4
11	2P	134	ALA	2.4
36	1e	91	LEU	2.4
42	1k	63	LEU	2.4
42	2k	66	LEU	2.4
50	2s	38	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	1A	2134	A	2.4
1	2A	653	A	2.4
6	2G	134	GLY	2.4
32	2a	1039	C	2.4
34	2c	76	VAL	2.4
16	2U	76	TYR	2.4
25	23	44	ARG	2.4
35	2d	122	ARG	2.4
17	2V	43	GLU	2.4
36	2e	88	LYS	2.4
41	2j	51	ARG	2.4
50	2s	61	TYR	2.4
42	2k	92	GLU	2.4
1	1A	1176	G	2.4
3	2D	177	LEU	2.4
5	2F	181	LEU	2.4
7	2H	68	THR	2.4
8	2I	30	LEU	2.4
37	2f	99	ALA	2.4
38	1g	86	GLN	2.4
43	1l	107	ALA	2.4
43	2l	104	VAL	2.4
50	2s	67	VAL	2.4
37	1f	62	TRP	2.4
1	2A	272(A)	U	2.4
1	2A	2134	A	2.4
16	2U	61	TRP	2.4
33	2b	75	LYS	2.4
35	2d	115	ARG	2.4
42	2k	70	LYS	2.4
45	2n	31	ARG	2.4
55	1x	72	A	2.4
34	2c	193	TYR	2.4
12	2Q	4	PRO	2.4
8	2I	49	ALA	2.4
34	1c	52	LEU	2.4
34	2c	67	THR	2.4
42	1k	23	ALA	2.4
42	2k	64	ALA	2.4
43	2l	62	SER	2.4
49	2r	20	ALA	2.4
6	2G	77	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
7	2H	30	LYS	2.4
7	2H	140	LYS	2.4
30	28	36	LYS	2.4
54	2y	71	G	2.4
55	2x	6	G	2.4
7	2H	116	GLU	2.4
33	2b	59	GLU	2.4
33	2b	217	ARG	2.4
35	1d	75	PHE	2.4
1	2A	2111	C	2.3
3	2D	126	GLN	2.3
32	2a	1066	C	2.3
53	1v	23	A	2.3
42	2k	22	HIS	2.3
6	2G	139	LEU	2.3
49	1r	30	ASP	2.3
4	2E	41	LYS	2.3
11	2P	57	THR	2.3
21	2Z	150	LEU	2.3
21	2Z	173	ALA	2.3
7	2H	161	GLY	2.3
22	20	65	GLY	2.3
33	2b	8	LYS	2.3
49	1r	84	LYS	2.3
33	1b	41	ILE	2.3
36	1e	11	ILE	2.3
37	2f	87	ARG	2.3
5	2F	37	VAL	2.3
28	26	52	VAL	2.3
32	1a	1001(A)	G	2.3
35	1d	116	GLN	2.3
17	2V	76	LYS	2.3
35	1d	136	PRO	2.3
54	2w	51	U	2.3
12	2Q	17	LEU	2.3
36	1e	5	ASP	2.3
37	1f	45	LEU	2.3
39	1h	133	LEU	2.3
8	2I	70	GLU	2.3
32	1a	722	A	2.3
32	2a	1028	C	2.3
32	2a	1043	C	2.3

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Mol	Chain	Res	Type	RSRZ
33	2b	151	GLY	2.3
38	2g	109	ASN	2.3
33	1b	42	ILE	2.3
33	2b	182	ILE	2.3
36	2e	41	VAL	2.3
38	2g	26	PHE	2.3
23	11	48	LYS	2.3
1	2A	2115	G	2.3
35	1d	134	ASP	2.3
5	2F	21	ALA	2.3
8	2I	13	GLY	2.3
17	2V	28	GLU	2.3
32	1a	1036	G	2.3
34	2c	32	LEU	2.3
36	2e	50	GLU	2.3
36	2e	81	GLU	2.3
55	2x	53	G	2.3
28	26	23	THR	2.3
33	1b	23	ARG	2.3
33	2b	173	ALA	2.3
35	1d	50	ARG	2.3
41	2j	48	THR	2.3
43	2l	41	ARG	2.3
54	2y	68	C	2.3
1	2A	2126	A	2.3
17	2V	96	ILE	2.3
22	20	30	VAL	2.3
34	1c	76	VAL	2.3
37	2f	16	GLN	2.3
35	1d	34	GLU	2.3
6	2G	153	ARG	2.3
35	1d	36	ARG	2.3
36	2e	14	ARG	2.3
37	2f	14	LEU	2.3
37	2f	43	LEU	2.3
39	1h	2	LEU	2.3
39	1h	59	LEU	2.3
46	2o	89	GLY	2.3
49	1r	45	SER	2.3
34	2c	3	ASN	2.3
35	1d	147	ALA	2.3
1	2A	405	U	2.3

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Mol	Chain	Res	Type	RSRZ
1	2A	2895	U	2.3
23	21	33	LYS	2.3
23	21	78	LYS	2.3
44	2m	65	LYS	2.3
12	2Q	29	PHE	2.3
22	20	57	PHE	2.3
35	2d	158	ILE	2.3
49	2r	75	ILE	2.3
34	1c	18	TRP	2.3
55	2x	76	A	2.3
45	2n	3	ARG	2.3
7	2H	41	MET	2.3
35	1d	124	GLY	2.3
11	2P	59	LEU	2.3
37	1f	67	MET	2.3
8	2I	126	TYR	2.3
21	2Z	21	ALA	2.3
22	20	12	ASN	2.3
29	27	48	LYS	2.3
43	1l	30	ALA	2.3
49	2r	60	ALA	2.3
37	2f	81	ILE	2.3
7	2H	45	VAL	2.3
17	2V	61	VAL	2.3
1	1A	2121	G	2.3
1	1A	2148	G	2.3
32	2a	987	G	2.3
1	1A	2111	C	2.3
33	2b	14	GLY	2.3
50	2s	68	GLY	2.3
30	28	5	LYS	2.3
34	2c	20	SER	2.3
38	2g	88	PRO	2.3
32	1a	1030(D)	A	2.3
39	2h	119	LEU	2.3
41	1j	8	LEU	2.3
54	2y	9	A	2.3
5	2F	113	ALA	2.3
26	24	32	TYR	2.3
35	2d	68	TYR	2.3
42	1k	112	THR	2.3
44	2m	107	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
45	2n	24	CYS	2.3
9	2N	16	ILE	2.3
33	1b	211	ILE	2.3
46	1o	87	ILE	2.3
8	2I	27	ARG	2.3
9	2N	39	ARG	2.3
37	1f	88	VAL	2.3
43	1l	113	ARG	2.3
12	2Q	130	LYS	2.3
33	1b	43	ASP	2.3
35	2d	144	ASP	2.3
42	1k	36	ASP	2.3
42	1k	118	GLY	2.3
1	2A	2104	G	2.3
9	2N	107	LEU	2.3
38	2g	73	MET	2.3
42	2k	38	ASN	2.3
54	2y	15	G	2.3
7	2H	75	ALA	2.3
7	2H	150	ALA	2.3
54	2y	67	C	2.3
1	2A	2176	A	2.3
32	1a	161	A	2.3
32	2a	986	A	2.3
54	1y	7	A	2.3
3	1D	263	ARG	2.3
25	23	55	ARG	2.3
26	24	68	ARG	2.3
35	1d	100	ARG	2.3
44	2m	3	ARG	2.3
7	2H	90	LYS	2.3
39	2h	109	ILE	2.3
36	2e	90	VAL	2.3
8	2I	16	GLY	2.2
23	21	31	GLY	2.2
32	2a	1040	U	2.2
42	1k	88	GLY	2.2
12	2Q	39	PRO	2.2
22	20	84	LEU	2.2
30	28	32	LEU	2.2
37	1f	79	LEU	2.2
37	2f	56	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
39	2h	133	LEU	2.2
44	2m	81	LEU	2.2
35	1d	15	GLU	2.2
21	2Z	164	ALA	2.2
1	1A	2794	C	2.2
54	2y	27	G	2.2
54	2y	43	C	2.2
55	2x	71	C	2.2
9	2N	50	ASP	2.2
1	2A	2158	A	2.2
7	2H	9	ILE	2.2
17	2V	70	ILE	2.2
21	2Z	56	VAL	2.2
25	23	36	VAL	2.2
54	1y	58	A	2.2
54	1w	47	U	2.2
33	1b	61	LEU	2.2
35	1d	58	LEU	2.2
43	2l	77	LEU	2.2
3	2D	224	ALA	2.2
23	21	25	LYS	2.2
9	2N	134	ARG	2.2
30	28	10	ALA	2.2
35	2d	195	ALA	2.2
43	1l	67	THR	2.2
43	2l	15	ARG	2.2
37	2f	63	TYR	2.2
1	2A	894	C	2.2
43	2l	72	GLY	2.2
4	2E	198	VAL	2.2
7	2H	44	VAL	2.2
30	28	35	GLN	2.2
34	1c	106	VAL	2.2
39	2h	95	VAL	2.2
43	2l	85	ILE	2.2
33	2b	119	GLU	2.2
8	2I	128	LEU	2.2
34	1c	196	LEU	2.2
1	1A	1066	U	2.2
34	2c	18	TRP	2.2
39	1h	10	LEU	2.2
39	2h	2	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
35	1d	14	ARG	2.2
43	2l	97	ARG	2.2
9	2N	124	ALA	2.2
10	2O	1	MET	2.2
11	2P	90	ARG	2.2
16	2U	78	THR	2.2
43	1l	38	THR	2.2
41	2j	89	ASP	2.2
37	2f	57	GLN	2.2
34	2c	151	VAL	2.2
35	1d	137	SER	2.2
23	21	98	LEU	2.2
33	2b	53	ARG	2.2
45	2n	41	ARG	2.2
45	2n	45	ARG	2.2
6	2G	110	ALA	2.2
32	1a	1532	U	2.2
11	2P	136	GLU	2.2
17	2V	6	LYS	2.2
45	2n	21	TYR	2.2
3	1D	229	VAL	2.2
8	1I	79	ILE	2.2
10	1O	86	ILE	2.2
31	29	3	VAL	2.2
3	2D	267	SER	2.2
16	2U	94	ASN	2.2
21	2Z	142	SER	2.2
23	11	2	SER	2.2
36	1e	40	ARG	2.2
37	1f	77	ARG	2.2
42	1k	43	SER	2.2
50	2s	37	ARG	2.2
3	2D	257	LEU	2.2
26	24	7	PRO	2.2
35	1d	108	LEU	2.2
35	2d	94	LEU	2.2
42	1k	103	LEU	2.2
32	1a	720	C	2.2
32	2a	89	C	2.2
36	2e	30	ALA	2.2
1	1A	883	G	2.2
3	2D	170	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
43	1l	95	GLY	2.2
54	1y	66	U	2.2
1	1A	229	A	2.2
21	2Z	48	PHE	2.2
25	23	15	TYR	2.2
8	2I	57	ARG	2.2
9	2N	53	VAL	2.2
25	23	3	ARG	2.2
25	23	13	ILE	2.2
33	1b	36	ARG	2.2
37	2f	93	SER	2.2
11	1P	100	LEU	2.2
46	2o	57	LEU	2.2
49	2r	78	LEU	2.2
37	1f	66	GLU	2.2
1	2A	2804	C	2.2
33	1b	207	ALA	2.2
42	1k	73	MET	2.2
22	20	10	THR	2.2
44	2m	89	GLY	2.2
54	1w	48	C	2.2
1	2A	2109	U	2.2
35	2d	13	ARG	2.2
37	2f	2	ARG	2.2
45	2n	26	ARG	2.2
1	2A	2123	G	2.2
54	1y	65	G	2.2
7	2H	26	VAL	2.2
14	2S	40	ILE	2.2
34	2c	154	SER	2.2
35	2d	126	ILE	2.2
36	1e	89	ILE	2.2
10	1O	53	LYS	2.2
28	26	38	LYS	2.2
54	2y	14	A	2.2
33	1b	131	PRO	2.2
34	1c	188	LEU	2.2
46	1o	66	LEU	2.2
12	2Q	40	ALA	2.2
21	2Z	106	GLY	2.2
25	23	18	ASP	2.2
9	2N	27	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
35	2d	2	GLY	2.2
49	2r	69	THR	2.2
38	2g	143	ARG	2.2
42	1k	54	ARG	2.2
1	1A	886	C	2.2
21	2Z	88	PHE	2.2
32	2a	1045	C	2.2
1	2A	2506	U	2.1
1	2A	2585	U	2.1
12	2Q	74	TYR	2.1
8	2I	71	ILE	2.1
23	21	57	GLU	2.1
30	28	31	HIS	2.1
38	2g	101	LEU	2.1
42	2k	62	GLN	2.1
9	2N	125	GLY	2.1
30	28	9	GLY	2.1
17	2V	27	ALA	2.1
11	2P	67	MET	2.1
21	2Z	98	MET	2.1
33	1b	137	ARG	2.1
34	1c	85	ARG	2.1
36	2e	21	ALA	2.1
38	2g	100	ALA	2.1
42	2k	65	ALA	2.1
35	2d	181	MET	2.1
37	1f	1	MET	2.1
50	2s	78	ARG	2.1
35	1d	18	LYS	2.1
7	2H	46	GLU	2.1
9	2N	45	ASN	2.1
34	1c	82	GLU	2.1
1	1A	2136	C	2.1
1	2A	1181	C	2.1
3	2D	145	VAL	2.1
9	2N	52	VAL	2.1
12	2Q	42	ILE	2.1
17	2V	11	GLN	2.1
26	24	67	TYR	2.1
33	1b	197	VAL	2.1
36	2e	76	ILE	2.1
5	2F	148	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
7	2H	64	LEU	2.1
9	2N	38	HIS	2.1
30	28	50	LEU	2.1
30	28	20	GLY	2.1
31	29	12	ASP	2.1
33	2b	159	PRO	2.1
36	2e	5	ASP	2.1
36	2e	29	GLY	2.1
7	2H	130	ARG	2.1
9	2N	74	ARG	2.1
23	11	21	ARG	2.1
33	1b	209	ARG	2.1
33	2b	30	ARG	2.1
34	2c	164	ARG	2.1
42	1k	65	ALA	2.1
1	1A	2127	G	2.1
1	2A	843	G	2.1
30	28	4	MET	2.1
36	2e	136	MET	2.1
6	2G	59	GLU	2.1
32	2a	958	A	2.1
50	2s	27	GLU	2.1
4	2E	31	CYS	2.1
3	2D	185	VAL	2.1
10	2O	38	VAL	2.1
30	28	22	VAL	2.1
35	1d	198	VAL	2.1
8	2I	68	LEU	2.1
43	2l	7	ILE	2.1
1	2A	271(N)	U	2.1
7	2H	117	PRO	2.1
22	20	22	GLY	2.1
33	2b	60	ASP	2.1
45	2n	58	LYS	2.1
48	1q	100	LYS	2.1
10	1O	108	GLU	2.1
5	2F	129	PHE	2.1
1	1A	2110	G	2.1
1	2A	2106	G	2.1
1	2A	2411	A	2.1
32	1a	1003	G	2.1
3	1D	49	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
8	2I	116	LEU	2.1
9	2N	119	ARG	2.1
35	1d	64	LEU	2.1
43	1l	94	PRO	2.1
1	1A	2177	C	2.1
42	1k	60	ALA	2.1
49	2r	73	ALA	2.1
23	21	35	THR	2.1
40	2i	7	THR	2.1
9	2N	104	LYS	2.1
25	23	5	LYS	2.1
34	1c	199	LYS	2.1
11	2P	66	GLY	2.1
34	2c	131	ARG	2.1
36	1e	43	LEU	2.1
36	2e	105	VAL	2.1
37	2f	72	VAL	2.1
43	1l	39	VAL	2.1
1	1A	652(F)	G	2.1
7	2H	157	TYR	2.1
8	2I	132	PRO	2.1
9	2N	86	PRO	2.1
17	2V	34	GLU	2.1
28	26	21	TYR	2.1
33	1b	35	GLU	2.1
55	1x	70	G	2.1
1	1A	1963	U	2.1
9	2N	47	ALA	2.1
11	2P	81	GLN	2.1
34	1c	160	ALA	2.1
32	2a	1109	C	2.1
43	1l	123	LYS	2.1
54	2w	62	C	2.1
7	2H	69	ARG	2.1
33	2b	21	ARG	2.1
34	1c	179	ARG	2.1
41	2j	46	ARG	2.1
36	1e	42	GLY	2.1
7	2H	169	VAL	2.1
8	2I	15	VAL	2.1
17	2V	47	VAL	2.1
28	26	48	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
34	2c	86	VAL	2.1
39	1h	65	TYR	2.1
41	2j	38	ILE	2.1
43	2l	100	ILE	2.1
1	2A	1042	G	2.1
1	2A	2147	G	2.1
3	2D	5	LYS	2.1
11	2P	46	LYS	2.1
42	2k	23	ALA	2.1
33	1b	56	ARG	2.1
35	1d	159	ARG	2.1
36	2e	27	ARG	2.1
43	2l	44	THR	2.1
1	2A	2105	C	2.1
7	1H	174	GLY	2.1
21	2Z	2	GLU	2.1
41	2j	64	GLU	2.1
5	2F	24	LEU	2.1
10	2O	8	LEU	2.1
21	2Z	96	VAL	2.1
31	29	10	ILE	2.1
33	1b	208	ILE	2.1
35	1d	133	VAL	2.1
23	21	71	TYR	2.1
17	2V	55	ALA	2.1
8	2I	78	THR	2.1
1	2A	2159	G	2.0
22	20	6	GLY	2.1
32	2a	780	A	2.1
32	2a	1101	A	2.1
34	1c	186	PHE	2.1
54	1w	64	A	2.1
54	2w	63	G	2.0
54	2y	29	G	2.0
45	2n	4	LYS	2.0
22	20	66	VAL	2.0
30	28	23	VAL	2.0
32	2a	1223	C	2.0
33	1b	93	VAL	2.0
33	2b	16	HIS	2.0
36	1e	115	VAL	2.0
50	2s	57	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
7	2H	4	ILE	2.0
14	2S	82	ILE	2.0
49	1r	65	ILE	2.0
9	2N	18	ALA	2.0
21	2Z	82	ARG	2.0
33	1b	52	GLU	2.0
33	2b	186	ALA	2.0
42	1k	27	ASN	2.0
42	2k	119	CYS	2.0
45	2n	38	GLY	2.0
3	2D	261	LYS	2.0
33	2b	24	TRP	2.0
33	2b	132	LYS	2.0
32	1a	1257	U	2.0
35	1d	155	LEU	2.0
39	2h	112	LEU	2.0
41	1j	71	LEU	2.0
41	2j	85	LEU	2.0
1	2A	2101	G	2.0
8	1I	132	PRO	2.0
28	26	39	TYR	2.0
34	2c	58	GLU	2.0
37	2f	66	GLU	2.0
49	2r	38	GLU	2.0
3	2D	156	ALA	2.0
16	2U	66	ASN	2.0
21	2Z	51	ALA	2.0
34	1c	71	ALA	2.0
50	2s	75	ALA	2.0
6	2G	154	GLY	2.0
7	2H	134	SER	2.0
14	2S	41	ASP	2.0
33	2b	73	THR	2.0
35	2d	109	GLY	2.0
9	2N	69	GLN	2.0
35	2d	45	GLN	2.0
38	2g	64	GLN	2.0
3	1D	133	LEU	2.0
35	2d	135	LEU	2.0
1	2A	2098	U	2.0
1	2A	2118	U	2.0
9	2N	114	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
9	2N	126	PRO	2.0
10	2O	17	ARG	2.0
12	2Q	102	VAL	2.0
17	2V	36	PRO	2.0
34	1c	70	VAL	2.0
34	2c	75	VAL	2.0
23	21	37	ILE	2.0
39	1h	83	ILE	2.0
1	2A	228	A	2.0
1	2A	849	A	2.0
6	2G	36	LYS	2.0
1	1A	2106	G	2.0
7	2H	163	TYR	2.0
34	2c	102	ASN	2.0
36	2e	61	TYR	2.0
42	2k	75	TYR	2.0
1	1A	2164	C	2.0
1	1A	2188	C	2.0
1	2A	2110	G	2.0
8	2I	115	ALA	2.0
12	2Q	15	GLY	2.0
32	2a	1058	G	2.0
33	2b	29	ALA	2.0
36	2e	84	PHE	2.0
37	1f	89	MET	2.0
38	1g	89	MET	2.0
43	1l	37	CYS	2.0
7	1H	103	LEU	2.0
25	13	60	GLU	2.0
36	2e	139	LEU	2.0
37	1f	2	ARG	2.0
39	2h	84	ARG	2.0
39	2h	122	ARG	2.0
46	1o	41	GLU	2.0
49	2r	72	ARG	2.0
4	2E	33	VAL	2.0
7	2H	77	LYS	2.0
33	1b	202	PRO	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	PSU	1y	55	20/21	0.74	0.30	88,97,106,113	0
54	G7M	2y	46	24/25	0.74	0.40	93,103,108,124	0
54	G7M	2w	46	24/25	0.75	0.47	92,100,108,128	0
54	5MU	2y	54	21/22	0.76	0.47	89,99,108,126	0
54	PSU	2y	55	20/21	0.76	0.38	95,103,112,114	0
54	PSU	2w	55	20/21	0.77	0.45	83,96,105,108	0
54	4SU	2w	8	20/21	0.77	0.43	95,104,113,122	0
54	4SU	2y	8	20/21	0.79	0.26	95,102,115,124	0
54	5MU	1y	54	21/22	0.79	0.34	83,89,100,115	0
54	MIA	2y	37	22/30	0.82	0.32	84,95,103,113	0
55	4SU	2x	8	20/21	0.83	0.25	84,89,98,98	0
54	4SU	1y	8	20/21	0.83	0.28	93,96,106,109	0
54	G7M	1w	46	24/25	0.84	0.31	83,91,108,125	0
54	PSU	2y	32	20/21	0.84	0.25	86,95,106,107	0
54	MIA	1y	37	22/30	0.84	0.23	78,88,99,105	0
54	PSU	2y	39	20/21	0.85	0.31	87,90,101,107	0
54	5MU	2w	54	21/22	0.85	0.27	76,89,94,97	0
54	PSU	2w	32	20/21	0.86	0.36	85,92,99,107	0
32	2MG	2a	1207	24/25	0.87	0.20	84,90,101,109	0
54	4SU	1w	8	20/21	0.87	0.24	83,88,96,99	0
54	PSU	2w	39	20/21	0.88	0.34	80,90,96,98	0
32	5MC	2a	967	21/22	0.89	0.16	65,74,83,86	0
54	PSU	1y	39	20/21	0.89	0.27	78,85,93,95	0
32	PSU	2a	516	20/21	0.89	0.22	76,82,88,90	0
32	M2G	2a	966	25/26	0.89	0.19	64,73,88,95	0
54	PSU	1y	32	20/21	0.90	0.24	82,90,99,99	0
54	G7M	1y	46	24/25	0.90	0.34	91,98,104,115	0
55	5MU	2x	54	21/22	0.91	0.25	81,85,90,105	0
55	PSU	2x	55	20/21	0.91	0.23	81,84,92,96	0
54	PSU	1w	55	20/21	0.91	0.17	69,81,87,90	0
54	MIA	2w	37	25/30	0.92	0.24	84,88,95,97	0
1	PSU	2A	1911	20/21	0.92	0.19	63,72,76,81	0
43	0TD	2l	92	10/11	0.92	0.25	71,74,75,87	0
32	G7M	2a	527	24/25	0.93	0.17	64,71,78,84	0
32	5MC	2a	1404	21/22	0.93	0.20	61,67,73,73	0
55	5MC	2x	32	21/22	0.94	0.17	72,81,83,87	0
55	5MU	1x	54	21/22	0.94	0.15	60,70,76,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
43	0TD	1l	92	10/11	0.94	0.31	50,55,58,79	0
32	2MG	1a	1207	24/25	0.94	0.14	65,71,76,78	0
55	4SU	1x	8	20/21	0.94	0.18	64,70,78,88	0
32	5MC	2a	1400	21/22	0.95	0.18	71,77,83,87	0
32	4OC	2a	1402	22/23	0.95	0.16	64,71,77,80	0
1	PSU	2A	1917	20/21	0.95	0.16	66,75,81,83	0
32	5MC	2a	1407	21/22	0.95	0.22	58,63,67,75	0
32	MA6	2a	1519	24/25	0.95	0.27	50,68,74,78	0
1	OMC	2A	1920	21/22	0.95	0.20	63,71,74,77	0
1	5MC	2A	1962	21/22	0.95	0.19	42,54,61,72	0
54	PSU	1w	32	20/21	0.95	0.14	63,69,88,88	0
54	MIA	1w	37	29/30	0.95	0.20	49,59,67,72	0
1	5MU	1A	1915	21/22	0.95	0.22	51,58,62,70	0
55	PSU	1x	55	20/21	0.95	0.14	58,65,73,77	0
1	5MU	2A	1915	21/22	0.95	0.14	77,82,91,99	0
32	G7M	1a	527	24/25	0.96	0.17	36,46,53,59	0
32	M2G	1a	966	25/26	0.96	0.17	51,55,62,65	0
32	UR3	2a	1498	21/22	0.96	0.18	60,66,71,76	0
32	MA6	2a	1518	24/25	0.96	0.20	53,68,73,74	0
1	PSU	1A	1917	20/21	0.96	0.21	45,53,65,68	0
32	5MC	1a	1404	21/22	0.96	0.21	39,43,49,54	0
1	PSU	1A	1911	20/21	0.97	0.21	41,46,50,53	0
54	PSU	1w	39	20/21	0.97	0.15	57,66,72,77	0
32	MA6	1a	1519	24/25	0.97	0.22	37,43,49,51	0
54	5MU	1w	54	21/22	0.97	0.17	60,71,78,82	0
1	OMC	1A	1920	21/22	0.97	0.21	35,43,46,50	0
1	5MC	2A	1942	21/22	0.97	0.19	55,61,67,68	0
32	5MC	1a	967	21/22	0.97	0.15	53,59,63,69	0
1	2MA	2A	2503	23/24	0.97	0.21	32,39,44,48	0
1	PSU	2A	2605	20/21	0.97	0.20	35,42,46,46	0
32	PSU	1a	516	20/21	0.97	0.14	55,61,66,68	0
32	MA6	1a	1518	24/25	0.98	0.22	32,41,45,46	0
55	5MC	1x	32	21/22	0.98	0.15	52,55,60,63	0
1	5MC	1A	1942	21/22	0.98	0.20	35,41,46,52	0
1	5MC	1A	1962	21/22	0.98	0.21	28,34,42,44	0
1	5MU	2A	1939	21/22	0.98	0.19	38,44,50,51	0
1	OMU	1A	2552	21/22	0.98	0.20	23,28,35,36	0
1	PSU	1A	2605	20/21	0.98	0.20	24,28,30,35	0
1	OMG	2A	2251	24/25	0.98	0.25	37,47,52,53	0
32	5MC	1a	1400	21/22	0.98	0.17	43,51,56,67	0
1	OMU	2A	2552	21/22	0.98	0.20	38,45,48,54	0
32	4OC	1a	1402	22/23	0.98	0.18	41,46,53,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MU	1A	1939	21/22	0.98	0.21	23,26,32,40	0
32	5MC	1a	1407	21/22	0.98	0.22	37,40,44,45	0
32	UR3	1a	1498	21/22	0.98	0.20	37,42,47,48	0
1	2MA	1A	2503	23/24	0.99	0.19	16,21,24,25	0
1	OMG	1A	2251	24/25	0.99	0.19	18,26,32,37	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	3763	1/1	0.10	0.65	80,80,80,80	0
56	MG	2a	1733	1/1	0.15	0.10	105,105,105,105	0
56	MG	2a	1689	1/1	0.23	0.37	80,80,80,80	0
56	MG	2A	3591	1/1	0.32	0.74	74,74,74,74	0
56	MG	1A	3856	1/1	0.32	0.14	66,66,66,66	0
56	MG	2A	3821	1/1	0.34	0.16	79,79,79,79	0
56	MG	2a	1822	1/1	0.34	2.61	94,94,94,94	0
56	MG	2A	3230	1/1	0.42	0.84	90,90,90,90	0
56	MG	2A	3218	1/1	0.43	0.53	82,82,82,82	0
56	MG	1A	3292	1/1	0.43	0.56	78,78,78,78	0
56	MG	2a	1771	1/1	0.44	0.37	84,84,84,84	0
56	MG	1A	3424	1/1	0.45	0.28	59,59,59,59	0
56	MG	2a	1751	1/1	0.46	0.33	85,85,85,85	0
56	MG	1x	109	1/1	0.46	0.23	85,85,85,85	0
56	MG	1a	1728	1/1	0.46	0.08	80,80,80,80	0
56	MG	1B	229	1/1	0.48	0.21	77,77,77,77	0
56	MG	2A	3155	1/1	0.48	0.31	65,65,65,65	0
56	MG	1w	107	1/1	0.48	0.40	95,95,95,95	0
56	MG	2w	103	1/1	0.48	0.35	73,73,73,73	0
56	MG	1A	3696	1/1	0.49	0.13	60,60,60,60	0
56	MG	1A	3992	1/1	0.49	0.49	88,88,88,88	0
56	MG	2A	3878	1/1	0.49	0.20	82,82,82,82	0
56	MG	1a	1755	1/1	0.51	0.10	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1629	1/1	0.51	0.14	74,74,74,74	0
56	MG	1A	3817	1/1	0.52	0.15	67,67,67,67	0
56	MG	1A	3989	1/1	0.53	0.20	94,94,94,94	0
56	MG	2x	103	1/1	0.53	0.40	86,86,86,86	0
56	MG	2A	3341	1/1	0.54	0.59	74,74,74,74	0
56	MG	1A	3947	1/1	0.54	0.23	70,70,70,70	0
56	MG	2A	3325	1/1	0.54	0.89	70,70,70,70	0
56	MG	1A	3335	1/1	0.55	0.30	72,72,72,72	0
56	MG	2a	1622	1/1	0.56	0.27	71,71,71,71	0
56	MG	2A	3581	1/1	0.56	0.42	82,82,82,82	0
56	MG	1a	1778	1/1	0.56	0.14	60,60,60,60	0
56	MG	2A	3608	1/1	0.56	0.24	76,76,76,76	0
56	MG	2A	3659	1/1	0.57	0.12	81,81,81,81	0
56	MG	2A	3346	1/1	0.58	0.35	74,74,74,74	0
56	MG	2A	3194	1/1	0.58	0.48	77,77,77,77	0
56	MG	2a	1708	1/1	0.59	0.35	80,80,80,80	0
56	MG	2A	3087	1/1	0.60	0.28	71,71,71,71	0
56	MG	2A	3797	1/1	0.61	0.16	89,89,89,89	0
56	MG	2a	1738	1/1	0.61	0.17	62,62,62,62	0
56	MG	2A	3168	1/1	0.61	0.30	67,67,67,67	0
56	MG	2A	3619	1/1	0.61	0.48	75,75,75,75	0
56	MG	1A	3476	1/1	0.61	0.25	56,56,56,56	0
56	MG	2A	3716	1/1	0.61	0.28	81,81,81,81	0
56	MG	2A	3162	1/1	0.61	0.52	78,78,78,78	0
56	MG	2A	3283	1/1	0.62	0.45	70,70,70,70	0
56	MG	1A	3421	1/1	0.62	0.34	56,56,56,56	0
56	MG	1w	109	1/1	0.62	0.07	86,86,86,86	0
56	MG	2A	3233	1/1	0.62	0.13	73,73,73,73	0
56	MG	2A	3569	1/1	0.62	0.23	54,54,54,54	0
56	MG	2A	3291	1/1	0.63	0.11	73,73,73,73	0
56	MG	1a	1764	1/1	0.63	0.14	60,60,60,60	0
56	MG	2A	3498	1/1	0.63	0.11	61,61,61,61	0
56	MG	1A	3049	1/1	0.64	0.14	52,52,52,52	0
56	MG	10	102	1/1	0.64	0.62	56,56,56,56	0
56	MG	2A	3729	1/1	0.64	0.36	87,87,87,87	0
56	MG	2A	3263	1/1	0.64	0.30	65,65,65,65	0
56	MG	1A	3347	1/1	0.64	0.39	64,64,64,64	0
56	MG	1A	3363	1/1	0.64	0.45	54,54,54,54	0
56	MG	1A	4138	1/1	0.64	0.25	50,50,50,50	0
56	MG	2A	3060	1/1	0.64	0.18	66,66,66,66	0
56	MG	2a	1624	1/1	0.64	0.22	71,71,71,71	0
56	MG	1A	3209	1/1	0.65	0.20	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3193	1/1	0.65	0.27	74,74,74,74	0
56	MG	1A	3433	1/1	0.65	0.26	54,54,54,54	0
56	MG	25	105	1/1	0.66	0.28	57,57,57,57	0
56	MG	1A	3826	1/1	0.66	0.14	49,49,49,49	0
56	MG	2A	3239	1/1	0.66	0.18	72,72,72,72	0
56	MG	1a	1666	1/1	0.66	0.18	63,63,63,63	0
56	MG	2A	3624	1/1	0.67	0.30	86,86,86,86	0
56	MG	1A	3048	1/1	0.67	0.36	53,53,53,53	0
56	MG	2A	3067	1/1	0.67	0.41	73,73,73,73	0
56	MG	1Y	203	1/1	0.67	0.16	69,69,69,69	0
56	MG	1A	3629	1/1	0.68	0.25	56,56,56,56	0
56	MG	2A	3667	1/1	0.68	0.17	54,54,54,54	0
56	MG	2A	3237	1/1	0.68	0.36	76,76,76,76	0
56	MG	1a	1758	1/1	0.68	0.35	81,81,81,81	0
56	MG	1A	3384	1/1	0.68	0.36	77,77,77,77	0
56	MG	2A	3025	1/1	0.68	0.51	70,70,70,70	0
56	MG	18	105	1/1	0.68	0.38	46,46,46,46	0
56	MG	1a	1799	1/1	0.68	0.11	62,62,62,62	0
56	MG	2A	3620	1/1	0.68	0.33	72,72,72,72	0
56	MG	1f	202	1/1	0.68	0.26	66,66,66,66	0
56	MG	2A	3149	1/1	0.69	0.13	87,87,87,87	0
56	MG	1A	3435	1/1	0.69	0.18	85,85,85,85	0
56	MG	1A	3844	1/1	0.69	0.12	48,48,48,48	0
56	MG	2A	3764	1/1	0.69	0.19	74,74,74,74	0
56	MG	2A	3268	1/1	0.69	0.34	62,62,62,62	0
56	MG	2A	3521	1/1	0.69	0.33	65,65,65,65	0
56	MG	2A	3847	1/1	0.69	0.40	86,86,86,86	0
56	MG	2A	3867	1/1	0.69	0.19	75,75,75,75	0
56	MG	2A	3027	1/1	0.69	0.21	58,58,58,58	0
56	MG	2A	3185	1/1	0.69	0.43	63,63,63,63	0
56	MG	2a	1617	1/1	0.69	0.25	82,82,82,82	0
56	MG	1A	3977	1/1	0.70	0.29	63,63,63,63	0
56	MG	2A	3173	1/1	0.70	0.28	70,70,70,70	0
56	MG	2A	3499	1/1	0.70	0.46	78,78,78,78	0
56	MG	2A	3647	1/1	0.70	0.37	69,69,69,69	0
56	MG	1A	3056	1/1	0.70	0.45	61,61,61,61	0
56	MG	1A	3368	1/1	0.70	0.55	45,45,45,45	0
56	MG	1A	3293	1/1	0.70	0.19	53,53,53,53	0
56	MG	2a	1807	1/1	0.70	0.12	81,81,81,81	0
56	MG	2a	1605	1/1	0.70	0.18	68,68,68,68	0
56	MG	2A	3338	1/1	0.70	0.31	55,55,55,55	0
56	MG	2w	105	1/1	0.70	1.62	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	3251	1/1	0.70	0.39	68,68,68,68	0
56	MG	1A	4078	1/1	0.71	0.51	73,73,73,73	0
56	MG	2A	3190	1/1	0.71	0.36	63,63,63,63	0
56	MG	2A	3192	1/1	0.71	0.59	59,59,59,59	0
56	MG	1A	3325	1/1	0.71	0.41	71,71,71,71	0
56	MG	2a	1728	1/1	0.71	0.21	82,82,82,82	0
56	MG	1a	1756	1/1	0.71	0.39	75,75,75,75	0
56	MG	2A	3297	1/1	0.71	0.11	81,81,81,81	0
56	MG	2A	3845	1/1	0.71	0.18	71,71,71,71	0
56	MG	1A	3365	1/1	0.71	0.28	49,49,49,49	0
56	MG	2A	3327	1/1	0.71	0.13	64,64,64,64	0
56	MG	1x	102	1/1	0.71	0.26	67,67,67,67	0
56	MG	2a	1837	1/1	0.71	0.13	70,70,70,70	0
56	MG	2j	201	1/1	0.71	0.08	83,83,83,83	0
56	MG	1A	3391	1/1	0.71	0.50	55,55,55,55	0
56	MG	1a	1667	1/1	0.71	0.32	64,64,64,64	0
56	MG	1a	1788	1/1	0.71	0.23	71,71,71,71	0
56	MG	2a	1621	1/1	0.72	0.59	75,75,75,75	0
56	MG	1a	1805	1/1	0.72	0.38	71,71,71,71	0
56	MG	2A	3723	1/1	0.72	0.16	47,47,47,47	0
56	MG	2a	1639	1/1	0.72	0.10	72,72,72,72	0
56	MG	2a	1823	1/1	0.72	0.40	81,81,81,81	0
56	MG	2A	3228	1/1	0.72	0.25	55,55,55,55	0
56	MG	2g	201	1/1	0.72	0.59	84,84,84,84	0
56	MG	1A	3375	1/1	0.72	0.48	61,61,61,61	0
56	MG	2A	3258	1/1	0.72	0.26	79,79,79,79	0
56	MG	2A	3488	1/1	0.72	0.19	41,41,41,41	0
56	MG	1a	1699	1/1	0.72	0.09	84,84,84,84	0
56	MG	2A	3664	1/1	0.73	0.42	72,72,72,72	0
56	MG	1A	3263	1/1	0.73	0.42	56,56,56,56	0
56	MG	1A	3734	1/1	0.73	0.18	52,52,52,52	0
56	MG	2a	1796	1/1	0.73	0.16	69,69,69,69	0
56	MG	1A	3925	1/1	0.73	0.31	52,52,52,52	0
56	MG	1v	101	1/1	0.73	0.20	78,78,78,78	0
56	MG	2A	3607	1/1	0.73	0.12	55,55,55,55	0
56	MG	1A	3377	1/1	0.73	0.14	54,54,54,54	0
56	MG	1A	3408	1/1	0.73	1.38	45,45,45,45	0
56	MG	2A	3366	1/1	0.73	0.35	60,60,60,60	0
56	MG	1a	1787	1/1	0.73	0.18	75,75,75,75	0
56	MG	1A	3836	1/1	0.73	0.12	68,68,68,68	0
56	MG	2A	3020	1/1	0.73	0.30	67,67,67,67	0
56	MG	2y	101	1/1	0.73	0.51	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	1625	1/1	0.74	0.18	51,51,51,51	0
56	MG	2A	3342	1/1	0.74	0.11	67,67,67,67	0
56	MG	1A	3894	1/1	0.74	0.26	26,26,26,26	0
56	MG	2a	1663	1/1	0.74	0.29	73,73,73,73	0
56	MG	2A	3249	1/1	0.74	0.81	79,79,79,79	0
56	MG	1A	3914	1/1	0.74	0.35	82,82,82,82	0
56	MG	2A	3494	1/1	0.74	0.18	49,49,49,49	0
56	MG	1A	4100	1/1	0.74	0.15	53,53,53,53	0
56	MG	1A	3176	1/1	0.74	0.18	69,69,69,69	0
56	MG	1A	3182	1/1	0.74	0.23	50,50,50,50	0
56	MG	2A	3271	1/1	0.74	0.43	70,70,70,70	0
56	MG	2A	3844	1/1	0.74	0.19	82,82,82,82	0
56	MG	1a	1829	1/1	0.74	0.12	63,63,63,63	0
56	MG	1A	3961	1/1	0.74	0.15	42,42,42,42	0
56	MG	2A	3854	1/1	0.74	0.09	72,72,72,72	0
56	MG	2A	3224	1/1	0.74	0.18	70,70,70,70	0
56	MG	2A	3316	1/1	0.74	0.40	77,77,77,77	0
56	MG	2A	3320	1/1	0.74	0.33	61,61,61,61	0
56	MG	2a	1604	1/1	0.74	0.24	85,85,85,85	0
56	MG	1A	3539	1/1	0.74	0.14	68,68,68,68	0
56	MG	1A	3581	1/1	0.74	0.28	57,57,57,57	0
56	MG	1a	1759	1/1	0.74	0.16	76,76,76,76	0
56	MG	2A	3145	1/1	0.75	0.43	64,64,64,64	0
56	MG	2a	1704	1/1	0.75	1.04	72,72,72,72	0
56	MG	2A	3439	1/1	0.75	0.24	74,74,74,74	0
56	MG	1G	202	1/1	0.75	0.30	57,57,57,57	0
56	MG	1a	1732	1/1	0.75	0.17	82,82,82,82	0
56	MG	2A	3648	1/1	0.75	0.51	75,75,75,75	0
56	MG	2A	3212	1/1	0.75	1.36	79,79,79,79	0
56	MG	2A	3252	1/1	0.75	0.11	67,67,67,67	0
56	MG	1m	3001	1/1	0.75	0.11	63,63,63,63	0
56	MG	28	101	1/1	0.75	0.92	77,77,77,77	0
56	MG	2A	3561	1/1	0.75	0.28	50,50,50,50	0
56	MG	1O	201	1/1	0.75	0.93	66,66,66,66	0
56	MG	1A	3489	1/1	0.75	0.20	48,48,48,48	0
56	MG	1B	223	1/1	0.75	0.24	72,72,72,72	0
56	MG	1A	4114	1/1	0.75	0.20	61,61,61,61	0
56	MG	2A	3785	1/1	0.75	0.22	76,76,76,76	0
56	MG	2A	3353	1/1	0.75	0.18	78,78,78,78	0
56	MG	2A	3820	1/1	0.75	0.11	79,79,79,79	0
56	MG	2a	1665	1/1	0.75	0.12	69,69,69,69	0
56	MG	2a	1691	1/1	0.76	0.27	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3125	1/1	0.76	0.76	39,39,39,39	0
56	MG	2A	3395	1/1	0.76	0.57	70,70,70,70	0
56	MG	2a	1725	1/1	0.76	0.20	90,90,90,90	0
56	MG	1w	108	1/1	0.76	0.30	82,82,82,82	0
56	MG	2A	3450	1/1	0.76	0.18	69,69,69,69	0
56	MG	1A	3252	1/1	0.76	0.27	49,49,49,49	0
56	MG	1A	3849	1/1	0.76	0.11	55,55,55,55	0
56	MG	2a	1752	1/1	0.76	0.09	72,72,72,72	0
56	MG	2A	3235	1/1	0.76	0.49	65,65,65,65	0
56	MG	2a	1780	1/1	0.76	0.19	72,72,72,72	0
56	MG	1A	3705	1/1	0.76	0.17	54,54,54,54	0
56	MG	1A	4035	1/1	0.76	0.52	71,71,71,71	0
56	MG	1a	1751	1/1	0.76	0.13	75,75,75,75	0
56	MG	2A	3740	1/1	0.76	0.18	52,52,52,52	0
56	MG	1A	3334	1/1	0.76	0.22	59,59,59,59	0
56	MG	1A	3790	1/1	0.76	0.13	23,23,23,23	0
56	MG	1A	3599	1/1	0.76	0.19	50,50,50,50	0
56	MG	2A	3789	1/1	0.76	0.05	77,77,77,77	0
56	MG	2A	3345	1/1	0.76	0.18	78,78,78,78	0
56	MG	1A	3621	1/1	0.76	0.15	76,76,76,76	0
56	MG	1w	101	1/1	0.76	0.29	74,74,74,74	0
56	MG	2A	3279	1/1	0.77	0.32	60,60,60,60	0
56	MG	1A	3871	1/1	0.77	0.15	63,63,63,63	0
56	MG	2a	1632	1/1	0.77	0.18	77,77,77,77	0
56	MG	1A	3452	1/1	0.77	0.20	60,60,60,60	0
56	MG	2A	3748	1/1	0.77	0.21	44,44,44,44	0
56	MG	2A	3758	1/1	0.77	0.17	57,57,57,57	0
56	MG	2a	1668	1/1	0.77	0.22	72,72,72,72	0
56	MG	2a	1678	1/1	0.77	0.21	74,74,74,74	0
56	MG	2a	1682	1/1	0.77	0.15	79,79,79,79	0
56	MG	1A	3619	1/1	0.77	0.17	52,52,52,52	0
56	MG	1A	3276	1/1	0.77	0.24	49,49,49,49	0
56	MG	2A	3545	1/1	0.77	0.09	40,40,40,40	0
56	MG	2A	3091	1/1	0.77	0.09	70,70,70,70	0
56	MG	2A	3110	1/1	0.77	0.21	67,67,67,67	0
56	MG	1a	1736	1/1	0.77	0.07	70,70,70,70	0
56	MG	1A	3409	1/1	0.77	0.83	71,71,71,71	0
56	MG	2a	1735	1/1	0.77	0.07	83,83,83,83	0
56	MG	2A	3153	1/1	0.77	0.27	51,51,51,51	0
56	MG	1A	3838	1/1	0.77	0.13	25,25,25,25	0
56	MG	1A	3538	1/1	0.77	0.28	65,65,65,65	0
56	MG	1A	3434	1/1	0.77	0.26	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	2A	3862	1/1	0.77	0.26	60,60,60,60	0
56	MG	1A	3991	1/1	0.77	0.18	69,69,69,69	0
56	MG	1A	3850	1/1	0.77	0.22	68,68,68,68	0
56	MG	2A	3880	1/1	0.77	0.55	74,74,74,74	0
56	MG	2Q	202	1/1	0.77	1.00	66,66,66,66	0
56	MG	2a	1834	1/1	0.77	0.10	63,63,63,63	0
56	MG	2a	1835	1/1	0.77	0.14	64,64,64,64	0
56	MG	1A	4019	1/1	0.77	0.34	44,44,44,44	0
56	MG	1A	3851	1/1	0.77	0.08	59,59,59,59	0
56	MG	1A	3228	1/1	0.77	0.19	39,39,39,39	0
56	MG	2A	3455	1/1	0.77	0.13	53,53,53,53	0
56	MG	2a	1608	1/1	0.77	0.14	72,72,72,72	0
56	MG	2A	3685	1/1	0.77	0.34	49,49,49,49	0
56	MG	2A	3464	1/1	0.77	0.15	49,49,49,49	0
56	MG	2a	1701	1/1	0.78	0.13	75,75,75,75	0
56	MG	2A	3092	1/1	0.78	0.17	72,72,72,72	0
56	MG	2A	3292	1/1	0.78	0.17	72,72,72,72	0
56	MG	1B	206	1/1	0.78	0.35	49,49,49,49	0
56	MG	2A	3309	1/1	0.78	0.32	70,70,70,70	0
56	MG	2A	3678	1/1	0.78	0.19	66,66,66,66	0
56	MG	1A	3951	1/1	0.78	0.18	59,59,59,59	0
56	MG	2A	3492	1/1	0.78	0.20	73,73,73,73	0
56	MG	2A	3319	1/1	0.78	0.57	56,56,56,56	0
56	MG	1A	3912	1/1	0.78	0.19	43,43,43,43	0
56	MG	2a	1757	1/1	0.78	0.11	65,65,65,65	0
56	MG	2a	1764	1/1	0.78	0.15	81,81,81,81	0
56	MG	2A	3324	1/1	0.78	0.25	75,75,75,75	0
56	MG	2A	3509	1/1	0.78	0.27	63,63,63,63	0
56	MG	1A	3257	1/1	0.78	0.26	57,57,57,57	0
56	MG	1A	4090	1/1	0.78	0.15	70,70,70,70	0
56	MG	2A	3220	1/1	0.78	1.66	73,73,73,73	0
56	MG	1A	3919	1/1	0.78	0.13	56,56,56,56	0
56	MG	2a	1828	1/1	0.78	0.12	80,80,80,80	0
56	MG	2a	1830	1/1	0.78	0.11	87,87,87,87	0
56	MG	2a	1637	1/1	0.78	0.15	61,61,61,61	0
56	MG	1A	3877	1/1	0.78	0.14	58,58,58,58	0
56	MG	2A	3344	1/1	0.78	0.25	70,70,70,70	0
56	MG	2A	3269	1/1	0.78	0.27	76,76,76,76	0
56	MG	1A	3338	1/1	0.78	0.16	66,66,66,66	0
56	MG	2k	201	1/1	0.78	0.09	68,68,68,68	0
56	MG	2q	201	1/1	0.78	0.12	86,86,86,86	0
56	MG	2A	3274	1/1	0.78	1.11	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1603	1/1	0.78	0.14	67,67,67,67	0
56	MG	2A	3234	1/1	0.78	0.51	68,68,68,68	0
56	MG	2A	3411	1/1	0.78	0.23	67,67,67,67	0
56	MG	2A	3811	1/1	0.79	0.31	70,70,70,70	0
56	MG	1a	1808	1/1	0.79	0.08	65,65,65,65	0
56	MG	2a	1694	1/1	0.79	0.24	66,66,66,66	0
56	MG	1A	3140	1/1	0.79	0.43	41,41,41,41	0
56	MG	2a	1703	1/1	0.79	0.26	70,70,70,70	0
56	MG	2A	3265	1/1	0.79	0.21	68,68,68,68	0
56	MG	2a	1706	1/1	0.79	0.28	76,76,76,76	0
56	MG	1A	3950	1/1	0.79	0.16	53,53,53,53	0
56	MG	2a	1715	1/1	0.79	0.18	70,70,70,70	0
56	MG	2A	3215	1/1	0.79	0.48	76,76,76,76	0
56	MG	1A	3874	1/1	0.79	0.08	69,69,69,69	0
56	MG	1A	3955	1/1	0.79	0.21	46,46,46,46	0
56	MG	2A	3354	1/1	0.79	0.50	71,71,71,71	0
56	MG	2A	3632	1/1	0.79	0.26	51,51,51,51	0
56	MG	2a	1744	1/1	0.79	0.08	79,79,79,79	0
56	MG	1A	3618	1/1	0.79	0.24	70,70,70,70	0
56	MG	2B	202	1/1	0.79	0.46	63,63,63,63	0
56	MG	2B	213	1/1	0.79	0.13	76,76,76,76	0
56	MG	2F	303	1/1	0.79	0.10	64,64,64,64	0
56	MG	2A	3282	1/1	0.79	0.32	58,58,58,58	0
56	MG	1A	3392	1/1	0.79	0.20	68,68,68,68	0
56	MG	2A	3427	1/1	0.79	0.32	43,43,43,43	0
56	MG	1A	3407	1/1	0.79	0.38	54,54,54,54	0
56	MG	1a	1653	1/1	0.79	0.34	61,61,61,61	0
56	MG	2A	3293	1/1	0.79	0.17	69,69,69,69	0
56	MG	2a	1611	1/1	0.79	0.17	67,67,67,67	0
56	MG	1A	3628	1/1	0.79	0.10	67,67,67,67	0
56	MG	2A	3306	1/1	0.79	0.29	53,53,53,53	0
56	MG	2A	3490	1/1	0.79	0.34	71,71,71,71	0
56	MG	1A	3822	1/1	0.79	0.19	27,27,27,27	0
56	MG	1a	1697	1/1	0.79	0.17	64,64,64,64	0
56	MG	2A	3756	1/1	0.79	0.13	64,64,64,64	0
56	MG	2A	3238	1/1	0.79	0.21	61,61,61,61	0
56	MG	1D	313	1/1	0.79	0.59	40,40,40,40	0
56	MG	2A	3189	1/1	0.79	0.21	52,52,52,52	0
56	MG	1a	1801	1/1	0.79	0.09	89,89,89,89	0
56	MG	2w	106	1/1	0.79	0.34	71,71,71,71	0
56	MG	2w	107	1/1	0.79	0.64	86,86,86,86	0
56	MG	1A	3020	1/1	0.79	0.26	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3335	1/1	0.79	0.18	81,81,81,81	0
56	MG	1a	1830	1/1	0.80	0.19	63,63,63,63	0
56	MG	1a	1840	1/1	0.80	0.15	75,75,75,75	0
56	MG	1A	3432	1/1	0.80	0.21	44,44,44,44	0
56	MG	2A	3159	1/1	0.80	0.18	66,66,66,66	0
56	MG	1A	3207	1/1	0.80	0.13	53,53,53,53	0
56	MG	2A	3259	1/1	0.80	0.25	61,61,61,61	0
56	MG	2A	3884	1/1	0.80	0.47	75,75,75,75	0
56	MG	2a	1730	1/1	0.80	0.18	68,68,68,68	0
56	MG	2A	3261	1/1	0.80	0.26	71,71,71,71	0
56	MG	2B	211	1/1	0.80	0.16	77,77,77,77	0
56	MG	1A	3719	1/1	0.80	0.12	33,33,33,33	0
56	MG	1A	3245	1/1	0.80	0.30	44,44,44,44	0
56	MG	2N	201	1/1	0.80	0.42	72,72,72,72	0
56	MG	2A	3174	1/1	0.80	0.34	57,57,57,57	0
56	MG	1A	3551	1/1	0.80	0.17	52,52,52,52	0
56	MG	2A	3673	1/1	0.80	0.26	64,64,64,64	0
56	MG	1A	3891	1/1	0.80	0.17	48,48,48,48	0
56	MG	1A	3246	1/1	0.80	0.14	53,53,53,53	0
56	MG	2a	1791	1/1	0.80	0.12	81,81,81,81	0
56	MG	2a	1795	1/1	0.80	0.10	78,78,78,78	0
56	MG	13	101	1/1	0.80	0.28	46,46,46,46	0
56	MG	1A	3443	1/1	0.80	0.16	53,53,53,53	0
56	MG	2a	1819	1/1	0.80	0.12	91,91,91,91	0
56	MG	2a	1612	1/1	0.80	0.26	69,69,69,69	0
56	MG	2A	3002	1/1	0.80	0.09	59,59,59,59	0
56	MG	1A	4036	1/1	0.80	0.32	62,62,62,62	0
56	MG	1A	3450	1/1	0.80	0.26	48,48,48,48	0
56	MG	1A	3266	1/1	0.80	0.38	40,40,40,40	0
56	MG	1a	1792	1/1	0.80	0.20	61,61,61,61	0
56	MG	1A	3458	1/1	0.80	0.27	39,39,39,39	0
56	MG	1A	3470	1/1	0.80	0.17	37,37,37,37	0
56	MG	2A	3782	1/1	0.80	0.29	77,77,77,77	0
56	MG	2A	3089	1/1	0.80	0.26	61,61,61,61	0
56	MG	2A	3515	1/1	0.80	0.28	51,51,51,51	0
56	MG	1A	4130	1/1	0.80	0.25	69,69,69,69	0
56	MG	1A	3251	1/1	0.80	0.16	65,65,65,65	0
56	MG	1a	1825	1/1	0.80	0.12	77,77,77,77	0
56	MG	2A	3236	1/1	0.80	0.45	68,68,68,68	0
56	MG	2A	3116	1/1	0.80	0.24	65,65,65,65	0
56	MG	1A	3643	1/1	0.80	0.17	57,57,57,57	0
56	MG	1A	3415	1/1	0.81	0.34	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1699	1/1	0.81	0.22	64,64,64,64	0
56	MG	1B	224	1/1	0.81	0.18	76,76,76,76	0
56	MG	2A	3143	1/1	0.81	0.13	51,51,51,51	0
56	MG	1A	3840	1/1	0.81	0.08	56,56,56,56	0
56	MG	1l	201	1/1	0.81	0.28	68,68,68,68	0
56	MG	1A	3336	1/1	0.81	0.21	61,61,61,61	0
56	MG	2A	3587	1/1	0.81	0.16	68,68,68,68	0
56	MG	2A	3590	1/1	0.81	0.16	58,58,58,58	0
56	MG	1F	308	1/1	0.81	0.16	49,49,49,49	0
56	MG	1A	3997	1/1	0.81	0.28	64,64,64,64	0
56	MG	1A	3446	1/1	0.81	0.54	55,55,55,55	0
56	MG	1A	3784	1/1	0.81	0.28	58,58,58,58	0
56	MG	2B	201	1/1	0.81	0.28	76,76,76,76	0
56	MG	2a	1742	1/1	0.81	0.09	75,75,75,75	0
56	MG	1Z	302	1/1	0.81	0.17	64,64,64,64	0
56	MG	1A	3929	1/1	0.81	0.17	63,63,63,63	0
56	MG	1x	105	1/1	0.81	0.26	73,73,73,73	0
56	MG	2D	306	1/1	0.81	0.42	69,69,69,69	0
56	MG	2A	3351	1/1	0.81	0.42	75,75,75,75	0
56	MG	2A	3188	1/1	0.81	0.17	60,60,60,60	0
56	MG	1A	3935	1/1	0.81	0.15	33,33,33,33	0
56	MG	1A	3227	1/1	0.81	0.28	60,60,60,60	0
56	MG	2A	3370	1/1	0.81	0.40	72,72,72,72	0
56	MG	2A	3388	1/1	0.81	0.74	46,46,46,46	0
56	MG	2A	3012	1/1	0.81	0.49	42,42,42,42	0
56	MG	1A	3814	1/1	0.81	0.28	34,34,34,34	0
56	MG	1A	3028	1/1	0.81	0.19	44,44,44,44	0
56	MG	2A	3276	1/1	0.81	0.15	69,69,69,69	0
56	MG	2A	3724	1/1	0.81	0.21	57,57,57,57	0
56	MG	2A	3446	1/1	0.81	0.14	46,46,46,46	0
56	MG	2A	3732	1/1	0.81	0.27	48,48,48,48	0
56	MG	2A	3210	1/1	0.81	1.24	64,64,64,64	0
56	MG	1A	3349	1/1	0.81	0.30	43,43,43,43	0
56	MG	2a	1840	1/1	0.81	0.21	73,73,73,73	0
56	MG	1a	1644	1/1	0.81	0.12	54,54,54,54	0
56	MG	1A	3663	1/1	0.81	0.16	37,37,37,37	0
56	MG	2a	1660	1/1	0.81	0.17	69,69,69,69	0
56	MG	1a	1660	1/1	0.81	0.23	64,64,64,64	0
56	MG	1a	1663	1/1	0.81	0.19	65,65,65,65	0
56	MG	1A	3299	1/1	0.81	1.38	57,57,57,57	0
56	MG	2A	3783	1/1	0.81	0.20	56,56,56,56	0
56	MG	2A	3303	1/1	0.81	0.42	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	220	1/1	0.81	0.20	68,68,68,68	0
56	MG	2A	3231	1/1	0.81	0.14	70,70,70,70	0
56	MG	2y	103	1/1	0.81	0.42	72,72,72,72	0
56	MG	2A	3382	1/1	0.82	0.19	51,51,51,51	0
56	MG	1A	3934	1/1	0.82	0.10	33,33,33,33	0
56	MG	1A	3889	1/1	0.82	0.13	54,54,54,54	0
56	MG	2A	3788	1/1	0.82	0.11	60,60,60,60	0
56	MG	2A	3398	1/1	0.82	0.41	60,60,60,60	0
56	MG	2A	3314	1/1	0.82	0.15	67,67,67,67	0
56	MG	2A	3417	1/1	0.82	0.36	67,67,67,67	0
56	MG	1A	3188	1/1	0.82	0.94	65,65,65,65	0
56	MG	2a	1631	1/1	0.82	0.15	64,64,64,64	0
56	MG	1x	113	1/1	0.82	0.21	79,79,79,79	0
56	MG	2a	1785	1/1	0.82	0.16	67,67,67,67	0
56	MG	2A	3262	1/1	0.82	0.20	64,64,64,64	0
56	MG	2A	3151	1/1	0.82	0.38	70,70,70,70	0
56	MG	1A	3191	1/1	0.82	0.25	43,43,43,43	0
56	MG	1A	3900	1/1	0.82	0.20	75,75,75,75	0
56	MG	2a	1810	1/1	0.82	0.14	76,76,76,76	0
56	MG	1A	3469	1/1	0.82	0.55	44,44,44,44	0
56	MG	1A	3396	1/1	0.82	0.33	50,50,50,50	0
56	MG	2a	1671	1/1	0.82	0.16	55,55,55,55	0
56	MG	2A	3869	1/1	0.82	0.07	76,76,76,76	0
56	MG	1A	3078	1/1	0.82	0.22	60,60,60,60	0
56	MG	2a	1688	1/1	0.82	0.12	70,70,70,70	0
56	MG	2A	3058	1/1	0.82	0.17	66,66,66,66	0
56	MG	1A	3451	1/1	0.82	0.18	63,63,63,63	0
56	MG	2A	3721	1/1	0.82	0.25	68,68,68,68	0
56	MG	2A	3175	1/1	0.82	0.35	66,66,66,66	0
56	MG	2A	3507	1/1	0.82	0.10	65,65,65,65	0
56	MG	1A	4117	1/1	0.82	0.13	47,47,47,47	0
56	MG	1T	204	1/1	0.82	0.17	41,41,41,41	0
56	MG	1V	205	1/1	0.82	0.16	51,51,51,51	0
56	MG	1A	4128	1/1	0.82	0.07	65,65,65,65	0
56	MG	1a	1798	1/1	0.82	0.12	64,64,64,64	0
56	MG	2X	103	1/1	0.82	0.23	58,58,58,58	0
56	MG	1A	3666	1/1	0.82	0.17	24,24,24,24	0
56	MG	2A	3380	1/1	0.82	0.20	66,66,66,66	0
56	MG	2A	3381	1/1	0.82	0.16	50,50,50,50	0
56	MG	1A	3921	1/1	0.83	0.11	74,74,74,74	0
56	MG	2A	3347	1/1	0.83	0.30	75,75,75,75	0
56	MG	2A	3824	1/1	0.83	0.21	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3828	1/1	0.83	0.23	73,73,73,73	0
56	MG	1a	1633	1/1	0.83	0.25	67,67,67,67	0
56	MG	1A	3511	1/1	0.83	0.17	37,37,37,37	0
56	MG	2A	3057	1/1	0.83	0.14	79,79,79,79	0
56	MG	1a	1645	1/1	0.83	0.13	64,64,64,64	0
56	MG	2A	3209	1/1	0.83	0.71	68,68,68,68	0
56	MG	1A	3926	1/1	0.83	0.19	45,45,45,45	0
56	MG	1A	4021	1/1	0.83	0.25	44,44,44,44	0
56	MG	1A	3873	1/1	0.83	0.16	57,57,57,57	0
56	MG	1A	3740	1/1	0.83	0.12	55,55,55,55	0
56	MG	1F	313	1/1	0.83	0.54	63,63,63,63	0
56	MG	2A	3396	1/1	0.83	0.18	55,55,55,55	0
56	MG	1a	1670	1/1	0.83	0.55	57,57,57,57	0
56	MG	2A	3409	1/1	0.83	0.51	63,63,63,63	0
56	MG	2a	1741	1/1	0.83	0.08	70,70,70,70	0
56	MG	1a	1679	1/1	0.83	0.17	58,58,58,58	0
56	MG	2D	302	1/1	0.83	0.62	49,49,49,49	0
56	MG	1a	1692	1/1	0.83	0.10	43,43,43,43	0
56	MG	2E	301	1/1	0.83	0.16	67,67,67,67	0
56	MG	2E	303	1/1	0.83	0.16	57,57,57,57	0
56	MG	2a	1763	1/1	0.83	0.14	62,62,62,62	0
56	MG	2F	301	1/1	0.83	0.37	49,49,49,49	0
56	MG	1A	4061	1/1	0.83	0.12	61,61,61,61	0
56	MG	1A	4074	1/1	0.83	0.14	59,59,59,59	0
56	MG	2A	3690	1/1	0.83	0.19	55,55,55,55	0
56	MG	2A	3700	1/1	0.83	0.32	64,64,64,64	0
56	MG	2A	3704	1/1	0.83	0.17	70,70,70,70	0
56	MG	2A	3710	1/1	0.83	0.23	66,66,66,66	0
56	MG	1O	203	1/1	0.83	0.13	66,66,66,66	0
56	MG	1A	3178	1/1	0.83	0.31	43,43,43,43	0
56	MG	2A	3452	1/1	0.83	0.12	57,57,57,57	0
56	MG	1U	204	1/1	0.83	0.74	56,56,56,56	0
56	MG	1A	3881	1/1	0.83	0.26	20,20,20,20	0
56	MG	2a	1824	1/1	0.83	0.30	76,76,76,76	0
56	MG	2a	1616	1/1	0.83	0.15	85,85,85,85	0
56	MG	2A	3486	1/1	0.83	0.21	30,30,30,30	0
56	MG	1A	3344	1/1	0.83	0.25	54,54,54,54	0
56	MG	2A	3323	1/1	0.83	0.52	47,47,47,47	0
56	MG	1A	3679	1/1	0.83	0.05	68,68,68,68	0
56	MG	2a	1630	1/1	0.83	0.12	77,77,77,77	0
56	MG	1A	3180	1/1	0.83	0.20	50,50,50,50	0
56	MG	2A	3250	1/1	0.83	0.49	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3494	1/1	0.83	0.12	46,46,46,46	0
56	MG	1A	3595	1/1	0.83	0.16	55,55,55,55	0
56	MG	1y	102	1/1	0.83	0.99	90,90,90,90	0
56	MG	2A	3177	1/1	0.83	0.41	78,78,78,78	0
56	MG	2A	3519	1/1	0.83	0.18	38,38,38,38	0
56	MG	2A	3343	1/1	0.83	0.51	72,72,72,72	0
56	MG	1A	3867	1/1	0.83	0.21	55,55,55,55	0
56	MG	2x	106	1/1	0.83	0.21	72,72,72,72	0
56	MG	1A	3868	1/1	0.83	0.22	66,66,66,66	0
56	MG	2A	3819	1/1	0.83	0.14	66,66,66,66	0
56	MG	2a	1642	1/1	0.84	0.14	75,75,75,75	0
56	MG	2A	3198	1/1	0.84	0.19	60,60,60,60	0
56	MG	2A	3207	1/1	0.84	1.10	57,57,57,57	0
56	MG	1A	3226	1/1	0.84	0.29	62,62,62,62	0
56	MG	2A	3467	1/1	0.84	0.10	45,45,45,45	0
56	MG	1A	3787	1/1	0.84	0.19	18,18,18,18	0
56	MG	1A	4093	1/1	0.84	0.11	58,58,58,58	0
56	MG	2a	1681	1/1	0.84	0.19	71,71,71,71	0
56	MG	2A	3311	1/1	0.84	0.20	65,65,65,65	0
56	MG	2a	1685	1/1	0.84	0.23	50,50,50,50	0
56	MG	1A	4095	1/1	0.84	0.29	67,67,67,67	0
56	MG	1A	3269	1/1	0.84	0.16	50,50,50,50	0
56	MG	2A	3317	1/1	0.84	0.26	59,59,59,59	0
56	MG	1a	1626	1/1	0.84	0.15	47,47,47,47	0
56	MG	2A	3814	1/1	0.84	0.16	68,68,68,68	0
56	MG	2A	3062	1/1	0.84	0.31	45,45,45,45	0
56	MG	2A	3064	1/1	0.84	0.31	55,55,55,55	0
56	MG	2A	3229	1/1	0.84	0.22	61,61,61,61	0
56	MG	1A	3806	1/1	0.84	0.14	42,42,42,42	0
56	MG	2A	3085	1/1	0.84	0.25	46,46,46,46	0
56	MG	2a	1712	1/1	0.84	0.17	75,75,75,75	0
56	MG	2A	3830	1/1	0.84	0.07	57,57,57,57	0
56	MG	2A	3232	1/1	0.84	0.11	67,67,67,67	0
56	MG	2a	1727	1/1	0.84	0.08	66,66,66,66	0
56	MG	1A	3639	1/1	0.84	0.11	47,47,47,47	0
56	MG	1A	3417	1/1	0.84	0.23	64,64,64,64	0
56	MG	1A	3883	1/1	0.84	0.15	33,33,33,33	0
56	MG	1a	1819	1/1	0.84	0.16	61,61,61,61	0
56	MG	2A	3094	1/1	0.84	0.15	79,79,79,79	0
56	MG	1a	1823	1/1	0.84	0.16	69,69,69,69	0
56	MG	1A	3418	1/1	0.84	0.21	59,59,59,59	0
56	MG	1A	3364	1/1	0.84	0.35	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3612	1/1	0.84	0.21	68,68,68,68	0
56	MG	2A	3349	1/1	0.84	0.47	60,60,60,60	0
56	MG	1B	218	1/1	0.84	0.25	60,60,60,60	0
56	MG	2a	1760	1/1	0.84	0.23	86,86,86,86	0
56	MG	2B	210	1/1	0.84	0.29	72,72,72,72	0
56	MG	1A	3127	1/1	0.84	0.58	35,35,35,35	0
56	MG	2A	3627	1/1	0.84	0.14	73,73,73,73	0
56	MG	1f	201	1/1	0.84	0.17	52,52,52,52	0
56	MG	2D	304	1/1	0.84	0.92	51,51,51,51	0
56	MG	2A	3363	1/1	0.84	0.29	58,58,58,58	0
56	MG	2D	307	1/1	0.84	0.35	74,74,74,74	0
56	MG	1A	3466	1/1	0.84	0.23	47,47,47,47	0
56	MG	1A	3328	1/1	0.84	0.51	41,41,41,41	0
56	MG	1A	4015	1/1	0.84	0.19	65,65,65,65	0
56	MG	1A	3399	1/1	0.84	0.13	63,63,63,63	0
56	MG	1v	102	1/1	0.84	0.12	77,77,77,77	0
56	MG	2A	3385	1/1	0.84	0.42	53,53,53,53	0
56	MG	1A	3725	1/1	0.84	0.42	50,50,50,50	0
56	MG	2A	3389	1/1	0.84	0.15	63,63,63,63	0
56	MG	2A	3694	1/1	0.84	0.15	78,78,78,78	0
56	MG	2a	1831	1/1	0.84	0.17	70,70,70,70	0
56	MG	1A	4034	1/1	0.84	0.16	56,56,56,56	0
56	MG	1A	3095	1/1	0.84	0.37	34,34,34,34	0
56	MG	1A	3737	1/1	0.84	0.34	49,49,49,49	0
56	MG	2A	3714	1/1	0.84	0.13	66,66,66,66	0
56	MG	1A	4038	1/1	0.84	0.38	52,52,52,52	0
56	MG	2a	1613	1/1	0.84	0.12	67,67,67,67	0
56	MG	2A	3719	1/1	0.84	0.09	82,82,82,82	0
56	MG	1a	1746	1/1	0.84	0.07	55,55,55,55	0
56	MG	2q	202	1/1	0.84	0.18	79,79,79,79	0
56	MG	1A	4046	1/1	0.84	0.15	68,68,68,68	0
56	MG	2A	3424	1/1	0.84	0.19	70,70,70,70	0
56	MG	1A	4056	1/1	0.84	0.16	47,47,47,47	0
56	MG	1A	3376	1/1	0.84	0.15	51,51,51,51	0
56	MG	1A	3768	1/1	0.84	0.11	35,35,35,35	0
56	MG	2A	3742	1/1	0.84	0.17	73,73,73,73	0
56	MG	2A	3747	1/1	0.84	0.07	68,68,68,68	0
56	MG	1A	4077	1/1	0.84	0.30	64,64,64,64	0
56	MG	1A	3268	1/1	0.85	0.11	50,50,50,50	0
56	MG	1A	3333	1/1	0.85	0.49	51,51,51,51	0
56	MG	2a	1644	1/1	0.85	0.18	80,80,80,80	0
56	MG	2a	1653	1/1	0.85	0.14	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	3759	1/1	0.85	0.13	25,25,25,25	0
56	MG	2A	3312	1/1	0.85	0.21	67,67,67,67	0
56	MG	1A	4029	1/1	0.85	0.36	65,65,65,65	0
56	MG	2A	3765	1/1	0.85	0.15	38,38,38,38	0
56	MG	2A	3773	1/1	0.85	0.16	56,56,56,56	0
56	MG	2a	1677	1/1	0.85	0.12	73,73,73,73	0
56	MG	1A	3121	1/1	0.85	0.25	45,45,45,45	0
56	MG	1A	3741	1/1	0.85	0.25	62,62,62,62	0
56	MG	1A	3754	1/1	0.85	0.20	49,49,49,49	0
56	MG	2A	3074	1/1	0.85	0.35	54,54,54,54	0
56	MG	2a	1687	1/1	0.85	0.15	75,75,75,75	0
56	MG	2A	3077	1/1	0.85	0.45	58,58,58,58	0
56	MG	1a	1814	1/1	0.85	0.12	66,66,66,66	0
56	MG	2A	3810	1/1	0.85	0.20	63,63,63,63	0
56	MG	1a	1651	1/1	0.85	0.14	57,57,57,57	0
56	MG	1a	1822	1/1	0.85	0.18	60,60,60,60	0
56	MG	2A	3532	1/1	0.85	0.18	32,32,32,32	0
56	MG	1A	3640	1/1	0.85	0.15	18,18,18,18	0
56	MG	1a	1824	1/1	0.85	0.13	63,63,63,63	0
56	MG	2A	3340	1/1	0.85	0.25	71,71,71,71	0
56	MG	1D	309	1/1	0.85	0.30	41,41,41,41	0
56	MG	2A	3584	1/1	0.85	0.12	53,53,53,53	0
56	MG	2A	3100	1/1	0.85	0.12	68,68,68,68	0
56	MG	1A	3780	1/1	0.85	0.17	19,19,19,19	0
56	MG	1A	3478	1/1	0.85	0.33	37,37,37,37	0
56	MG	2A	3595	1/1	0.85	0.20	58,58,58,58	0
56	MG	1F	311	1/1	0.85	0.29	64,64,64,64	0
56	MG	1A	3484	1/1	0.85	0.11	56,56,56,56	0
56	MG	2A	3240	1/1	0.85	0.14	50,50,50,50	0
56	MG	2A	3872	1/1	0.85	0.32	63,63,63,63	0
56	MG	2A	3614	1/1	0.85	0.28	61,61,61,61	0
56	MG	2A	3246	1/1	0.85	0.38	68,68,68,68	0
56	MG	2A	3148	1/1	0.85	0.47	70,70,70,70	0
56	MG	1A	3184	1/1	0.85	1.01	49,49,49,49	0
56	MG	1I	201	1/1	0.85	0.11	64,64,64,64	0
56	MG	1A	3793	1/1	0.85	0.17	43,43,43,43	0
56	MG	2A	3254	1/1	0.85	0.38	74,74,74,74	0
56	MG	1n	101	1/1	0.85	0.18	53,53,53,53	0
56	MG	2A	3651	1/1	0.85	0.42	67,67,67,67	0
56	MG	2A	3652	1/1	0.85	0.16	73,73,73,73	0
56	MG	2a	1777	1/1	0.85	0.10	75,75,75,75	0
56	MG	1A	3797	1/1	0.85	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3660	1/1	0.85	0.27	51,51,51,51	0
56	MG	2A	3663	1/1	0.85	0.20	51,51,51,51	0
56	MG	2A	3161	1/1	0.85	0.19	55,55,55,55	0
56	MG	1a	1700	1/1	0.85	0.20	49,49,49,49	0
56	MG	1S	203	1/1	0.85	0.15	69,69,69,69	0
56	MG	2F	306	1/1	0.85	0.17	59,59,59,59	0
56	MG	2G	201	1/1	0.85	0.17	79,79,79,79	0
56	MG	2A	3264	1/1	0.85	0.25	77,77,77,77	0
56	MG	1A	4081	1/1	0.85	0.16	60,60,60,60	0
56	MG	2T	202	1/1	0.85	0.20	53,53,53,53	0
56	MG	1A	3676	1/1	0.85	0.14	56,56,56,56	0
56	MG	20	103	1/1	0.85	0.15	60,60,60,60	0
56	MG	1A	3601	1/1	0.85	0.17	31,31,31,31	0
56	MG	1A	3985	1/1	0.85	0.30	52,52,52,52	0
56	MG	2a	1602	1/1	0.85	0.11	82,82,82,82	0
56	MG	2A	3408	1/1	0.85	0.28	66,66,66,66	0
56	MG	2A	3178	1/1	0.85	0.46	68,68,68,68	0
56	MG	2A	3711	1/1	0.85	0.15	71,71,71,71	0
56	MG	1A	3609	1/1	0.85	0.31	66,66,66,66	0
56	MG	2A	3186	1/1	0.85	0.46	43,43,43,43	0
56	MG	2m	201	1/1	0.85	0.09	81,81,81,81	0
56	MG	2A	3280	1/1	0.85	0.51	67,67,67,67	0
56	MG	1A	3697	1/1	0.85	0.08	36,36,36,36	0
56	MG	2r	101	1/1	0.85	0.25	75,75,75,75	0
56	MG	2A	3433	1/1	0.85	0.31	63,63,63,63	0
56	MG	10	105	1/1	0.85	0.11	74,74,74,74	0
56	MG	1A	3361	1/1	0.85	0.41	62,62,62,62	0
56	MG	1a	1761	1/1	0.85	0.07	51,51,51,51	0
56	MG	1A	3282	1/1	0.85	0.36	39,39,39,39	0
56	MG	1A	3524	1/1	0.85	0.12	33,33,33,33	0
56	MG	1a	1612	1/1	0.85	0.18	57,57,57,57	0
56	MG	1a	1620	1/1	0.85	0.18	63,63,63,63	0
57	ZN	24	501	1/1	0.85	0.05	128,128,128,128	0
56	MG	1A	3751	1/1	0.86	0.17	21,21,21,21	0
56	MG	1A	3096	1/1	0.86	0.14	44,44,44,44	0
56	MG	1A	3142	1/1	0.86	0.24	56,56,56,56	0
56	MG	1A	3423	1/1	0.86	0.39	57,57,57,57	0
56	MG	2A	3442	1/1	0.86	0.24	58,58,58,58	0
56	MG	1A	3382	1/1	0.86	0.17	53,53,53,53	0
56	MG	1A	4059	1/1	0.86	0.20	53,53,53,53	0
56	MG	2A	3156	1/1	0.86	0.22	59,59,59,59	0
56	MG	19	101	1/1	0.86	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3760	1/1	0.86	0.18	76,76,76,76	0
56	MG	1A	3430	1/1	0.86	0.19	47,47,47,47	0
56	MG	1A	4073	1/1	0.86	0.15	55,55,55,55	0
56	MG	2A	3482	1/1	0.86	0.16	36,36,36,36	0
56	MG	2A	3772	1/1	0.86	0.13	58,58,58,58	0
56	MG	2A	3281	1/1	0.86	0.56	75,75,75,75	0
56	MG	1A	3637	1/1	0.86	0.21	21,21,21,21	0
56	MG	1A	3261	1/1	0.86	0.22	60,60,60,60	0
56	MG	1A	3490	1/1	0.86	0.13	56,56,56,56	0
56	MG	1A	3799	1/1	0.86	0.21	42,42,42,42	0
56	MG	1a	1841	1/1	0.86	0.11	68,68,68,68	0
56	MG	1A	3388	1/1	0.86	0.13	48,48,48,48	0
56	MG	2A	3804	1/1	0.86	0.27	66,66,66,66	0
56	MG	1A	3923	1/1	0.86	0.17	44,44,44,44	0
56	MG	1A	3809	1/1	0.86	0.78	35,35,35,35	0
56	MG	2A	3307	1/1	0.86	0.33	70,70,70,70	0
56	MG	1a	1647	1/1	0.86	0.25	66,66,66,66	0
56	MG	1A	3645	1/1	0.86	0.16	35,35,35,35	0
56	MG	1A	3658	1/1	0.86	0.15	18,18,18,18	0
56	MG	1a	1659	1/1	0.86	0.16	59,59,59,59	0
56	MG	2a	1713	1/1	0.86	0.08	77,77,77,77	0
56	MG	1A	3496	1/1	0.86	0.13	55,55,55,55	0
56	MG	2a	1721	1/1	0.86	0.27	57,57,57,57	0
56	MG	2a	1722	1/1	0.86	0.10	89,89,89,89	0
56	MG	1A	3300	1/1	0.86	0.53	41,41,41,41	0
56	MG	2A	3195	1/1	0.86	0.65	48,48,48,48	0
56	MG	1a	1664	1/1	0.86	0.15	61,61,61,61	0
56	MG	2A	3203	1/1	0.86	0.42	66,66,66,66	0
56	MG	2A	3848	1/1	0.86	0.36	64,64,64,64	0
56	MG	1A	3832	1/1	0.86	0.10	40,40,40,40	0
56	MG	2A	3859	1/1	0.86	0.11	67,67,67,67	0
56	MG	1A	3948	1/1	0.86	0.15	73,73,73,73	0
56	MG	2A	3866	1/1	0.86	0.13	78,78,78,78	0
56	MG	1A	3194	1/1	0.86	0.65	34,34,34,34	0
56	MG	2A	3601	1/1	0.86	0.11	73,73,73,73	0
56	MG	2A	3331	1/1	0.86	0.29	59,59,59,59	0
56	MG	2A	3333	1/1	0.86	0.23	71,71,71,71	0
56	MG	1A	3232	1/1	0.86	0.24	44,44,44,44	0
56	MG	1a	1684	1/1	0.86	0.20	60,60,60,60	0
56	MG	1A	3954	1/1	0.86	0.15	46,46,46,46	0
56	MG	1a	1696	1/1	0.86	0.20	71,71,71,71	0
56	MG	1A	3155	1/1	0.86	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3058	1/1	0.86	0.16	56,56,56,56	0
56	MG	2a	1784	1/1	0.86	0.22	81,81,81,81	0
56	MG	1A	3967	1/1	0.86	0.14	54,54,54,54	0
56	MG	1a	1720	1/1	0.86	0.14	46,46,46,46	0
56	MG	2A	3032	1/1	0.86	0.24	51,51,51,51	0
56	MG	2A	3045	1/1	0.86	0.21	67,67,67,67	0
56	MG	1A	3975	1/1	0.86	0.21	67,67,67,67	0
56	MG	1a	1730	1/1	0.86	0.08	63,63,63,63	0
56	MG	2a	1811	1/1	0.86	0.24	75,75,75,75	0
56	MG	1A	3847	1/1	0.86	0.18	45,45,45,45	0
56	MG	1a	1733	1/1	0.86	0.14	66,66,66,66	0
56	MG	1E	301	1/1	0.86	0.31	49,49,49,49	0
56	MG	1E	312	1/1	0.86	0.38	64,64,64,64	0
56	MG	2A	3669	1/1	0.86	0.15	60,60,60,60	0
56	MG	1A	3574	1/1	0.86	0.14	48,48,48,48	0
56	MG	1A	3988	1/1	0.86	0.25	60,60,60,60	0
56	MG	2A	3242	1/1	0.86	0.25	71,71,71,71	0
56	MG	2A	3243	1/1	0.86	0.27	54,54,54,54	0
56	MG	1A	3367	1/1	0.86	0.40	36,36,36,36	0
56	MG	1A	3585	1/1	0.86	0.23	21,21,21,21	0
56	MG	1A	3853	1/1	0.86	0.23	65,65,65,65	0
56	MG	2A	3705	1/1	0.86	0.08	49,49,49,49	0
56	MG	2A	3706	1/1	0.86	0.09	63,63,63,63	0
56	MG	1A	3733	1/1	0.86	0.38	55,55,55,55	0
56	MG	1A	3250	1/1	0.86	0.13	60,60,60,60	0
56	MG	2a	1609	1/1	0.86	0.17	60,60,60,60	0
56	MG	1A	3372	1/1	0.86	0.21	51,51,51,51	0
56	MG	2w	101	1/1	0.86	0.16	79,79,79,79	0
56	MG	2A	3405	1/1	0.86	0.59	59,59,59,59	0
56	MG	1A	3739	1/1	0.86	0.14	68,68,68,68	0
56	MG	2a	1615	1/1	0.86	0.14	63,63,63,63	0
56	MG	2A	3720	1/1	0.86	0.10	73,73,73,73	0
56	MG	2x	101	1/1	0.86	0.11	55,55,55,55	0
56	MG	1A	3214	1/1	0.86	0.21	59,59,59,59	0
56	MG	1A	3468	1/1	0.86	0.31	39,39,39,39	0
56	MG	1V	206	1/1	0.86	0.19	41,41,41,41	0
56	MG	2A	3725	1/1	0.86	0.08	65,65,65,65	0
56	MG	2A	3728	1/1	0.86	0.14	61,61,61,61	0
56	MG	1A	3437	1/1	0.87	0.13	57,57,57,57	0
56	MG	18	101	1/1	0.87	0.57	64,64,64,64	0
56	MG	2a	1647	1/1	0.87	0.26	58,58,58,58	0
56	MG	2A	3781	1/1	0.87	0.10	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	3480	1/1	0.87	0.23	42,42,42,42	0
56	MG	2A	3524	1/1	0.87	0.20	64,64,64,64	0
56	MG	2A	3219	1/1	0.87	0.62	50,50,50,50	0
56	MG	2A	3059	1/1	0.87	0.20	44,44,44,44	0
56	MG	1A	3979	1/1	0.87	0.17	31,31,31,31	0
56	MG	1A	3378	1/1	0.87	0.14	46,46,46,46	0
56	MG	2A	3799	1/1	0.87	0.12	61,61,61,61	0
56	MG	2a	1680	1/1	0.87	0.13	57,57,57,57	0
56	MG	1A	3112	1/1	0.87	0.17	36,36,36,36	0
56	MG	2A	3336	1/1	0.87	0.26	60,60,60,60	0
56	MG	1a	1615	1/1	0.87	0.13	56,56,56,56	0
56	MG	2A	3072	1/1	0.87	0.30	57,57,57,57	0
56	MG	1a	1786	1/1	0.87	0.11	57,57,57,57	0
56	MG	1a	1616	1/1	0.87	0.09	60,60,60,60	0
56	MG	2A	3078	1/1	0.87	0.48	58,58,58,58	0
56	MG	2A	3082	1/1	0.87	0.18	49,49,49,49	0
56	MG	1A	3331	1/1	0.87	0.32	40,40,40,40	0
56	MG	1B	203	1/1	0.87	0.12	61,61,61,61	0
56	MG	1A	3616	1/1	0.87	0.21	45,45,45,45	0
56	MG	1A	3491	1/1	0.87	0.09	61,61,61,61	0
56	MG	2A	3350	1/1	0.87	0.15	64,64,64,64	0
56	MG	1a	1630	1/1	0.87	0.15	44,44,44,44	0
56	MG	1A	3829	1/1	0.87	0.12	50,50,50,50	0
56	MG	2A	3857	1/1	0.87	0.14	64,64,64,64	0
56	MG	2A	3097	1/1	0.87	0.50	73,73,73,73	0
56	MG	2a	1720	1/1	0.87	0.10	72,72,72,72	0
56	MG	2A	3640	1/1	0.87	0.16	52,52,52,52	0
56	MG	2A	3865	1/1	0.87	0.26	58,58,58,58	0
56	MG	1a	1636	1/1	0.87	0.09	62,62,62,62	0
56	MG	1a	1640	1/1	0.87	0.13	47,47,47,47	0
56	MG	1A	3206	1/1	0.87	0.67	38,38,38,38	0
56	MG	2A	3121	1/1	0.87	0.46	52,52,52,52	0
56	MG	1A	3071	1/1	0.87	0.12	40,40,40,40	0
56	MG	1A	3507	1/1	0.87	0.14	35,35,35,35	0
56	MG	2A	3662	1/1	0.87	0.16	69,69,69,69	0
56	MG	2A	3383	1/1	0.87	0.18	57,57,57,57	0
56	MG	1A	3453	1/1	0.87	0.12	66,66,66,66	0
56	MG	1A	3295	1/1	0.87	0.18	55,55,55,55	0
56	MG	2a	1749	1/1	0.87	0.07	77,77,77,77	0
56	MG	2a	1750	1/1	0.87	0.13	67,67,67,67	0
56	MG	1A	3002	1/1	0.87	0.28	47,47,47,47	0
56	MG	2A	3670	1/1	0.87	0.19	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1E	310	1/1	0.87	0.14	30,30,30,30	0
56	MG	1A	3145	1/1	0.87	0.20	39,39,39,39	0
56	MG	2A	3683	1/1	0.87	0.15	44,44,44,44	0
56	MG	1A	3933	1/1	0.87	0.21	61,61,61,61	0
56	MG	1A	3304	1/1	0.87	0.51	35,35,35,35	0
56	MG	2a	1773	1/1	0.87	0.15	78,78,78,78	0
56	MG	1A	4050	1/1	0.87	0.09	52,52,52,52	0
56	MG	1A	3557	1/1	0.87	0.20	22,22,22,22	0
56	MG	2A	3166	1/1	0.87	1.34	71,71,71,71	0
56	MG	1a	1671	1/1	0.87	0.66	67,67,67,67	0
56	MG	1A	3941	1/1	0.87	0.21	28,28,28,28	0
56	MG	2A	3426	1/1	0.87	0.15	52,52,52,52	0
56	MG	2P	201	1/1	0.87	0.30	50,50,50,50	0
56	MG	2a	1805	1/1	0.87	0.18	72,72,72,72	0
56	MG	2P	202	1/1	0.87	0.15	56,56,56,56	0
56	MG	1A	3945	1/1	0.87	0.10	35,35,35,35	0
56	MG	1A	3773	1/1	0.87	0.36	61,61,61,61	0
56	MG	2X	101	1/1	0.87	0.20	72,72,72,72	0
56	MG	2a	1820	1/1	0.87	0.35	84,84,84,84	0
56	MG	1Q	203	1/1	0.87	0.15	47,47,47,47	0
56	MG	2Z	301	1/1	0.87	0.09	85,85,85,85	0
56	MG	1S	201	1/1	0.87	0.56	44,44,44,44	0
56	MG	2A	3444	1/1	0.87	0.17	32,32,32,32	0
56	MG	2A	3184	1/1	0.87	0.13	68,68,68,68	0
56	MG	28	103	1/1	0.87	0.14	45,45,45,45	0
56	MG	2A	3290	1/1	0.87	0.27	82,82,82,82	0
56	MG	1A	3646	1/1	0.87	0.08	52,52,52,52	0
56	MG	1A	3861	1/1	0.87	0.10	23,23,23,23	0
56	MG	2a	1838	1/1	0.87	0.14	67,67,67,67	0
56	MG	1a	1716	1/1	0.87	0.07	53,53,53,53	0
56	MG	2A	3466	1/1	0.87	0.13	42,42,42,42	0
56	MG	1A	3652	1/1	0.87	0.23	52,52,52,52	0
56	MG	2A	3481	1/1	0.87	0.19	60,60,60,60	0
56	MG	1a	1726	1/1	0.87	0.15	59,59,59,59	0
56	MG	1A	4080	1/1	0.87	0.13	36,36,36,36	0
56	MG	1A	3316	1/1	0.87	0.12	41,41,41,41	0
56	MG	1A	4083	1/1	0.87	0.34	56,56,56,56	0
56	MG	2a	1618	1/1	0.87	0.19	65,65,65,65	0
56	MG	1A	3659	1/1	0.87	0.15	27,27,27,27	0
56	MG	2w	104	1/1	0.87	0.22	73,73,73,73	0
56	MG	1A	3258	1/1	0.87	0.13	55,55,55,55	0
56	MG	1a	1742	1/1	0.87	0.17	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	10	104	1/1	0.87	0.48	43,43,43,43	0
56	MG	2w	108	1/1	0.87	0.39	85,85,85,85	0
56	MG	1A	3582	1/1	0.87	0.11	28,28,28,28	0
56	MG	2A	3044	1/1	0.87	0.24	55,55,55,55	0
56	MG	2a	1633	1/1	0.87	0.28	67,67,67,67	0
56	MG	2A	3766	1/1	0.87	0.18	47,47,47,47	0
56	MG	2a	1638	1/1	0.87	0.25	71,71,71,71	0
56	MG	2A	3770	1/1	0.87	0.21	61,61,61,61	0
56	MG	2A	3170	1/1	0.88	0.32	67,67,67,67	0
56	MG	1A	3684	1/1	0.88	0.10	39,39,39,39	0
56	MG	2A	3628	1/1	0.88	0.12	53,53,53,53	0
56	MG	1a	1757	1/1	0.88	0.11	69,69,69,69	0
56	MG	2A	3634	1/1	0.88	0.22	64,64,64,64	0
56	MG	2A	3635	1/1	0.88	0.18	62,62,62,62	0
56	MG	2A	3008	1/1	0.88	0.12	55,55,55,55	0
56	MG	2A	3176	1/1	0.88	0.39	61,61,61,61	0
56	MG	2A	3855	1/1	0.88	0.19	62,62,62,62	0
56	MG	2a	1690	1/1	0.88	0.16	77,77,77,77	0
56	MG	1A	3870	1/1	0.88	0.23	71,71,71,71	0
56	MG	1A	3256	1/1	0.88	0.15	53,53,53,53	0
56	MG	1A	3804	1/1	0.88	0.13	40,40,40,40	0
56	MG	2A	3402	1/1	0.88	0.31	62,62,62,62	0
56	MG	1A	3374	1/1	0.88	0.37	55,55,55,55	0
56	MG	1a	1767	1/1	0.88	0.12	75,75,75,75	0
56	MG	2A	3039	1/1	0.88	0.28	80,80,80,80	0
56	MG	2a	1707	1/1	0.88	0.09	60,60,60,60	0
56	MG	1A	3957	1/1	0.88	0.15	26,26,26,26	0
56	MG	2a	1710	1/1	0.88	0.20	55,55,55,55	0
56	MG	2a	1711	1/1	0.88	0.22	64,64,64,64	0
56	MG	1A	3274	1/1	0.88	0.24	55,55,55,55	0
56	MG	2A	3418	1/1	0.88	0.18	67,67,67,67	0
56	MG	1A	3341	1/1	0.88	0.22	51,51,51,51	0
56	MG	1N	206	1/1	0.88	0.17	44,44,44,44	0
56	MG	1a	1791	1/1	0.88	0.22	68,68,68,68	0
56	MG	1A	3307	1/1	0.88	0.88	56,56,56,56	0
56	MG	2A	3295	1/1	0.88	0.11	72,72,72,72	0
56	MG	2A	3686	1/1	0.88	0.23	61,61,61,61	0
56	MG	2A	3296	1/1	0.88	0.09	83,83,83,83	0
56	MG	1A	3346	1/1	0.88	0.24	59,59,59,59	0
56	MG	2A	3697	1/1	0.88	0.13	64,64,64,64	0
56	MG	1A	3240	1/1	0.88	0.60	34,34,34,34	0
56	MG	2A	3447	1/1	0.88	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3205	1/1	0.88	0.58	43,43,43,43	0
56	MG	2E	304	1/1	0.88	0.20	34,34,34,34	0
56	MG	1A	3324	1/1	0.88	0.42	60,60,60,60	0
56	MG	2a	1746	1/1	0.88	0.05	77,77,77,77	0
56	MG	1A	3555	1/1	0.88	0.17	27,27,27,27	0
56	MG	1a	1806	1/1	0.88	0.18	53,53,53,53	0
56	MG	1A	4098	1/1	0.88	0.27	60,60,60,60	0
56	MG	1A	3279	1/1	0.88	0.20	42,42,42,42	0
56	MG	2a	1756	1/1	0.88	0.11	65,65,65,65	0
56	MG	2A	3718	1/1	0.88	0.15	63,63,63,63	0
56	MG	2A	3081	1/1	0.88	0.10	86,86,86,86	0
56	MG	1A	3075	1/1	0.88	0.15	44,44,44,44	0
56	MG	1A	3120	1/1	0.88	0.18	49,49,49,49	0
56	MG	2a	1765	1/1	0.88	0.22	65,65,65,65	0
56	MG	2a	1769	1/1	0.88	0.13	72,72,72,72	0
56	MG	1A	4119	1/1	0.88	0.11	39,39,39,39	0
56	MG	2A	3321	1/1	0.88	0.50	74,74,74,74	0
56	MG	1a	1683	1/1	0.88	0.14	48,48,48,48	0
56	MG	1A	4120	1/1	0.88	0.37	49,49,49,49	0
56	MG	1a	1691	1/1	0.88	0.12	54,54,54,54	0
56	MG	27	102	1/1	0.88	0.43	55,55,55,55	0
56	MG	1A	3842	1/1	0.88	0.12	62,62,62,62	0
56	MG	2a	1792	1/1	0.88	0.20	66,66,66,66	0
56	MG	2A	3734	1/1	0.88	0.16	33,33,33,33	0
56	MG	10	103	1/1	0.88	0.30	53,53,53,53	0
56	MG	2A	3098	1/1	0.88	0.36	64,64,64,64	0
56	MG	1A	3479	1/1	0.88	0.37	42,42,42,42	0
56	MG	2a	1808	1/1	0.88	0.09	76,76,76,76	0
56	MG	2a	1607	1/1	0.88	0.19	79,79,79,79	0
56	MG	1A	4017	1/1	0.88	0.12	44,44,44,44	0
56	MG	2a	1818	1/1	0.88	0.08	79,79,79,79	0
56	MG	1A	3133	1/1	0.88	0.32	37,37,37,37	0
56	MG	2A	3120	1/1	0.88	0.33	55,55,55,55	0
56	MG	2A	3528	1/1	0.88	0.16	55,55,55,55	0
56	MG	1A	3587	1/1	0.88	0.11	24,24,24,24	0
56	MG	2a	1614	1/1	0.88	0.24	73,73,73,73	0
56	MG	1A	3777	1/1	0.88	0.13	41,41,41,41	0
56	MG	2A	3551	1/1	0.88	0.17	58,58,58,58	0
56	MG	2A	3560	1/1	0.88	0.22	46,46,46,46	0
56	MG	1A	3661	1/1	0.88	0.15	29,29,29,29	0
56	MG	2A	3147	1/1	0.88	0.19	79,79,79,79	0
56	MG	1A	3173	1/1	0.88	0.08	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1623	1/1	0.88	0.38	71,71,71,71	0
56	MG	2A	3244	1/1	0.88	0.42	62,62,62,62	0
56	MG	2a	1626	1/1	0.88	0.31	87,87,87,87	0
56	MG	2A	3774	1/1	0.88	0.39	63,63,63,63	0
56	MG	1a	1605	1/1	0.88	0.12	65,65,65,65	0
56	MG	2A	3248	1/1	0.88	0.13	70,70,70,70	0
56	MG	1a	1731	1/1	0.88	0.09	80,80,80,80	0
56	MG	2a	1636	1/1	0.88	0.20	55,55,55,55	0
56	MG	2A	3594	1/1	0.88	0.11	63,63,63,63	0
56	MG	1w	102	1/1	0.88	0.12	46,46,46,46	0
56	MG	2A	3597	1/1	0.88	0.38	63,63,63,63	0
56	MG	2A	3599	1/1	0.88	0.42	85,85,85,85	0
56	MG	1A	3401	1/1	0.88	0.14	44,44,44,44	0
56	MG	2a	1645	1/1	0.88	0.11	79,79,79,79	0
56	MG	2A	3603	1/1	0.88	0.20	57,57,57,57	0
56	MG	2a	1648	1/1	0.88	0.12	70,70,70,70	0
56	MG	1A	3406	1/1	0.88	0.69	51,51,51,51	0
56	MG	1B	237	1/1	0.88	0.10	47,47,47,47	0
56	MG	1a	1618	1/1	0.88	0.86	57,57,57,57	0
56	MG	1D	306	1/1	0.88	0.69	48,48,48,48	0
56	MG	2y	102	1/1	0.88	0.35	87,87,87,87	0
56	MG	1A	3865	1/1	0.88	0.39	50,50,50,50	0
56	MG	1A	3055	1/1	0.88	0.24	32,32,32,32	0
56	MG	1A	3776	1/1	0.89	0.09	60,60,60,60	0
56	MG	1A	3069	1/1	0.89	0.23	29,29,29,29	0
56	MG	1A	3136	1/1	0.89	0.36	32,32,32,32	0
56	MG	1a	1745	1/1	0.89	0.07	65,65,65,65	0
56	MG	1A	3350	1/1	0.89	0.16	38,38,38,38	0
56	MG	2A	3440	1/1	0.89	0.24	45,45,45,45	0
56	MG	1a	1747	1/1	0.89	0.22	69,69,69,69	0
56	MG	1A	4052	1/1	0.89	0.21	44,44,44,44	0
56	MG	2A	3253	1/1	0.89	0.10	64,64,64,64	0
56	MG	2A	3736	1/1	0.89	0.19	44,44,44,44	0
56	MG	1A	3354	1/1	0.89	0.20	50,50,50,50	0
56	MG	1A	3025	1/1	0.89	0.20	54,54,54,54	0
56	MG	1A	3486	1/1	0.89	0.17	33,33,33,33	0
56	MG	1A	3234	1/1	0.89	0.14	31,31,31,31	0
56	MG	2A	3749	1/1	0.89	0.21	49,49,49,49	0
56	MG	2A	3751	1/1	0.89	0.10	58,58,58,58	0
56	MG	1A	3305	1/1	0.89	0.65	46,46,46,46	0
56	MG	11	104	1/1	0.89	0.28	43,43,43,43	0
56	MG	1a	1763	1/1	0.89	0.07	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1650	1/1	0.89	0.19	52,52,52,52	0
56	MG	1A	3306	1/1	0.89	0.73	48,48,48,48	0
56	MG	2a	1656	1/1	0.89	0.22	62,62,62,62	0
56	MG	1a	1766	1/1	0.89	0.10	73,73,73,73	0
56	MG	15	103	1/1	0.89	0.36	44,44,44,44	0
56	MG	2A	3102	1/1	0.89	0.12	65,65,65,65	0
56	MG	1A	3204	1/1	0.89	0.35	37,37,37,37	0
56	MG	1A	3309	1/1	0.89	0.53	40,40,40,40	0
56	MG	2A	3117	1/1	0.89	0.11	79,79,79,79	0
56	MG	1A	3931	1/1	0.89	0.08	48,48,48,48	0
56	MG	1a	1601	1/1	0.89	0.36	52,52,52,52	0
56	MG	2A	3776	1/1	0.89	0.18	59,59,59,59	0
56	MG	2A	3778	1/1	0.89	0.12	53,53,53,53	0
56	MG	2A	3138	1/1	0.89	0.26	55,55,55,55	0
56	MG	1A	3499	1/1	0.89	0.15	28,28,28,28	0
56	MG	2A	3514	1/1	0.89	0.27	63,63,63,63	0
56	MG	2A	3285	1/1	0.89	0.18	65,65,65,65	0
56	MG	2A	3787	1/1	0.89	0.14	83,83,83,83	0
56	MG	1A	3503	1/1	0.89	0.20	27,27,27,27	0
56	MG	1A	3310	1/1	0.89	0.10	47,47,47,47	0
56	MG	2A	3791	1/1	0.89	0.20	69,69,69,69	0
56	MG	1A	3937	1/1	0.89	0.09	50,50,50,50	0
56	MG	1A	3124	1/1	0.89	0.60	41,41,41,41	0
56	MG	2A	3800	1/1	0.89	0.07	59,59,59,59	0
56	MG	2A	3802	1/1	0.89	0.36	67,67,67,67	0
56	MG	1A	3270	1/1	0.89	0.28	51,51,51,51	0
56	MG	2A	3533	1/1	0.89	0.17	47,47,47,47	0
56	MG	1A	3272	1/1	0.89	0.14	57,57,57,57	0
56	MG	1A	3671	1/1	0.89	0.11	64,64,64,64	0
56	MG	2A	3300	1/1	0.89	0.15	73,73,73,73	0
56	MG	1A	4118	1/1	0.89	0.28	36,36,36,36	0
56	MG	2A	3564	1/1	0.89	0.16	64,64,64,64	0
56	MG	2A	3823	1/1	0.89	0.15	54,54,54,54	0
56	MG	1A	3181	1/1	0.89	0.19	49,49,49,49	0
56	MG	2A	3826	1/1	0.89	0.18	58,58,58,58	0
56	MG	2a	1724	1/1	0.89	0.12	86,86,86,86	0
56	MG	2A	3827	1/1	0.89	0.36	66,66,66,66	0
56	MG	2A	3577	1/1	0.89	0.26	67,67,67,67	0
56	MG	2A	3829	1/1	0.89	0.17	66,66,66,66	0
56	MG	1A	3098	1/1	0.89	0.20	35,35,35,35	0
56	MG	2a	1732	1/1	0.89	0.22	75,75,75,75	0
56	MG	2A	3831	1/1	0.89	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3833	1/1	0.89	0.07	58,58,58,58	0
56	MG	2A	3582	1/1	0.89	0.28	67,67,67,67	0
56	MG	1A	4122	1/1	0.89	0.16	47,47,47,47	0
56	MG	1A	3953	1/1	0.89	0.17	55,55,55,55	0
56	MG	1A	3380	1/1	0.89	0.26	52,52,52,52	0
56	MG	1A	4132	1/1	0.89	0.12	38,38,38,38	0
56	MG	1A	3686	1/1	0.89	0.19	74,74,74,74	0
56	MG	1a	1835	1/1	0.89	0.11	73,73,73,73	0
56	MG	1A	3846	1/1	0.89	0.10	54,54,54,54	0
56	MG	1a	1649	1/1	0.89	0.73	51,51,51,51	0
56	MG	1A	3278	1/1	0.89	0.74	52,52,52,52	0
56	MG	1A	3568	1/1	0.89	0.18	21,21,21,21	0
56	MG	2A	3179	1/1	0.89	0.28	64,64,64,64	0
56	MG	2A	3868	1/1	0.89	0.20	68,68,68,68	0
56	MG	1h	201	1/1	0.89	0.20	58,58,58,58	0
56	MG	1A	3704	1/1	0.89	0.28	53,53,53,53	0
56	MG	1A	3447	1/1	0.89	0.10	62,62,62,62	0
56	MG	1A	3978	1/1	0.89	0.10	51,51,51,51	0
56	MG	1A	3210	1/1	0.89	0.12	43,43,43,43	0
56	MG	1A	3183	1/1	0.89	0.26	41,41,41,41	0
56	MG	1A	3860	1/1	0.89	0.16	55,55,55,55	0
56	MG	1A	3728	1/1	0.89	0.16	59,59,59,59	0
56	MG	1A	3990	1/1	0.89	0.10	62,62,62,62	0
56	MG	2a	1789	1/1	0.89	0.12	73,73,73,73	0
56	MG	1A	3284	1/1	0.89	0.12	38,38,38,38	0
56	MG	2B	215	1/1	0.89	0.16	84,84,84,84	0
56	MG	2a	1793	1/1	0.89	0.17	75,75,75,75	0
56	MG	2B	218	1/1	0.89	0.09	82,82,82,82	0
56	MG	1A	3287	1/1	0.89	0.12	60,60,60,60	0
56	MG	2A	3639	1/1	0.89	0.07	62,62,62,62	0
56	MG	2D	305	1/1	0.89	0.52	42,42,42,42	0
56	MG	1A	3996	1/1	0.89	0.27	60,60,60,60	0
56	MG	2A	3204	1/1	0.89	0.54	59,59,59,59	0
56	MG	1a	1690	1/1	0.89	0.09	64,64,64,64	0
56	MG	2a	1815	1/1	0.89	0.17	75,75,75,75	0
56	MG	1A	3592	1/1	0.89	0.17	20,20,20,20	0
56	MG	2A	3208	1/1	0.89	0.53	69,69,69,69	0
56	MG	1A	4012	1/1	0.89	0.22	45,45,45,45	0
56	MG	2a	1821	1/1	0.89	0.21	95,95,95,95	0
56	MG	1x	114	1/1	0.89	0.29	68,68,68,68	0
56	MG	1A	4014	1/1	0.89	0.17	54,54,54,54	0
56	MG	1A	3395	1/1	0.89	0.14	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1825	1/1	0.89	0.14	53,53,53,53	0
56	MG	2a	1827	1/1	0.89	0.18	77,77,77,77	0
56	MG	2A	3003	1/1	0.89	0.09	57,57,57,57	0
56	MG	1a	1698	1/1	0.89	0.09	52,52,52,52	0
56	MG	1G	203	1/1	0.89	0.10	67,67,67,67	0
56	MG	2A	3221	1/1	0.89	0.09	69,69,69,69	0
56	MG	2A	3671	1/1	0.89	0.20	56,56,56,56	0
56	MG	2A	3014	1/1	0.89	0.34	52,52,52,52	0
56	MG	2X	102	1/1	0.89	0.21	68,68,68,68	0
56	MG	1G	205	1/1	0.89	0.23	66,66,66,66	0
56	MG	2d	301	1/1	0.89	0.13	73,73,73,73	0
56	MG	2f	201	1/1	0.89	0.18	51,51,51,51	0
56	MG	1a	1706	1/1	0.89	0.13	55,55,55,55	0
56	MG	20	102	1/1	0.89	0.21	68,68,68,68	0
56	MG	1a	1708	1/1	0.89	0.08	57,57,57,57	0
56	MG	2A	3028	1/1	0.89	0.39	49,49,49,49	0
56	MG	26	101	1/1	0.89	0.57	68,68,68,68	0
56	MG	2A	3687	1/1	0.89	0.09	70,70,70,70	0
56	MG	2A	3688	1/1	0.89	0.07	63,63,63,63	0
56	MG	2v	101	1/1	0.89	0.14	64,64,64,64	0
56	MG	2A	3030	1/1	0.89	0.23	53,53,53,53	0
56	MG	2A	3692	1/1	0.89	0.12	71,71,71,71	0
56	MG	2A	3391	1/1	0.89	0.58	57,57,57,57	0
56	MG	1A	3223	1/1	0.89	0.14	55,55,55,55	0
56	MG	1A	3398	1/1	0.89	0.42	40,40,40,40	0
56	MG	2A	3040	1/1	0.89	0.28	61,61,61,61	0
56	MG	1a	1721	1/1	0.89	0.33	72,72,72,72	0
56	MG	1a	1722	1/1	0.89	0.10	64,64,64,64	0
56	MG	1A	3607	1/1	0.89	0.18	51,51,51,51	0
56	MG	1A	3086	1/1	0.89	0.39	35,35,35,35	0
56	MG	1A	4032	1/1	0.89	0.17	61,61,61,61	0
56	MG	1A	3613	1/1	0.89	0.13	51,51,51,51	0
56	MG	1A	3294	1/1	0.89	0.17	45,45,45,45	0
56	MG	2y	104	1/1	0.89	0.63	79,79,79,79	0
56	MG	2A	3420	1/1	0.89	0.13	65,65,65,65	0
58	Y7K	2a	1841	33/33	0.89	0.23	75,81,88,93	0
56	MG	1A	3694	1/1	0.90	0.15	35,35,35,35	0
56	MG	1A	3944	1/1	0.90	0.14	43,43,43,43	0
56	MG	2A	3390	1/1	0.90	0.12	57,57,57,57	0
56	MG	1A	4082	1/1	0.90	0.14	50,50,50,50	0
56	MG	1A	3329	1/1	0.90	0.46	41,41,41,41	0
56	MG	2A	3036	1/1	0.90	0.59	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3225	1/1	0.90	0.31	62,62,62,62	0
56	MG	1A	3052	1/1	0.90	0.24	52,52,52,52	0
56	MG	1A	3597	1/1	0.90	0.13	20,20,20,20	0
56	MG	2A	3041	1/1	0.90	0.11	57,57,57,57	0
56	MG	1A	3151	1/1	0.90	0.17	35,35,35,35	0
56	MG	1A	3710	1/1	0.90	0.18	59,59,59,59	0
56	MG	16	101	1/1	0.90	0.29	44,44,44,44	0
56	MG	1A	3054	1/1	0.90	0.07	49,49,49,49	0
56	MG	2A	3419	1/1	0.90	0.26	65,65,65,65	0
56	MG	2a	1635	1/1	0.90	0.21	65,65,65,65	0
56	MG	1A	3158	1/1	0.90	0.21	60,60,60,60	0
56	MG	2A	3739	1/1	0.90	0.16	45,45,45,45	0
56	MG	18	107	1/1	0.90	0.20	46,46,46,46	0
56	MG	1A	3165	1/1	0.90	0.47	36,36,36,36	0
56	MG	1a	1760	1/1	0.90	0.08	75,75,75,75	0
56	MG	2A	3066	1/1	0.90	0.12	52,52,52,52	0
56	MG	2A	3436	1/1	0.90	0.08	68,68,68,68	0
56	MG	1A	3337	1/1	0.90	0.39	39,39,39,39	0
56	MG	2A	3069	1/1	0.90	0.30	46,46,46,46	0
56	MG	1A	3381	1/1	0.90	0.29	42,42,42,42	0
56	MG	2a	1651	1/1	0.90	0.13	72,72,72,72	0
56	MG	1A	3965	1/1	0.90	0.05	39,39,39,39	0
56	MG	2A	3245	1/1	0.90	0.15	58,58,58,58	0
56	MG	2a	1659	1/1	0.90	0.10	66,66,66,66	0
56	MG	2A	3075	1/1	0.90	0.17	53,53,53,53	0
56	MG	1A	3855	1/1	0.90	0.10	39,39,39,39	0
56	MG	2a	1664	1/1	0.90	0.35	61,61,61,61	0
56	MG	1A	3260	1/1	0.90	0.29	47,47,47,47	0
56	MG	1A	3171	1/1	0.90	0.12	38,38,38,38	0
56	MG	2a	1670	1/1	0.90	0.24	71,71,71,71	0
56	MG	1a	1779	1/1	0.90	0.15	52,52,52,52	0
56	MG	2A	3083	1/1	0.90	0.44	44,44,44,44	0
56	MG	1a	1780	1/1	0.90	0.15	60,60,60,60	0
56	MG	1A	3620	1/1	0.90	0.18	55,55,55,55	0
56	MG	1A	4133	1/1	0.90	0.27	55,55,55,55	0
56	MG	2A	3777	1/1	0.90	0.51	63,63,63,63	0
56	MG	2A	3485	1/1	0.90	0.20	44,44,44,44	0
56	MG	1A	3436	1/1	0.90	0.15	79,79,79,79	0
56	MG	1A	3092	1/1	0.90	0.20	43,43,43,43	0
56	MG	1a	1627	1/1	0.90	0.15	62,62,62,62	0
56	MG	1B	205	1/1	0.90	0.16	51,51,51,51	0
56	MG	1A	3070	1/1	0.90	0.19	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	209	1/1	0.90	0.26	61,61,61,61	0
56	MG	1a	1802	1/1	0.90	0.13	51,51,51,51	0
56	MG	2A	3105	1/1	0.90	0.25	48,48,48,48	0
56	MG	2A	3792	1/1	0.90	0.37	62,62,62,62	0
56	MG	1a	1803	1/1	0.90	0.09	66,66,66,66	0
56	MG	2A	3510	1/1	0.90	0.13	54,54,54,54	0
56	MG	2A	3272	1/1	0.90	0.18	56,56,56,56	0
56	MG	2A	3273	1/1	0.90	0.57	70,70,70,70	0
56	MG	2A	3115	1/1	0.90	0.23	52,52,52,52	0
56	MG	2A	3805	1/1	0.90	0.07	73,73,73,73	0
56	MG	2A	3806	1/1	0.90	0.36	67,67,67,67	0
56	MG	2A	3275	1/1	0.90	0.16	64,64,64,64	0
56	MG	1a	1804	1/1	0.90	0.26	62,62,62,62	0
56	MG	2A	3525	1/1	0.90	0.18	61,61,61,61	0
56	MG	2A	3818	1/1	0.90	0.27	74,74,74,74	0
56	MG	1A	3869	1/1	0.90	0.17	58,58,58,58	0
56	MG	2A	3531	1/1	0.90	0.18	30,30,30,30	0
56	MG	2A	3119	1/1	0.90	0.43	46,46,46,46	0
56	MG	1A	3509	1/1	0.90	0.16	46,46,46,46	0
56	MG	1B	222	1/1	0.90	0.14	38,38,38,38	0
56	MG	2A	3128	1/1	0.90	0.17	45,45,45,45	0
56	MG	2A	3554	1/1	0.90	0.15	53,53,53,53	0
56	MG	1a	1810	1/1	0.90	0.15	65,65,65,65	0
56	MG	2A	3287	1/1	0.90	0.32	71,71,71,71	0
56	MG	2A	3140	1/1	0.90	0.12	63,63,63,63	0
56	MG	2A	3567	1/1	0.90	0.17	68,68,68,68	0
56	MG	1A	3769	1/1	0.90	0.31	41,41,41,41	0
56	MG	2A	3835	1/1	0.90	0.12	75,75,75,75	0
56	MG	2A	3839	1/1	0.90	0.09	77,77,77,77	0
56	MG	2a	1747	1/1	0.90	0.13	70,70,70,70	0
56	MG	1a	1817	1/1	0.90	0.11	84,84,84,84	0
56	MG	1A	3872	1/1	0.90	0.11	35,35,35,35	0
56	MG	1B	227	1/1	0.90	0.16	62,62,62,62	0
56	MG	2A	3583	1/1	0.90	0.17	39,39,39,39	0
56	MG	2a	1753	1/1	0.90	0.19	62,62,62,62	0
56	MG	1A	3995	1/1	0.90	0.14	56,56,56,56	0
56	MG	2A	3150	1/1	0.90	0.30	63,63,63,63	0
56	MG	1B	232	1/1	0.90	0.26	52,52,52,52	0
56	MG	2a	1762	1/1	0.90	0.20	77,77,77,77	0
56	MG	2A	3858	1/1	0.90	0.17	64,64,64,64	0
56	MG	1A	3772	1/1	0.90	0.32	31,31,31,31	0
56	MG	2A	3304	1/1	0.90	0.25	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3863	1/1	0.90	0.09	74,74,74,74	0
56	MG	2A	3864	1/1	0.90	0.10	67,67,67,67	0
56	MG	1A	3019	1/1	0.90	0.16	42,42,42,42	0
56	MG	1A	3876	1/1	0.90	0.14	62,62,62,62	0
56	MG	2a	1778	1/1	0.90	0.12	79,79,79,79	0
56	MG	2A	3308	1/1	0.90	0.28	64,64,64,64	0
56	MG	1A	3128	1/1	0.90	0.41	42,42,42,42	0
56	MG	1A	3878	1/1	0.90	0.17	67,67,67,67	0
56	MG	2a	1787	1/1	0.90	0.07	80,80,80,80	0
56	MG	2A	3606	1/1	0.90	0.32	69,69,69,69	0
56	MG	2A	3875	1/1	0.90	0.15	42,42,42,42	0
56	MG	1E	302	1/1	0.90	0.56	42,42,42,42	0
56	MG	1e	201	1/1	0.90	0.09	72,72,72,72	0
56	MG	2A	3883	1/1	0.90	0.18	57,57,57,57	0
56	MG	2A	3315	1/1	0.90	0.28	69,69,69,69	0
56	MG	2a	1804	1/1	0.90	0.18	78,78,78,78	0
56	MG	1a	1669	1/1	0.90	0.49	61,61,61,61	0
56	MG	1E	309	1/1	0.90	0.26	62,62,62,62	0
56	MG	2B	205	1/1	0.90	0.16	60,60,60,60	0
56	MG	2B	207	1/1	0.90	0.12	59,59,59,59	0
56	MG	2A	3318	1/1	0.90	0.23	74,74,74,74	0
56	MG	2A	3171	1/1	0.90	0.44	49,49,49,49	0
56	MG	1A	3527	1/1	0.90	0.15	28,28,28,28	0
56	MG	1a	1673	1/1	0.90	0.08	68,68,68,68	0
56	MG	2A	3629	1/1	0.90	0.16	28,28,28,28	0
56	MG	2B	219	1/1	0.90	0.20	77,77,77,77	0
56	MG	2D	301	1/1	0.90	0.20	55,55,55,55	0
56	MG	2A	3322	1/1	0.90	0.31	66,66,66,66	0
56	MG	1A	3449	1/1	0.90	0.30	55,55,55,55	0
56	MG	1A	3073	1/1	0.90	0.52	29,29,29,29	0
56	MG	1F	309	1/1	0.90	0.10	47,47,47,47	0
56	MG	1A	3650	1/1	0.90	0.05	42,42,42,42	0
56	MG	1A	3351	1/1	0.90	1.43	56,56,56,56	0
56	MG	2A	3182	1/1	0.90	0.08	55,55,55,55	0
56	MG	1A	3135	1/1	0.90	0.17	36,36,36,36	0
56	MG	1w	106	1/1	0.90	0.16	63,63,63,63	0
56	MG	2F	302	1/1	0.90	0.39	61,61,61,61	0
56	MG	1A	3104	1/1	0.90	0.17	51,51,51,51	0
56	MG	1A	3138	1/1	0.90	0.33	58,58,58,58	0
56	MG	1A	3802	1/1	0.90	0.39	25,25,25,25	0
56	MG	1A	3322	1/1	0.90	0.62	41,41,41,41	0
56	MG	2O	202	1/1	0.90	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1x	103	1/1	0.90	0.17	66,66,66,66	0
56	MG	1A	3664	1/1	0.90	0.16	32,32,32,32	0
56	MG	2A	3668	1/1	0.90	0.19	74,74,74,74	0
56	MG	1x	107	1/1	0.90	0.16	82,82,82,82	0
56	MG	1A	3579	1/1	0.90	0.08	40,40,40,40	0
56	MG	1A	3111	1/1	0.90	0.39	41,41,41,41	0
56	MG	2A	3200	1/1	0.90	0.20	46,46,46,46	0
56	MG	2A	3201	1/1	0.90	0.42	45,45,45,45	0
56	MG	2w	102	1/1	0.90	0.66	80,80,80,80	0
56	MG	2A	3680	1/1	0.90	0.19	55,55,55,55	0
56	MG	1A	3190	1/1	0.90	0.26	38,38,38,38	0
56	MG	1a	1719	1/1	0.90	0.13	67,67,67,67	0
56	MG	1A	3818	1/1	0.90	0.20	37,37,37,37	0
56	MG	1T	203	1/1	0.90	0.27	53,53,53,53	0
56	MG	1A	4071	1/1	0.90	0.13	58,58,58,58	0
56	MG	2A	3369	1/1	0.90	0.55	62,62,62,62	0
56	MG	2x	102	1/1	0.90	0.17	62,62,62,62	0
56	MG	1A	3413	1/1	0.90	0.12	44,44,44,44	0
56	MG	2A	3374	1/1	0.90	0.35	71,71,71,71	0
56	MG	1A	3004	1/1	0.90	0.13	30,30,30,30	0
56	MG	2A	3211	1/1	0.90	0.71	63,63,63,63	0
56	MG	1A	3590	1/1	0.90	0.18	44,44,44,44	0
56	MG	2A	3213	1/1	0.90	0.34	66,66,66,66	0
56	MG	1A	3693	1/1	0.90	0.15	18,18,18,18	0
56	MG	2A	3709	1/1	0.90	0.22	88,88,88,88	0
56	MG	2A	3005	1/1	0.91	0.21	60,60,60,60	0
56	MG	1a	1705	1/1	0.91	0.16	62,62,62,62	0
56	MG	1A	3438	1/1	0.91	0.17	62,62,62,62	0
56	MG	1A	3440	1/1	0.91	0.17	34,34,34,34	0
56	MG	2A	3019	1/1	0.91	0.06	70,70,70,70	0
56	MG	1a	1713	1/1	0.91	0.09	57,57,57,57	0
56	MG	2A	3410	1/1	0.91	0.20	38,38,38,38	0
56	MG	2A	3222	1/1	0.91	0.56	62,62,62,62	0
56	MG	1a	1715	1/1	0.91	0.16	71,71,71,71	0
56	MG	2A	3026	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	3641	1/1	0.91	0.32	65,65,65,65	0
56	MG	1A	3397	1/1	0.91	0.25	41,41,41,41	0
56	MG	1A	3162	1/1	0.91	0.08	42,42,42,42	0
56	MG	1A	4037	1/1	0.91	0.08	39,39,39,39	0
56	MG	2A	3035	1/1	0.91	0.29	62,62,62,62	0
56	MG	2A	3430	1/1	0.91	0.17	32,32,32,32	0
56	MG	2A	3745	1/1	0.91	0.24	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1N	201	1/1	0.91	0.16	55,55,55,55	0
56	MG	2A	3038	1/1	0.91	0.11	57,57,57,57	0
56	MG	1N	203	1/1	0.91	0.24	42,42,42,42	0
56	MG	2a	1641	1/1	0.91	0.10	94,94,94,94	0
56	MG	1A	3533	1/1	0.91	0.15	39,39,39,39	0
56	MG	2a	1643	1/1	0.91	0.17	58,58,58,58	0
56	MG	2A	3752	1/1	0.91	0.17	48,48,48,48	0
56	MG	1A	3534	1/1	0.91	0.14	36,36,36,36	0
56	MG	1A	3303	1/1	0.91	0.17	40,40,40,40	0
56	MG	1P	204	1/1	0.91	0.52	35,35,35,35	0
56	MG	2A	3046	1/1	0.91	0.14	56,56,56,56	0
56	MG	2A	3047	1/1	0.91	0.19	65,65,65,65	0
56	MG	2A	3053	1/1	0.91	0.09	58,58,58,58	0
56	MG	2A	3056	1/1	0.91	0.16	74,74,74,74	0
56	MG	2A	3456	1/1	0.91	0.31	60,60,60,60	0
56	MG	2A	3461	1/1	0.91	0.21	31,31,31,31	0
56	MG	1A	3400	1/1	0.91	0.33	53,53,53,53	0
56	MG	1A	3195	1/1	0.91	0.18	46,46,46,46	0
56	MG	1a	1741	1/1	0.91	0.12	60,60,60,60	0
56	MG	2a	1666	1/1	0.91	0.22	72,72,72,72	0
56	MG	2A	3476	1/1	0.91	0.25	43,43,43,43	0
56	MG	2A	3478	1/1	0.91	0.18	23,23,23,23	0
56	MG	1A	3403	1/1	0.91	0.33	49,49,49,49	0
56	MG	2a	1673	1/1	0.91	0.36	67,67,67,67	0
56	MG	1T	201	1/1	0.91	0.16	43,43,43,43	0
56	MG	1A	3662	1/1	0.91	0.24	24,24,24,24	0
56	MG	2A	3065	1/1	0.91	0.12	60,60,60,60	0
56	MG	1A	4065	1/1	0.91	0.26	73,73,73,73	0
56	MG	1A	4067	1/1	0.91	0.12	51,51,51,51	0
56	MG	1V	202	1/1	0.91	0.33	42,42,42,42	0
56	MG	2A	3493	1/1	0.91	0.28	48,48,48,48	0
56	MG	1A	4068	1/1	0.91	0.08	49,49,49,49	0
56	MG	2A	3495	1/1	0.91	0.08	36,36,36,36	0
56	MG	2A	3793	1/1	0.91	0.10	71,71,71,71	0
56	MG	1A	3366	1/1	0.91	0.29	38,38,38,38	0
56	MG	1W	202	1/1	0.91	0.23	39,39,39,39	0
56	MG	1A	3558	1/1	0.91	0.10	44,44,44,44	0
56	MG	1A	3248	1/1	0.91	0.47	60,60,60,60	0
56	MG	1A	4075	1/1	0.91	0.15	53,53,53,53	0
56	MG	1a	1762	1/1	0.91	0.08	68,68,68,68	0
56	MG	2a	1705	1/1	0.91	0.07	71,71,71,71	0
56	MG	1A	3215	1/1	0.91	0.16	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3807	1/1	0.91	0.18	59,59,59,59	0
56	MG	1A	3675	1/1	0.91	0.11	39,39,39,39	0
56	MG	1A	3824	1/1	0.91	0.17	42,42,42,42	0
56	MG	11	103	1/1	0.91	0.14	58,58,58,58	0
56	MG	1a	1768	1/1	0.91	0.12	62,62,62,62	0
56	MG	1a	1770	1/1	0.91	0.08	51,51,51,51	0
56	MG	1A	3283	1/1	0.91	0.34	36,36,36,36	0
56	MG	1A	3942	1/1	0.91	0.17	41,41,41,41	0
56	MG	1A	3231	1/1	0.91	0.15	36,36,36,36	0
56	MG	1a	1781	1/1	0.91	0.15	63,63,63,63	0
56	MG	1A	4087	1/1	0.91	0.11	55,55,55,55	0
56	MG	1A	3217	1/1	0.91	0.17	48,48,48,48	0
56	MG	2A	3555	1/1	0.91	0.09	30,30,30,30	0
56	MG	1A	3416	1/1	0.91	0.19	42,42,42,42	0
56	MG	2A	3112	1/1	0.91	0.12	50,50,50,50	0
56	MG	2a	1731	1/1	0.91	0.10	82,82,82,82	0
56	MG	2A	3288	1/1	0.91	0.83	63,63,63,63	0
56	MG	2A	3289	1/1	0.91	0.24	57,57,57,57	0
56	MG	1A	3474	1/1	0.91	0.16	69,69,69,69	0
56	MG	2a	1736	1/1	0.91	0.10	78,78,78,78	0
56	MG	1A	3342	1/1	0.91	0.20	71,71,71,71	0
56	MG	2A	3843	1/1	0.91	0.09	67,67,67,67	0
56	MG	1a	1795	1/1	0.91	0.17	79,79,79,79	0
56	MG	1a	1797	1/1	0.91	0.07	43,43,43,43	0
56	MG	2A	3294	1/1	0.91	0.07	75,75,75,75	0
56	MG	1A	3291	1/1	0.91	0.15	51,51,51,51	0
56	MG	2A	3853	1/1	0.91	0.21	52,52,52,52	0
56	MG	1A	4107	1/1	0.91	0.27	63,63,63,63	0
56	MG	1a	1604	1/1	0.91	0.10	59,59,59,59	0
56	MG	2A	3298	1/1	0.91	0.21	55,55,55,55	0
56	MG	2A	3592	1/1	0.91	0.17	48,48,48,48	0
56	MG	1A	4109	1/1	0.91	0.13	63,63,63,63	0
56	MG	2A	3301	1/1	0.91	0.28	57,57,57,57	0
56	MG	2a	1759	1/1	0.91	0.17	66,66,66,66	0
56	MG	1A	4113	1/1	0.91	0.08	43,43,43,43	0
56	MG	2a	1761	1/1	0.91	0.14	66,66,66,66	0
56	MG	1A	3222	1/1	0.91	0.22	56,56,56,56	0
56	MG	1A	3845	1/1	0.91	0.16	79,79,79,79	0
56	MG	1A	3698	1/1	0.91	0.16	56,56,56,56	0
56	MG	1a	1807	1/1	0.91	0.13	81,81,81,81	0
56	MG	1A	3271	1/1	0.91	0.18	44,44,44,44	0
56	MG	1A	3959	1/1	0.91	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3482	1/1	0.91	0.82	38,38,38,38	0
56	MG	1A	3963	1/1	0.91	0.09	43,43,43,43	0
56	MG	2A	3876	1/1	0.91	0.32	62,62,62,62	0
56	MG	2A	3616	1/1	0.91	0.15	69,69,69,69	0
56	MG	2A	3879	1/1	0.91	0.16	58,58,58,58	0
56	MG	1A	4129	1/1	0.91	0.18	61,61,61,61	0
56	MG	1A	3174	1/1	0.91	0.29	34,34,34,34	0
56	MG	2A	3623	1/1	0.91	0.09	36,36,36,36	0
56	MG	2A	3885	1/1	0.91	0.48	65,65,65,65	0
56	MG	1A	3604	1/1	0.91	0.17	43,43,43,43	0
56	MG	2A	3160	1/1	0.91	0.30	65,65,65,65	0
56	MG	1A	3972	1/1	0.91	0.11	46,46,46,46	0
56	MG	2B	206	1/1	0.91	0.12	69,69,69,69	0
56	MG	1a	1638	1/1	0.91	0.14	58,58,58,58	0
56	MG	1a	1827	1/1	0.91	0.16	75,75,75,75	0
56	MG	2A	3633	1/1	0.91	0.31	68,68,68,68	0
56	MG	2A	3167	1/1	0.91	0.50	64,64,64,64	0
56	MG	2a	1809	1/1	0.91	0.14	74,74,74,74	0
56	MG	1A	3606	1/1	0.91	0.19	60,60,60,60	0
56	MG	2A	3169	1/1	0.91	0.29	64,64,64,64	0
56	MG	1A	3426	1/1	0.91	0.29	30,30,30,30	0
56	MG	2a	1816	1/1	0.91	0.06	68,68,68,68	0
56	MG	2B	220	1/1	0.91	0.07	68,68,68,68	0
56	MG	1A	3488	1/1	0.91	0.20	53,53,53,53	0
56	MG	1a	1838	1/1	0.91	0.10	62,62,62,62	0
56	MG	1a	1839	1/1	0.91	0.46	57,57,57,57	0
56	MG	1A	3857	1/1	0.91	0.12	24,24,24,24	0
56	MG	1a	1648	1/1	0.91	0.08	69,69,69,69	0
56	MG	1B	207	1/1	0.91	0.32	61,61,61,61	0
56	MG	1A	3429	1/1	0.91	0.22	31,31,31,31	0
56	MG	2E	302	1/1	0.91	0.21	47,47,47,47	0
56	MG	1A	3986	1/1	0.91	0.23	52,52,52,52	0
56	MG	2A	3181	1/1	0.91	0.24	69,69,69,69	0
56	MG	2E	305	1/1	0.91	0.14	60,60,60,60	0
56	MG	1a	1655	1/1	0.91	0.21	71,71,71,71	0
56	MG	2A	3183	1/1	0.91	0.14	61,61,61,61	0
56	MG	1A	3327	1/1	0.91	0.41	40,40,40,40	0
56	MG	1A	3244	1/1	0.91	0.11	53,53,53,53	0
56	MG	1A	3353	1/1	0.91	0.16	63,63,63,63	0
56	MG	2A	3187	1/1	0.91	0.39	48,48,48,48	0
56	MG	2d	302	1/1	0.91	0.25	65,65,65,65	0
56	MG	1s	101	1/1	0.91	0.09	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	3275	1/1	0.91	0.15	53,53,53,53	0
56	MG	2A	3681	1/1	0.91	0.27	63,63,63,63	0
56	MG	1A	3749	1/1	0.91	0.10	62,62,62,62	0
56	MG	2l	203	1/1	0.91	0.20	68,68,68,68	0
56	MG	2l	204	1/1	0.91	0.07	68,68,68,68	0
56	MG	1A	3356	1/1	0.91	0.34	53,53,53,53	0
56	MG	2p	101	1/1	0.91	0.16	60,60,60,60	0
56	MG	1A	3624	1/1	0.91	0.17	53,53,53,53	0
56	MG	1B	233	1/1	0.91	0.15	67,67,67,67	0
56	MG	1B	235	1/1	0.91	0.16	65,65,65,65	0
56	MG	1A	3763	1/1	0.91	0.15	43,43,43,43	0
56	MG	20	101	1/1	0.91	0.21	56,56,56,56	0
56	MG	1A	4000	1/1	0.91	0.21	46,46,46,46	0
56	MG	1A	4009	1/1	0.91	0.17	60,60,60,60	0
56	MG	23	102	1/1	0.91	0.20	64,64,64,64	0
56	MG	2A	3695	1/1	0.91	0.20	63,63,63,63	0
56	MG	1A	3765	1/1	0.91	0.22	41,41,41,41	0
56	MG	27	101	1/1	0.91	0.26	39,39,39,39	0
56	MG	1A	3626	1/1	0.91	0.18	24,24,24,24	0
56	MG	2A	3701	1/1	0.91	0.11	50,50,50,50	0
56	MG	1A	3330	1/1	0.91	0.20	48,48,48,48	0
56	MG	1A	3771	1/1	0.91	0.61	35,35,35,35	0
56	MG	2x	105	1/1	0.91	0.14	71,71,71,71	0
56	MG	1A	3362	1/1	0.91	0.39	59,59,59,59	0
56	MG	2A	3708	1/1	0.91	0.14	55,55,55,55	0
56	MG	1A	4020	1/1	0.91	0.37	44,44,44,44	0
56	MG	1F	304	1/1	0.91	0.14	33,33,33,33	0
56	MG	1A	3508	1/1	0.91	0.17	43,43,43,43	0
56	MG	2y	106	1/1	0.91	0.18	89,89,89,89	0
56	MG	2A	3712	1/1	0.91	0.20	56,56,56,56	0
56	MG	1A	4025	1/1	0.91	0.13	33,33,33,33	0
56	MG	1A	3249	1/1	0.92	0.18	51,51,51,51	0
56	MG	2A	3015	1/1	0.92	0.17	33,33,33,33	0
56	MG	2A	3399	1/1	0.92	0.45	65,65,65,65	0
56	MG	1A	3762	1/1	0.92	0.12	32,32,32,32	0
56	MG	2A	3713	1/1	0.92	0.15	54,54,54,54	0
56	MG	1A	3339	1/1	0.92	0.24	37,37,37,37	0
56	MG	2A	3715	1/1	0.92	0.20	70,70,70,70	0
56	MG	2A	3406	1/1	0.92	0.30	59,59,59,59	0
56	MG	2A	3214	1/1	0.92	0.11	61,61,61,61	0
56	MG	1A	3018	1/1	0.92	0.18	29,29,29,29	0
56	MG	1A	3029	1/1	0.92	0.27	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3152	1/1	0.92	0.30	46,46,46,46	0
56	MG	1A	4033	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	3770	1/1	0.92	0.49	47,47,47,47	0
56	MG	2a	1629	1/1	0.92	0.18	75,75,75,75	0
56	MG	1A	3213	1/1	0.92	0.19	39,39,39,39	0
56	MG	1A	3084	1/1	0.92	0.09	67,67,67,67	0
56	MG	1A	3885	1/1	0.92	0.21	25,25,25,25	0
56	MG	2A	3731	1/1	0.92	0.11	39,39,39,39	0
56	MG	2A	3425	1/1	0.92	0.17	58,58,58,58	0
56	MG	1A	3630	1/1	0.92	0.30	68,68,68,68	0
56	MG	2A	3735	1/1	0.92	0.19	54,54,54,54	0
56	MG	1A	4041	1/1	0.92	0.26	50,50,50,50	0
56	MG	2A	3429	1/1	0.92	0.11	74,74,74,74	0
56	MG	1P	205	1/1	0.92	0.51	47,47,47,47	0
56	MG	1A	4045	1/1	0.92	0.09	49,49,49,49	0
56	MG	2A	3743	1/1	0.92	0.10	47,47,47,47	0
56	MG	2A	3043	1/1	0.92	0.39	64,64,64,64	0
56	MG	2A	3438	1/1	0.92	0.15	58,58,58,58	0
56	MG	1R	203	1/1	0.92	0.13	44,44,44,44	0
56	MG	1A	3525	1/1	0.92	0.13	35,35,35,35	0
56	MG	2A	3441	1/1	0.92	0.15	64,64,64,64	0
56	MG	1A	3892	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	3157	1/1	0.92	0.28	38,38,38,38	0
56	MG	2a	1655	1/1	0.92	0.12	67,67,67,67	0
56	MG	2A	3445	1/1	0.92	0.28	51,51,51,51	0
56	MG	2a	1657	1/1	0.92	0.19	51,51,51,51	0
56	MG	2A	3049	1/1	0.92	0.25	69,69,69,69	0
56	MG	2A	3050	1/1	0.92	0.26	61,61,61,61	0
56	MG	2a	1661	1/1	0.92	0.15	61,61,61,61	0
56	MG	2A	3761	1/1	0.92	0.14	56,56,56,56	0
56	MG	1A	3530	1/1	0.92	0.17	23,23,23,23	0
56	MG	2A	3054	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3903	1/1	0.92	0.13	30,30,30,30	0
56	MG	1A	3110	1/1	0.92	0.22	77,77,77,77	0
56	MG	2A	3460	1/1	0.92	0.10	58,58,58,58	0
56	MG	1a	1750	1/1	0.92	0.15	63,63,63,63	0
56	MG	1A	3913	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	3220	1/1	0.92	0.20	60,60,60,60	0
56	MG	1A	3915	1/1	0.92	0.23	66,66,66,66	0
56	MG	2A	3471	1/1	0.92	0.27	34,34,34,34	0
56	MG	2A	3474	1/1	0.92	0.10	43,43,43,43	0
56	MG	1V	207	1/1	0.92	0.20	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1683	1/1	0.92	0.14	60,60,60,60	0
56	MG	1A	3918	1/1	0.92	0.24	60,60,60,60	0
56	MG	2A	3480	1/1	0.92	0.26	65,65,65,65	0
56	MG	1X	102	1/1	0.92	0.20	30,30,30,30	0
56	MG	1Y	202	1/1	0.92	0.23	71,71,71,71	0
56	MG	1A	4072	1/1	0.92	0.23	44,44,44,44	0
56	MG	1A	3221	1/1	0.92	0.15	73,73,73,73	0
56	MG	2A	3255	1/1	0.92	0.38	62,62,62,62	0
56	MG	2A	3073	1/1	0.92	0.50	55,55,55,55	0
56	MG	1A	3185	1/1	0.92	0.30	35,35,35,35	0
56	MG	2A	3796	1/1	0.92	0.11	59,59,59,59	0
56	MG	2A	3260	1/1	0.92	0.34	66,66,66,66	0
56	MG	2A	3798	1/1	0.92	0.12	75,75,75,75	0
56	MG	1A	3794	1/1	0.92	0.20	31,31,31,31	0
56	MG	1A	3648	1/1	0.92	0.20	31,31,31,31	0
56	MG	1A	3545	1/1	0.92	0.10	61,61,61,61	0
56	MG	2A	3079	1/1	0.92	0.26	42,42,42,42	0
56	MG	2A	3505	1/1	0.92	0.23	60,60,60,60	0
56	MG	10	106	1/1	0.92	0.14	53,53,53,53	0
56	MG	10	107	1/1	0.92	0.12	61,61,61,61	0
56	MG	1a	1771	1/1	0.92	0.06	54,54,54,54	0
56	MG	1a	1775	1/1	0.92	0.09	64,64,64,64	0
56	MG	2A	3812	1/1	0.92	0.20	63,63,63,63	0
56	MG	11	102	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3355	1/1	0.92	0.21	41,41,41,41	0
56	MG	1A	3930	1/1	0.92	0.07	47,47,47,47	0
56	MG	2a	1726	1/1	0.92	0.09	80,80,80,80	0
56	MG	2A	3523	1/1	0.92	0.12	61,61,61,61	0
56	MG	12	101	1/1	0.92	0.19	44,44,44,44	0
56	MG	1a	1784	1/1	0.92	0.24	72,72,72,72	0
56	MG	2A	3277	1/1	0.92	0.13	56,56,56,56	0
56	MG	2A	3096	1/1	0.92	0.31	45,45,45,45	0
56	MG	1A	3654	1/1	0.92	0.14	14,14,14,14	0
56	MG	2a	1734	1/1	0.92	0.11	67,67,67,67	0
56	MG	13	102	1/1	0.92	0.63	56,56,56,56	0
56	MG	2A	3536	1/1	0.92	0.27	40,40,40,40	0
56	MG	1A	3552	1/1	0.92	0.23	46,46,46,46	0
56	MG	2A	3546	1/1	0.92	0.07	54,54,54,54	0
56	MG	2A	3832	1/1	0.92	0.20	63,63,63,63	0
56	MG	1A	3807	1/1	0.92	0.12	39,39,39,39	0
56	MG	1A	3808	1/1	0.92	0.24	38,38,38,38	0
56	MG	2A	3108	1/1	0.92	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1794	1/1	0.92	0.16	69,69,69,69	0
56	MG	18	103	1/1	0.92	0.32	39,39,39,39	0
56	MG	2A	3113	1/1	0.92	0.17	70,70,70,70	0
56	MG	2A	3565	1/1	0.92	0.36	62,62,62,62	0
56	MG	1A	3404	1/1	0.92	0.08	51,51,51,51	0
56	MG	2a	1754	1/1	0.92	0.13	77,77,77,77	0
56	MG	2A	3852	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3938	1/1	0.92	0.11	50,50,50,50	0
56	MG	2A	3571	1/1	0.92	0.47	71,71,71,71	0
56	MG	1A	3085	1/1	0.92	0.22	31,31,31,31	0
56	MG	2A	3118	1/1	0.92	0.21	49,49,49,49	0
56	MG	1A	3464	1/1	0.92	0.71	42,42,42,42	0
56	MG	1A	3943	1/1	0.92	0.17	43,43,43,43	0
56	MG	1A	3559	1/1	0.92	0.10	37,37,37,37	0
56	MG	2A	3122	1/1	0.92	0.32	45,45,45,45	0
56	MG	2a	1768	1/1	0.92	0.10	67,67,67,67	0
56	MG	2A	3299	1/1	0.92	0.61	69,69,69,69	0
56	MG	1A	4112	1/1	0.92	0.14	31,31,31,31	0
56	MG	2A	3133	1/1	0.92	0.30	53,53,53,53	0
56	MG	1a	1607	1/1	0.92	0.17	62,62,62,62	0
56	MG	1A	3819	1/1	0.92	0.09	41,41,41,41	0
56	MG	2A	3305	1/1	0.92	0.57	62,62,62,62	0
56	MG	2a	1781	1/1	0.92	0.10	71,71,71,71	0
56	MG	1A	3561	1/1	0.92	0.16	23,23,23,23	0
56	MG	2A	3600	1/1	0.92	0.11	39,39,39,39	0
56	MG	1A	3563	1/1	0.92	0.11	22,22,22,22	0
56	MG	1A	3567	1/1	0.92	0.15	24,24,24,24	0
56	MG	2A	3604	1/1	0.92	0.14	79,79,79,79	0
56	MG	1A	3827	1/1	0.92	0.10	17,17,17,17	0
56	MG	2A	3882	1/1	0.92	0.10	52,52,52,52	0
56	MG	1a	1621	1/1	0.92	0.10	51,51,51,51	0
56	MG	1a	1624	1/1	0.92	0.23	56,56,56,56	0
56	MG	1A	3952	1/1	0.92	0.18	43,43,43,43	0
56	MG	1A	3224	1/1	0.92	0.35	42,42,42,42	0
56	MG	1A	3831	1/1	0.92	0.12	32,32,32,32	0
56	MG	1A	3570	1/1	0.92	0.17	17,17,17,17	0
56	MG	1A	3834	1/1	0.92	0.16	34,34,34,34	0
56	MG	1a	1828	1/1	0.92	0.07	54,54,54,54	0
56	MG	1A	3958	1/1	0.92	0.07	48,48,48,48	0
56	MG	2A	3626	1/1	0.92	0.22	58,58,58,58	0
56	MG	2B	212	1/1	0.92	0.11	77,77,77,77	0
56	MG	1A	3311	1/1	0.92	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3189	1/1	0.92	0.29	40,40,40,40	0
56	MG	1A	3839	1/1	0.92	0.17	30,30,30,30	0
56	MG	2A	3631	1/1	0.92	0.17	42,42,42,42	0
56	MG	1A	3032	1/1	0.92	0.47	33,33,33,33	0
56	MG	1A	3414	1/1	0.92	0.23	38,38,38,38	0
56	MG	1A	3584	1/1	0.92	0.14	31,31,31,31	0
56	MG	1A	3168	1/1	0.92	0.17	38,38,38,38	0
56	MG	2A	3332	1/1	0.92	0.32	70,70,70,70	0
56	MG	1B	210	1/1	0.92	0.10	55,55,55,55	0
56	MG	1B	217	1/1	0.92	0.18	61,61,61,61	0
56	MG	1A	3273	1/1	0.92	0.26	49,49,49,49	0
56	MG	1A	3229	1/1	0.92	0.19	49,49,49,49	0
56	MG	1A	3848	1/1	0.92	0.08	54,54,54,54	0
56	MG	1A	3980	1/1	0.92	0.14	46,46,46,46	0
56	MG	1a	1661	1/1	0.92	0.42	62,62,62,62	0
56	MG	1A	3193	1/1	0.92	0.26	28,28,28,28	0
56	MG	1A	3481	1/1	0.92	0.61	34,34,34,34	0
56	MG	1A	3419	1/1	0.92	0.36	46,46,46,46	0
56	MG	2A	3666	1/1	0.92	0.24	57,57,57,57	0
56	MG	1A	3483	1/1	0.92	0.32	58,58,58,58	0
56	MG	1A	3038	1/1	0.92	0.30	57,57,57,57	0
56	MG	1A	3603	1/1	0.92	0.17	35,35,35,35	0
56	MG	2l	202	1/1	0.92	0.11	70,70,70,70	0
56	MG	1A	3094	1/1	0.92	0.16	29,29,29,29	0
56	MG	1a	1672	1/1	0.92	0.17	48,48,48,48	0
56	MG	1D	305	1/1	0.92	0.61	42,42,42,42	0
56	MG	2R	201	1/1	0.92	0.17	64,64,64,64	0
56	MG	1A	3198	1/1	0.92	0.31	60,60,60,60	0
56	MG	1a	1681	1/1	0.92	0.11	58,58,58,58	0
56	MG	1A	3243	1/1	0.92	0.13	39,39,39,39	0
56	MG	2t	201	1/1	0.92	0.11	56,56,56,56	0
56	MG	1D	312	1/1	0.92	0.16	56,56,56,56	0
56	MG	1A	3862	1/1	0.92	0.10	36,36,36,36	0
56	MG	2A	3371	1/1	0.92	0.27	57,57,57,57	0
56	MG	2A	3197	1/1	0.92	0.37	59,59,59,59	0
56	MG	2A	3375	1/1	0.92	0.11	45,45,45,45	0
56	MG	2A	3378	1/1	0.92	0.12	60,60,60,60	0
56	MG	25	103	1/1	0.92	0.56	58,58,58,58	0
56	MG	1A	3201	1/1	0.92	0.17	54,54,54,54	0
56	MG	2A	3199	1/1	0.92	0.21	49,49,49,49	0
56	MG	2w	109	1/1	0.92	0.12	75,75,75,75	0
56	MG	1A	4001	1/1	0.92	0.10	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3866	1/1	0.92	0.11	60,60,60,60	0
56	MG	27	103	1/1	0.92	0.17	60,60,60,60	0
56	MG	2A	3698	1/1	0.92	0.26	63,63,63,63	0
56	MG	28	102	1/1	0.92	0.24	54,54,54,54	0
56	MG	2x	107	1/1	0.92	0.15	55,55,55,55	0
56	MG	1A	3612	1/1	0.92	0.14	37,37,37,37	0
56	MG	1A	3202	1/1	0.92	0.38	34,34,34,34	0
56	MG	1A	3005	1/1	0.92	0.12	41,41,41,41	0
56	MG	2A	3010	1/1	0.92	0.21	51,51,51,51	0
56	MG	2a	1606	1/1	0.92	0.20	68,68,68,68	0
56	MG	1A	3144	1/1	0.92	0.25	38,38,38,38	0
56	MG	2A	3013	1/1	0.92	0.08	64,64,64,64	0
60	K	2A	3393	1/1	0.92	0.15	67,67,67,67	0
56	MG	1E	306	1/1	0.93	0.50	61,61,61,61	0
56	MG	2A	3001	1/1	0.93	0.39	51,51,51,51	0
56	MG	1A	3920	1/1	0.93	0.14	45,45,45,45	0
56	MG	1A	3039	1/1	0.93	0.13	35,35,35,35	0
56	MG	2A	3722	1/1	0.93	0.13	67,67,67,67	0
56	MG	1A	3614	1/1	0.93	0.18	41,41,41,41	0
56	MG	2a	1620	1/1	0.93	0.71	70,70,70,70	0
56	MG	2A	3423	1/1	0.93	0.10	56,56,56,56	0
56	MG	1a	1682	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	3924	1/1	0.93	0.07	41,41,41,41	0
56	MG	1F	306	1/1	0.93	0.39	25,25,25,25	0
56	MG	1a	1688	1/1	0.93	0.16	53,53,53,53	0
56	MG	1A	3425	1/1	0.93	0.32	65,65,65,65	0
56	MG	1A	4042	1/1	0.93	0.14	53,53,53,53	0
56	MG	2A	3227	1/1	0.93	0.36	58,58,58,58	0
56	MG	1A	3708	1/1	0.93	0.10	48,48,48,48	0
56	MG	2A	3737	1/1	0.93	0.14	37,37,37,37	0
56	MG	1A	3540	1/1	0.93	0.17	26,26,26,26	0
56	MG	1A	3715	1/1	0.93	0.09	39,39,39,39	0
56	MG	1A	3541	1/1	0.93	0.12	40,40,40,40	0
56	MG	1A	3543	1/1	0.93	0.08	31,31,31,31	0
56	MG	1A	3477	1/1	0.93	0.14	48,48,48,48	0
56	MG	1a	1703	1/1	0.93	0.17	66,66,66,66	0
56	MG	1A	3549	1/1	0.93	0.14	40,40,40,40	0
56	MG	1N	202	1/1	0.93	0.47	46,46,46,46	0
56	MG	1A	4064	1/1	0.93	0.15	54,54,54,54	0
56	MG	1A	3285	1/1	0.93	0.44	43,43,43,43	0
56	MG	2A	3451	1/1	0.93	0.12	29,29,29,29	0
56	MG	1A	3735	1/1	0.93	0.08	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1649	1/1	0.93	0.07	76,76,76,76	0
56	MG	1A	3736	1/1	0.93	0.13	40,40,40,40	0
56	MG	1A	3083	1/1	0.93	0.18	41,41,41,41	0
56	MG	1A	3167	1/1	0.93	0.70	52,52,52,52	0
56	MG	1A	3063	1/1	0.93	0.15	31,31,31,31	0
56	MG	1A	3067	1/1	0.93	0.16	48,48,48,48	0
56	MG	1a	1724	1/1	0.93	0.18	57,57,57,57	0
56	MG	1A	3638	1/1	0.93	0.26	26,26,26,26	0
56	MG	1S	202	1/1	0.93	0.30	48,48,48,48	0
56	MG	1A	3041	1/1	0.93	0.33	33,33,33,33	0
56	MG	2a	1662	1/1	0.93	0.17	59,59,59,59	0
56	MG	2A	3475	1/1	0.93	0.24	37,37,37,37	0
56	MG	1A	3044	1/1	0.93	0.12	30,30,30,30	0
56	MG	1A	3852	1/1	0.93	0.12	36,36,36,36	0
56	MG	1A	3485	1/1	0.93	0.10	41,41,41,41	0
56	MG	2a	1667	1/1	0.93	0.10	67,67,67,67	0
56	MG	1a	1734	1/1	0.93	0.09	55,55,55,55	0
56	MG	1A	3298	1/1	0.93	0.10	48,48,48,48	0
56	MG	2A	3256	1/1	0.93	0.41	58,58,58,58	0
56	MG	1U	207	1/1	0.93	0.23	35,35,35,35	0
56	MG	2a	1676	1/1	0.93	0.16	60,60,60,60	0
56	MG	1U	209	1/1	0.93	0.46	38,38,38,38	0
56	MG	1A	3175	1/1	0.93	0.31	47,47,47,47	0
56	MG	1A	3047	1/1	0.93	0.11	33,33,33,33	0
56	MG	1A	3956	1/1	0.93	0.13	35,35,35,35	0
56	MG	1a	1748	1/1	0.93	0.08	52,52,52,52	0
56	MG	1a	1749	1/1	0.93	0.06	49,49,49,49	0
56	MG	1A	3859	1/1	0.93	0.18	48,48,48,48	0
56	MG	1A	4094	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3072	1/1	0.93	0.20	31,31,31,31	0
56	MG	2A	3270	1/1	0.93	0.45	58,58,58,58	0
56	MG	1X	103	1/1	0.93	0.22	41,41,41,41	0
56	MG	1X	104	1/1	0.93	0.27	36,36,36,36	0
56	MG	2a	1693	1/1	0.93	0.27	68,68,68,68	0
56	MG	2A	3076	1/1	0.93	0.29	55,55,55,55	0
56	MG	2a	1697	1/1	0.93	0.41	86,86,86,86	0
56	MG	1X	105	1/1	0.93	0.20	56,56,56,56	0
56	MG	1Y	201	1/1	0.93	0.17	45,45,45,45	0
56	MG	1A	4096	1/1	0.93	0.10	55,55,55,55	0
56	MG	1A	3576	1/1	0.93	0.14	25,25,25,25	0
56	MG	2A	3809	1/1	0.93	0.25	71,71,71,71	0
56	MG	1A	3577	1/1	0.93	0.32	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1Z	303	1/1	0.93	0.14	52,52,52,52	0
56	MG	1A	4106	1/1	0.93	0.08	61,61,61,61	0
56	MG	2A	3086	1/1	0.93	0.17	39,39,39,39	0
56	MG	2A	3815	1/1	0.93	0.23	63,63,63,63	0
56	MG	2A	3816	1/1	0.93	0.19	52,52,52,52	0
56	MG	1a	1765	1/1	0.93	0.11	58,58,58,58	0
56	MG	1A	3653	1/1	0.93	0.13	42,42,42,42	0
56	MG	2A	3090	1/1	0.93	0.15	47,47,47,47	0
56	MG	2A	3540	1/1	0.93	0.12	69,69,69,69	0
56	MG	1A	3006	1/1	0.93	0.20	54,54,54,54	0
56	MG	1A	4110	1/1	0.93	0.13	60,60,60,60	0
56	MG	1a	1769	1/1	0.93	0.17	63,63,63,63	0
56	MG	2A	3553	1/1	0.93	0.33	40,40,40,40	0
56	MG	1A	3657	1/1	0.93	0.16	17,17,17,17	0
56	MG	1A	3970	1/1	0.93	0.16	38,38,38,38	0
56	MG	1A	3156	1/1	0.93	0.32	40,40,40,40	0
56	MG	1A	4115	1/1	0.93	0.28	66,66,66,66	0
56	MG	2A	3101	1/1	0.93	0.25	65,65,65,65	0
56	MG	1A	4116	1/1	0.93	0.12	51,51,51,51	0
56	MG	2A	3834	1/1	0.93	0.22	47,47,47,47	0
56	MG	1A	3779	1/1	0.93	0.19	52,52,52,52	0
56	MG	2A	3838	1/1	0.93	0.12	60,60,60,60	0
56	MG	1A	3976	1/1	0.93	0.19	45,45,45,45	0
56	MG	1A	3277	1/1	0.93	0.17	48,48,48,48	0
56	MG	1A	3781	1/1	0.93	0.13	18,18,18,18	0
56	MG	15	104	1/1	0.93	0.14	57,57,57,57	0
56	MG	2a	1745	1/1	0.93	0.12	63,63,63,63	0
56	MG	2A	3846	1/1	0.93	0.33	70,70,70,70	0
56	MG	1A	3660	1/1	0.93	0.15	35,35,35,35	0
56	MG	17	103	1/1	0.93	0.31	39,39,39,39	0
56	MG	1A	3412	1/1	0.93	0.42	34,34,34,34	0
56	MG	2A	3586	1/1	0.93	0.17	49,49,49,49	0
56	MG	1a	1793	1/1	0.93	0.18	45,45,45,45	0
56	MG	2A	3589	1/1	0.93	0.51	73,73,73,73	0
56	MG	1A	3983	1/1	0.93	0.10	42,42,42,42	0
56	MG	18	104	1/1	0.93	0.34	36,36,36,36	0
56	MG	1A	3502	1/1	0.93	0.22	43,43,43,43	0
56	MG	2A	3860	1/1	0.93	0.37	59,59,59,59	0
56	MG	2A	3310	1/1	0.93	0.35	67,67,67,67	0
56	MG	1A	4131	1/1	0.93	0.13	48,48,48,48	0
56	MG	1A	3875	1/1	0.93	0.21	52,52,52,52	0
56	MG	1a	1800	1/1	0.93	0.06	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3057	1/1	0.93	0.15	26,26,26,26	0
56	MG	1A	4135	1/1	0.93	0.18	68,68,68,68	0
56	MG	1A	4136	1/1	0.93	0.19	46,46,46,46	0
56	MG	1A	4137	1/1	0.93	0.35	37,37,37,37	0
56	MG	1A	3506	1/1	0.93	0.12	48,48,48,48	0
56	MG	1a	1610	1/1	0.93	0.08	70,70,70,70	0
56	MG	2a	1774	1/1	0.93	0.16	60,60,60,60	0
56	MG	2a	1775	1/1	0.93	0.13	51,51,51,51	0
56	MG	1a	1611	1/1	0.93	0.13	28,28,28,28	0
56	MG	2A	3877	1/1	0.93	0.29	60,60,60,60	0
56	MG	2a	1779	1/1	0.93	0.15	64,64,64,64	0
56	MG	2A	3611	1/1	0.93	0.17	35,35,35,35	0
56	MG	1A	4139	1/1	0.93	0.14	60,60,60,60	0
56	MG	1a	1614	1/1	0.93	0.11	57,57,57,57	0
56	MG	2A	3881	1/1	0.93	0.40	60,60,60,60	0
56	MG	1a	1812	1/1	0.93	0.07	81,81,81,81	0
56	MG	1B	202	1/1	0.93	0.36	48,48,48,48	0
56	MG	2A	3326	1/1	0.93	0.15	62,62,62,62	0
56	MG	1a	1815	1/1	0.93	0.14	71,71,71,71	0
56	MG	1A	3795	1/1	0.93	0.08	45,45,45,45	0
56	MG	1a	1617	1/1	0.93	0.06	53,53,53,53	0
56	MG	1A	3076	1/1	0.93	0.09	49,49,49,49	0
56	MG	2a	1801	1/1	0.93	0.10	77,77,77,77	0
56	MG	1A	3670	1/1	0.93	0.10	33,33,33,33	0
56	MG	1A	3993	1/1	0.93	0.18	39,39,39,39	0
56	MG	2B	209	1/1	0.93	0.29	80,80,80,80	0
56	MG	1a	1623	1/1	0.93	0.16	51,51,51,51	0
56	MG	1B	208	1/1	0.93	0.27	71,71,71,71	0
56	MG	1A	3801	1/1	0.93	0.14	34,34,34,34	0
56	MG	1A	3888	1/1	0.93	0.60	47,47,47,47	0
56	MG	1B	214	1/1	0.93	0.13	27,27,27,27	0
56	MG	2B	217	1/1	0.93	0.14	82,82,82,82	0
56	MG	2a	1817	1/1	0.93	0.19	66,66,66,66	0
56	MG	2A	3638	1/1	0.93	0.26	59,59,59,59	0
56	MG	1a	1834	1/1	0.93	0.06	67,67,67,67	0
56	MG	1A	3280	1/1	0.93	0.17	38,38,38,38	0
56	MG	1a	1836	1/1	0.93	0.04	45,45,45,45	0
56	MG	1A	3230	1/1	0.93	0.36	42,42,42,42	0
56	MG	1A	3312	1/1	0.93	0.33	39,39,39,39	0
56	MG	1A	4004	1/1	0.93	0.18	57,57,57,57	0
56	MG	1A	4006	1/1	0.93	0.28	55,55,55,55	0
56	MG	2A	3180	1/1	0.93	0.16	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	1b	301	1/1	0.93	0.06	84,84,84,84	0
56	MG	2A	3356	1/1	0.93	0.14	65,65,65,65	0
56	MG	2A	3360	1/1	0.93	0.24	40,40,40,40	0
56	MG	2A	3665	1/1	0.93	0.28	75,75,75,75	0
56	MG	1A	3677	1/1	0.93	0.13	41,41,41,41	0
56	MG	2a	1836	1/1	0.93	0.09	69,69,69,69	0
56	MG	2A	3365	1/1	0.93	0.34	55,55,55,55	0
56	MG	1B	225	1/1	0.93	0.14	67,67,67,67	0
56	MG	2A	3367	1/1	0.93	0.45	63,63,63,63	0
56	MG	1A	3896	1/1	0.93	0.26	46,46,46,46	0
56	MG	1a	1646	1/1	0.93	0.40	54,54,54,54	0
56	MG	1B	228	1/1	0.93	0.11	54,54,54,54	0
56	MG	2A	3675	1/1	0.93	0.18	67,67,67,67	0
56	MG	2A	3372	1/1	0.93	0.22	48,48,48,48	0
56	MG	2A	3679	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	4013	1/1	0.93	0.15	41,41,41,41	0
56	MG	1B	231	1/1	0.93	0.17	30,30,30,30	0
56	MG	2T	201	1/1	0.93	0.19	65,65,65,65	0
56	MG	2A	3376	1/1	0.93	0.14	44,44,44,44	0
56	MG	2T	203	1/1	0.93	0.07	61,61,61,61	0
56	MG	1a	1650	1/1	0.93	0.08	59,59,59,59	0
56	MG	2A	3379	1/1	0.93	0.13	52,52,52,52	0
56	MG	1t	201	1/1	0.93	0.10	60,60,60,60	0
56	MG	2A	3191	1/1	0.93	0.33	55,55,55,55	0
56	MG	1A	3460	1/1	0.93	0.13	41,41,41,41	0
56	MG	2A	3691	1/1	0.93	0.06	58,58,58,58	0
56	MG	1a	1652	1/1	0.93	0.25	63,63,63,63	0
56	MG	1A	3901	1/1	0.93	0.16	54,54,54,54	0
56	MG	1A	3902	1/1	0.93	0.16	51,51,51,51	0
56	MG	1w	105	1/1	0.93	0.10	69,69,69,69	0
56	MG	1A	3159	1/1	0.93	0.27	37,37,37,37	0
56	MG	1D	301	1/1	0.93	0.26	40,40,40,40	0
56	MG	2A	3392	1/1	0.93	0.16	66,66,66,66	0
56	MG	2A	3702	1/1	0.93	0.08	65,65,65,65	0
56	MG	27	104	1/1	0.93	0.24	50,50,50,50	0
56	MG	1A	3909	1/1	0.93	0.11	34,34,34,34	0
56	MG	1A	3813	1/1	0.93	0.16	43,43,43,43	0
56	MG	1A	3318	1/1	0.93	0.42	46,46,46,46	0
56	MG	2a	1601	1/1	0.93	0.35	74,74,74,74	0
56	MG	1A	3528	1/1	0.93	0.16	17,17,17,17	0
56	MG	2A	3401	1/1	0.93	0.25	65,65,65,65	0
56	MG	1A	3385	1/1	0.93	0.39	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1x	106	1/1	0.93	0.17	71,71,71,71	0
56	MG	1a	1668	1/1	0.93	0.12	39,39,39,39	0
56	MG	2A	3407	1/1	0.93	0.43	59,59,59,59	0
56	MG	1A	3422	1/1	0.93	0.37	39,39,39,39	0
56	MG	1A	3320	1/1	0.93	0.48	36,36,36,36	0
56	MG	1E	303	1/1	0.93	0.21	28,28,28,28	0
56	MG	1A	4097	1/1	0.94	0.09	61,61,61,61	0
56	MG	2A	3226	1/1	0.94	0.73	62,62,62,62	0
56	MG	2a	1603	1/1	0.94	0.23	53,53,53,53	0
56	MG	1A	3837	1/1	0.94	0.10	33,33,33,33	0
56	MG	2A	3422	1/1	0.94	0.24	65,65,65,65	0
56	MG	1A	3103	1/1	0.94	0.77	44,44,44,44	0
56	MG	1A	3357	1/1	0.94	0.24	37,37,37,37	0
56	MG	1a	1737	1/1	0.94	0.23	68,68,68,68	0
56	MG	1a	1739	1/1	0.94	0.22	61,61,61,61	0
56	MG	1a	1740	1/1	0.94	0.12	71,71,71,71	0
56	MG	1A	3716	1/1	0.94	0.10	26,26,26,26	0
56	MG	1A	3718	1/1	0.94	0.11	32,32,32,32	0
56	MG	1a	1744	1/1	0.94	0.10	75,75,75,75	0
56	MG	1A	3515	1/1	0.94	0.16	55,55,55,55	0
56	MG	1A	4111	1/1	0.94	0.09	24,24,24,24	0
56	MG	1A	3723	1/1	0.94	0.17	55,55,55,55	0
56	MG	1A	3402	1/1	0.94	0.15	28,28,28,28	0
56	MG	1A	3262	1/1	0.94	0.22	38,38,38,38	0
56	MG	1A	3731	1/1	0.94	0.13	30,30,30,30	0
56	MG	2A	3443	1/1	0.94	0.15	59,59,59,59	0
56	MG	1A	3732	1/1	0.94	0.18	58,58,58,58	0
56	MG	1A	3187	1/1	0.94	0.11	41,41,41,41	0
56	MG	2A	3727	1/1	0.94	0.18	63,63,63,63	0
56	MG	1A	3405	1/1	0.94	0.22	46,46,46,46	0
56	MG	1A	3968	1/1	0.94	0.15	38,38,38,38	0
56	MG	2A	3448	1/1	0.94	0.16	42,42,42,42	0
56	MG	1A	3265	1/1	0.94	0.16	58,58,58,58	0
56	MG	2A	3733	1/1	0.94	0.16	39,39,39,39	0
56	MG	2a	1634	1/1	0.94	0.13	57,57,57,57	0
56	MG	1A	3455	1/1	0.94	0.28	31,31,31,31	0
56	MG	1A	3854	1/1	0.94	0.08	36,36,36,36	0
56	MG	1A	3456	1/1	0.94	0.16	31,31,31,31	0
56	MG	1A	3233	1/1	0.94	0.16	42,42,42,42	0
56	MG	13	104	1/1	0.94	0.34	38,38,38,38	0
56	MG	1A	3170	1/1	0.94	0.18	27,27,27,27	0
56	MG	1A	3461	1/1	0.94	0.39	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3465	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3743	1/1	0.94	0.10	66,66,66,66	0
56	MG	2A	3746	1/1	0.94	0.15	66,66,66,66	0
56	MG	1A	3634	1/1	0.94	0.11	48,48,48,48	0
56	MG	2A	3469	1/1	0.94	0.06	54,54,54,54	0
56	MG	2A	3470	1/1	0.94	0.21	28,28,28,28	0
56	MG	2A	3750	1/1	0.94	0.11	41,41,41,41	0
56	MG	1A	3013	1/1	0.94	0.33	23,23,23,23	0
56	MG	2a	1652	1/1	0.94	0.11	62,62,62,62	0
56	MG	1A	3411	1/1	0.94	0.13	27,27,27,27	0
56	MG	2A	3755	1/1	0.94	0.17	60,60,60,60	0
56	MG	1A	3755	1/1	0.94	0.80	34,34,34,34	0
56	MG	1A	3758	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3477	1/1	0.94	0.12	50,50,50,50	0
56	MG	1a	1772	1/1	0.94	0.16	64,64,64,64	0
56	MG	1a	1774	1/1	0.94	0.10	69,69,69,69	0
56	MG	1A	3759	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3467	1/1	0.94	0.60	45,45,45,45	0
56	MG	1B	204	1/1	0.94	0.17	60,60,60,60	0
56	MG	1A	3126	1/1	0.94	0.44	31,31,31,31	0
56	MG	1A	3550	1/1	0.94	0.17	42,42,42,42	0
56	MG	1a	1783	1/1	0.94	0.12	68,68,68,68	0
56	MG	2A	3491	1/1	0.94	0.11	38,38,38,38	0
56	MG	1A	3994	1/1	0.94	0.23	46,46,46,46	0
56	MG	2A	3775	1/1	0.94	0.12	64,64,64,64	0
56	MG	1A	3767	1/1	0.94	0.44	28,28,28,28	0
56	MG	2a	1674	1/1	0.94	0.10	83,83,83,83	0
56	MG	1a	1608	1/1	0.94	0.10	55,55,55,55	0
56	MG	1a	1609	1/1	0.94	0.11	49,49,49,49	0
56	MG	2A	3780	1/1	0.94	0.22	67,67,67,67	0
56	MG	2A	3497	1/1	0.94	0.20	50,50,50,50	0
56	MG	1a	1789	1/1	0.94	0.23	82,82,82,82	0
56	MG	2A	3278	1/1	0.94	0.15	49,49,49,49	0
56	MG	2A	3501	1/1	0.94	0.24	67,67,67,67	0
56	MG	2A	3503	1/1	0.94	0.29	53,53,53,53	0
56	MG	2A	3095	1/1	0.94	0.18	53,53,53,53	0
56	MG	2A	3506	1/1	0.94	0.12	39,39,39,39	0
56	MG	2A	3790	1/1	0.94	0.23	64,64,64,64	0
56	MG	1A	3642	1/1	0.94	0.13	54,54,54,54	0
56	MG	1A	3109	1/1	0.94	0.09	50,50,50,50	0
56	MG	1B	212	1/1	0.94	0.16	46,46,46,46	0
56	MG	1B	213	1/1	0.94	0.24	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1696	1/1	0.94	0.06	77,77,77,77	0
56	MG	1A	3066	1/1	0.94	0.17	25,25,25,25	0
56	MG	2A	3518	1/1	0.94	0.12	75,75,75,75	0
56	MG	2A	3286	1/1	0.94	0.22	55,55,55,55	0
56	MG	2A	3520	1/1	0.94	0.49	82,82,82,82	0
56	MG	1A	3373	1/1	0.94	0.19	42,42,42,42	0
56	MG	2A	3103	1/1	0.94	0.23	62,62,62,62	0
56	MG	1A	4002	1/1	0.94	0.12	31,31,31,31	0
56	MG	1A	3475	1/1	0.94	0.12	34,34,34,34	0
56	MG	1A	4005	1/1	0.94	0.17	48,48,48,48	0
56	MG	2A	3530	1/1	0.94	0.23	58,58,58,58	0
56	MG	1A	3026	1/1	0.94	0.18	72,72,72,72	0
56	MG	1A	4007	1/1	0.94	0.27	48,48,48,48	0
56	MG	1A	3247	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3050	1/1	0.94	0.31	45,45,45,45	0
56	MG	2a	1716	1/1	0.94	0.11	67,67,67,67	0
56	MG	2a	1717	1/1	0.94	0.07	60,60,60,60	0
56	MG	2a	1718	1/1	0.94	0.19	69,69,69,69	0
56	MG	2A	3537	1/1	0.94	0.21	53,53,53,53	0
56	MG	1A	3884	1/1	0.94	0.11	30,30,30,30	0
56	MG	2A	3817	1/1	0.94	0.30	62,62,62,62	0
56	MG	2a	1723	1/1	0.94	0.07	61,61,61,61	0
56	MG	2A	3541	1/1	0.94	0.12	43,43,43,43	0
56	MG	1A	3179	1/1	0.94	0.57	37,37,37,37	0
56	MG	1A	3340	1/1	0.94	0.13	55,55,55,55	0
56	MG	2A	3547	1/1	0.94	0.23	42,42,42,42	0
56	MG	2A	3822	1/1	0.94	0.10	73,73,73,73	0
56	MG	1A	3379	1/1	0.94	0.15	35,35,35,35	0
56	MG	1a	1632	1/1	0.94	0.14	58,58,58,58	0
56	MG	2A	3825	1/1	0.94	0.31	78,78,78,78	0
56	MG	1A	3782	1/1	0.94	0.21	33,33,33,33	0
56	MG	1A	3783	1/1	0.94	0.22	34,34,34,34	0
56	MG	2A	3556	1/1	0.94	0.12	41,41,41,41	0
56	MG	2A	3557	1/1	0.94	0.09	39,39,39,39	0
56	MG	1A	3308	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3134	1/1	0.94	0.05	67,67,67,67	0
56	MG	2A	3136	1/1	0.94	0.26	57,57,57,57	0
56	MG	1a	1816	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3199	1/1	0.94	0.53	26,26,26,26	0
56	MG	2A	3141	1/1	0.94	0.28	62,62,62,62	0
56	MG	1A	3899	1/1	0.94	0.13	60,60,60,60	0
56	MG	2a	1748	1/1	0.94	0.06	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1820	1/1	0.94	0.17	73,73,73,73	0
56	MG	2A	3578	1/1	0.94	0.30	70,70,70,70	0
56	MG	2A	3146	1/1	0.94	0.05	75,75,75,75	0
56	MG	2A	3313	1/1	0.94	0.14	57,57,57,57	0
56	MG	1A	3343	1/1	0.94	0.22	58,58,58,58	0
56	MG	1A	3791	1/1	0.94	0.17	25,25,25,25	0
56	MG	2A	3585	1/1	0.94	0.25	52,52,52,52	0
56	MG	2A	3851	1/1	0.94	0.28	54,54,54,54	0
56	MG	2a	1758	1/1	0.94	0.16	50,50,50,50	0
56	MG	1A	3792	1/1	0.94	0.13	56,56,56,56	0
56	MG	1A	3225	1/1	0.94	0.43	37,37,37,37	0
56	MG	1a	1826	1/1	0.94	0.14	66,66,66,66	0
56	MG	1A	3906	1/1	0.94	0.22	28,28,28,28	0
56	MG	2A	3856	1/1	0.94	0.09	73,73,73,73	0
56	MG	2A	3154	1/1	0.94	0.26	72,72,72,72	0
56	MG	1A	3427	1/1	0.94	0.30	29,29,29,29	0
56	MG	2a	1767	1/1	0.94	0.14	67,67,67,67	0
56	MG	2A	3593	1/1	0.94	0.24	33,33,33,33	0
56	MG	1A	3487	1/1	0.94	0.32	57,57,57,57	0
56	MG	2A	3861	1/1	0.94	0.39	65,65,65,65	0
56	MG	2A	3157	1/1	0.94	0.21	49,49,49,49	0
56	MG	2A	3596	1/1	0.94	0.21	74,74,74,74	0
56	MG	1A	3665	1/1	0.94	0.13	34,34,34,34	0
56	MG	2a	1776	1/1	0.94	0.12	77,77,77,77	0
56	MG	1a	1832	1/1	0.94	0.11	58,58,58,58	0
56	MG	1A	3115	1/1	0.94	0.27	35,35,35,35	0
56	MG	1A	3800	1/1	0.94	0.10	32,32,32,32	0
56	MG	2A	3165	1/1	0.94	0.23	68,68,68,68	0
56	MG	1a	1656	1/1	0.94	0.17	50,50,50,50	0
56	MG	2a	1782	1/1	0.94	0.43	59,59,59,59	0
56	MG	1A	3917	1/1	0.94	0.21	53,53,53,53	0
56	MG	2A	3873	1/1	0.94	0.14	65,65,65,65	0
56	MG	2A	3334	1/1	0.94	0.16	69,69,69,69	0
56	MG	2a	1788	1/1	0.94	0.24	65,65,65,65	0
56	MG	1A	3253	1/1	0.94	0.24	37,37,37,37	0
56	MG	2A	3609	1/1	0.94	0.20	44,44,44,44	0
56	MG	1A	3390	1/1	0.94	0.40	66,66,66,66	0
56	MG	1A	4053	1/1	0.94	0.13	45,45,45,45	0
56	MG	1A	3313	1/1	0.94	0.08	19,19,19,19	0
56	MG	2A	3172	1/1	0.94	0.44	57,57,57,57	0
56	MG	2a	1797	1/1	0.94	0.19	64,64,64,64	0
56	MG	1A	4057	1/1	0.94	0.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1803	1/1	0.94	0.12	55,55,55,55	0
56	MG	1A	4058	1/1	0.94	0.34	44,44,44,44	0
56	MG	1G	201	1/1	0.94	0.27	33,33,33,33	0
56	MG	1A	3588	1/1	0.94	0.15	65,65,65,65	0
56	MG	1A	3314	1/1	0.94	0.47	41,41,41,41	0
56	MG	1A	4062	1/1	0.94	0.12	39,39,39,39	0
56	MG	1A	3495	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3682	1/1	0.94	0.07	36,36,36,36	0
56	MG	1A	3812	1/1	0.94	0.21	22,22,22,22	0
56	MG	1A	3393	1/1	0.94	0.44	45,45,45,45	0
56	MG	1N	205	1/1	0.94	0.16	32,32,32,32	0
56	MG	1A	4070	1/1	0.94	0.21	52,52,52,52	0
56	MG	1A	3497	1/1	0.94	0.17	39,39,39,39	0
56	MG	1w	104	1/1	0.94	0.24	83,83,83,83	0
56	MG	2B	214	1/1	0.94	0.08	70,70,70,70	0
56	MG	1A	3816	1/1	0.94	0.14	37,37,37,37	0
56	MG	1A	3688	1/1	0.94	0.15	53,53,53,53	0
56	MG	2A	3645	1/1	0.94	0.28	66,66,66,66	0
56	MG	1A	3692	1/1	0.94	0.17	22,22,22,22	0
56	MG	2a	1826	1/1	0.94	0.09	79,79,79,79	0
56	MG	1Q	201	1/1	0.94	0.07	35,35,35,35	0
56	MG	2A	3649	1/1	0.94	0.07	68,68,68,68	0
56	MG	2a	1829	1/1	0.94	0.23	53,53,53,53	0
56	MG	2A	3650	1/1	0.94	0.16	70,70,70,70	0
56	MG	1a	1694	1/1	0.94	0.14	32,32,32,32	0
56	MG	1a	1695	1/1	0.94	0.15	53,53,53,53	0
56	MG	2A	3653	1/1	0.94	0.15	56,56,56,56	0
56	MG	2A	3654	1/1	0.94	0.25	50,50,50,50	0
56	MG	2A	3655	1/1	0.94	0.10	61,61,61,61	0
56	MG	1A	3116	1/1	0.94	0.43	42,42,42,42	0
56	MG	2a	1839	1/1	0.94	0.13	93,93,93,93	0
56	MG	1Q	206	1/1	0.94	0.10	35,35,35,35	0
56	MG	1Q	207	1/1	0.94	0.12	41,41,41,41	0
56	MG	2A	3196	1/1	0.94	0.89	60,60,60,60	0
56	MG	2e	201	1/1	0.94	0.06	76,76,76,76	0
56	MG	2A	3377	1/1	0.94	0.54	48,48,48,48	0
56	MG	1R	202	1/1	0.94	0.26	38,38,38,38	0
56	MG	1A	3936	1/1	0.94	0.14	42,42,42,42	0
56	MG	1A	3500	1/1	0.94	0.17	45,45,45,45	0
56	MG	1A	4079	1/1	0.94	0.07	57,57,57,57	0
56	MG	1x	115	1/1	0.94	0.17	67,67,67,67	0
56	MG	2A	3202	1/1	0.94	0.28	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3384	1/1	0.94	0.24	53,53,53,53	0
56	MG	2A	3672	1/1	0.94	0.39	44,44,44,44	0
56	MG	1A	3695	1/1	0.94	0.10	36,36,36,36	0
56	MG	2Q	203	1/1	0.94	0.41	67,67,67,67	0
56	MG	1A	3352	1/1	0.94	0.70	55,55,55,55	0
56	MG	2A	3677	1/1	0.94	0.07	56,56,56,56	0
56	MG	1a	1709	1/1	0.94	0.06	68,68,68,68	0
56	MG	1A	3139	1/1	0.94	0.14	40,40,40,40	0
56	MG	2V	201	1/1	0.94	0.57	50,50,50,50	0
56	MG	2V	202	1/1	0.94	0.22	59,59,59,59	0
56	MG	2W	201	1/1	0.94	0.28	42,42,42,42	0
56	MG	1A	3605	1/1	0.94	0.16	52,52,52,52	0
56	MG	1A	4085	1/1	0.94	0.09	72,72,72,72	0
56	MG	2A	3009	1/1	0.94	0.09	50,50,50,50	0
56	MG	1U	206	1/1	0.94	0.44	32,32,32,32	0
56	MG	1A	3702	1/1	0.94	0.13	27,27,27,27	0
56	MG	1A	4089	1/1	0.94	0.09	58,58,58,58	0
56	MG	1A	3099	1/1	0.94	0.37	28,28,28,28	0
56	MG	1a	1723	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3216	1/1	0.94	0.10	68,68,68,68	0
56	MG	25	104	1/1	0.94	0.11	56,56,56,56	0
56	MG	2A	3217	1/1	0.94	0.14	89,89,89,89	0
56	MG	2A	3693	1/1	0.94	0.05	57,57,57,57	0
56	MG	1A	3833	1/1	0.94	0.16	50,50,50,50	0
56	MG	1A	3102	1/1	0.94	0.22	42,42,42,42	0
56	MG	1a	1727	1/1	0.94	0.10	60,60,60,60	0
56	MG	2y	105	1/1	0.94	0.09	94,94,94,94	0
56	MG	1A	3949	1/1	0.94	0.09	17,17,17,17	0
57	ZN	14	501	1/1	0.94	0.10	94,94,94,94	0
57	ZN	2Y	202	1/1	0.94	0.11	95,95,95,95	0
56	MG	2A	3699	1/1	0.94	0.06	77,77,77,77	0
56	MG	1W	201	1/1	0.94	0.24	40,40,40,40	0
56	MG	1A	3445	1/1	0.94	0.34	41,41,41,41	0
56	MG	1a	1818	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	4101	1/1	0.95	0.11	48,48,48,48	0
56	MG	1O	204	1/1	0.95	0.42	56,56,56,56	0
56	MG	2A	3744	1/1	0.95	0.19	56,56,56,56	0
56	MG	1a	1821	1/1	0.95	0.22	76,76,76,76	0
56	MG	2A	3502	1/1	0.95	0.27	59,59,59,59	0
56	MG	2A	3126	1/1	0.95	0.33	63,63,63,63	0
56	MG	2a	1625	1/1	0.95	0.10	82,82,82,82	0
56	MG	2A	3504	1/1	0.95	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1628	1/1	0.95	0.09	63,63,63,63	0
56	MG	1a	1662	1/1	0.95	0.19	55,55,55,55	0
56	MG	2A	3129	1/1	0.95	0.29	60,60,60,60	0
56	MG	1A	4103	1/1	0.95	0.10	42,42,42,42	0
56	MG	2A	3508	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3753	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3796	1/1	0.95	0.17	25,25,25,25	0
56	MG	2A	3135	1/1	0.95	0.31	66,66,66,66	0
56	MG	1A	3080	1/1	0.95	0.09	39,39,39,39	0
56	MG	2A	3137	1/1	0.95	0.24	59,59,59,59	0
56	MG	2A	3516	1/1	0.95	0.12	59,59,59,59	0
56	MG	1A	3798	1/1	0.95	0.20	47,47,47,47	0
56	MG	2A	3762	1/1	0.95	0.18	41,41,41,41	0
56	MG	2A	3302	1/1	0.95	0.35	53,53,53,53	0
56	MG	1Q	204	1/1	0.95	0.10	42,42,42,42	0
56	MG	1Q	205	1/1	0.95	0.33	36,36,36,36	0
56	MG	1A	3034	1/1	0.95	0.19	37,37,37,37	0
56	MG	2A	3767	1/1	0.95	0.16	59,59,59,59	0
56	MG	2A	3768	1/1	0.95	0.13	46,46,46,46	0
56	MG	2A	3769	1/1	0.95	0.19	52,52,52,52	0
56	MG	2A	3144	1/1	0.95	0.07	66,66,66,66	0
56	MG	2A	3771	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3699	1/1	0.95	0.09	23,23,23,23	0
56	MG	2A	3526	1/1	0.95	0.10	70,70,70,70	0
56	MG	2a	1654	1/1	0.95	0.12	61,61,61,61	0
56	MG	2A	3527	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3895	1/1	0.95	0.12	22,22,22,22	0
56	MG	1a	1833	1/1	0.95	0.22	62,62,62,62	0
56	MG	2a	1658	1/1	0.95	0.16	53,53,53,53	0
56	MG	1A	3297	1/1	0.95	0.10	40,40,40,40	0
56	MG	1a	1674	1/1	0.95	0.11	53,53,53,53	0
56	MG	1a	1675	1/1	0.95	0.17	52,52,52,52	0
56	MG	2A	3534	1/1	0.95	0.14	47,47,47,47	0
56	MG	1a	1677	1/1	0.95	0.14	46,46,46,46	0
56	MG	1A	3428	1/1	0.95	0.39	42,42,42,42	0
56	MG	2A	3784	1/1	0.95	0.27	39,39,39,39	0
56	MG	1A	3114	1/1	0.95	0.22	31,31,31,31	0
56	MG	1A	3706	1/1	0.95	0.13	33,33,33,33	0
56	MG	2A	3542	1/1	0.95	0.20	33,33,33,33	0
56	MG	1A	3358	1/1	0.95	0.14	39,39,39,39	0
56	MG	1A	3431	1/1	0.95	0.30	34,34,34,34	0
56	MG	2A	3158	1/1	0.95	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1686	1/1	0.95	0.10	51,51,51,51	0
56	MG	2a	1675	1/1	0.95	0.12	69,69,69,69	0
56	MG	2A	3552	1/1	0.95	0.16	35,35,35,35	0
56	MG	2A	3795	1/1	0.95	0.34	62,62,62,62	0
56	MG	1A	3904	1/1	0.95	0.14	22,22,22,22	0
56	MG	1U	203	1/1	0.95	0.40	33,33,33,33	0
56	MG	1A	3359	1/1	0.95	0.33	45,45,45,45	0
56	MG	2A	3163	1/1	0.95	0.17	67,67,67,67	0
56	MG	1A	3219	1/1	0.95	0.14	55,55,55,55	0
56	MG	2a	1684	1/1	0.95	0.24	64,64,64,64	0
56	MG	2A	3801	1/1	0.95	0.18	53,53,53,53	0
56	MG	2a	1686	1/1	0.95	0.15	50,50,50,50	0
56	MG	2A	3558	1/1	0.95	0.37	58,58,58,58	0
56	MG	2A	3803	1/1	0.95	0.14	46,46,46,46	0
56	MG	2A	3559	1/1	0.95	0.14	68,68,68,68	0
56	MG	1A	4124	1/1	0.95	0.25	67,67,67,67	0
56	MG	1A	4127	1/1	0.95	0.15	56,56,56,56	0
56	MG	2A	3562	1/1	0.95	0.26	57,57,57,57	0
56	MG	2A	3563	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3328	1/1	0.95	0.07	69,69,69,69	0
56	MG	2A	3330	1/1	0.95	0.26	50,50,50,50	0
56	MG	2a	1698	1/1	0.95	0.07	77,77,77,77	0
56	MG	1A	3717	1/1	0.95	0.06	27,27,27,27	0
56	MG	2a	1700	1/1	0.95	0.17	72,72,72,72	0
56	MG	2A	3813	1/1	0.95	0.33	64,64,64,64	0
56	MG	2a	1702	1/1	0.95	0.13	62,62,62,62	0
56	MG	2A	3568	1/1	0.95	0.44	43,43,43,43	0
56	MG	1V	203	1/1	0.95	0.53	34,34,34,34	0
56	MG	1A	3059	1/1	0.95	0.26	26,26,26,26	0
56	MG	2A	3573	1/1	0.95	0.12	59,59,59,59	0
56	MG	2A	3574	1/1	0.95	0.11	73,73,73,73	0
56	MG	1A	3177	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3720	1/1	0.95	0.13	31,31,31,31	0
56	MG	2A	3580	1/1	0.95	0.04	85,85,85,85	0
56	MG	1a	1702	1/1	0.95	0.18	36,36,36,36	0
56	MG	2A	3337	1/1	0.95	0.20	56,56,56,56	0
56	MG	1A	3556	1/1	0.95	0.18	18,18,18,18	0
56	MG	2A	3339	1/1	0.95	0.13	76,76,76,76	0
56	MG	1A	3100	1/1	0.95	0.18	33,33,33,33	0
56	MG	1W	206	1/1	0.95	0.30	25,25,25,25	0
56	MG	1a	1707	1/1	0.95	0.16	51,51,51,51	0
56	MG	1X	101	1/1	0.95	0.67	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4134	1/1	0.95	0.20	48,48,48,48	0
56	MG	1A	3197	1/1	0.95	0.45	42,42,42,42	0
56	MG	1x	104	1/1	0.95	0.09	74,74,74,74	0
56	MG	1A	3117	1/1	0.95	0.27	30,30,30,30	0
56	MG	1A	3439	1/1	0.95	0.12	45,45,45,45	0
56	MG	1a	1717	1/1	0.95	0.07	42,42,42,42	0
56	MG	2A	3837	1/1	0.95	0.29	73,73,73,73	0
56	MG	1a	1718	1/1	0.95	0.12	49,49,49,49	0
56	MG	1x	110	1/1	0.95	0.66	71,71,71,71	0
56	MG	2A	3840	1/1	0.95	0.34	60,60,60,60	0
56	MG	2A	3841	1/1	0.95	0.14	49,49,49,49	0
56	MG	1A	3562	1/1	0.95	0.11	26,26,26,26	0
56	MG	1A	4027	1/1	0.95	0.23	38,38,38,38	0
56	MG	1A	3160	1/1	0.95	0.14	28,28,28,28	0
56	MG	2a	1737	1/1	0.95	0.19	74,74,74,74	0
56	MG	1Z	301	1/1	0.95	0.17	45,45,45,45	0
56	MG	2a	1740	1/1	0.95	0.09	62,62,62,62	0
56	MG	1A	3564	1/1	0.95	0.15	21,21,21,21	0
56	MG	1A	3442	1/1	0.95	0.70	42,42,42,42	0
56	MG	2a	1743	1/1	0.95	0.14	58,58,58,58	0
56	MG	1A	3161	1/1	0.95	0.38	36,36,36,36	0
56	MG	2A	3004	1/1	0.95	0.09	52,52,52,52	0
56	MG	1A	3492	1/1	0.95	0.49	42,42,42,42	0
56	MG	2A	3610	1/1	0.95	0.09	76,76,76,76	0
56	MG	2A	3007	1/1	0.95	0.17	57,57,57,57	0
56	MG	1A	3370	1/1	0.95	0.18	60,60,60,60	0
56	MG	2A	3373	1/1	0.95	0.20	55,55,55,55	0
56	MG	1a	1729	1/1	0.95	0.08	77,77,77,77	0
56	MG	2A	3618	1/1	0.95	0.06	71,71,71,71	0
56	MG	1A	3371	1/1	0.95	0.20	36,36,36,36	0
56	MG	1A	3016	1/1	0.95	0.29	44,44,44,44	0
56	MG	2A	3621	1/1	0.95	0.05	60,60,60,60	0
56	MG	1A	3745	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3746	1/1	0.95	0.14	31,31,31,31	0
56	MG	1A	3748	1/1	0.95	0.24	44,44,44,44	0
56	MG	1A	3655	1/1	0.95	0.16	47,47,47,47	0
56	MG	1B	215	1/1	0.95	0.08	61,61,61,61	0
56	MG	2A	3023	1/1	0.95	0.18	37,37,37,37	0
56	MG	2A	3630	1/1	0.95	0.20	44,44,44,44	0
56	MG	2A	3870	1/1	0.95	0.09	70,70,70,70	0
56	MG	1A	3656	1/1	0.95	0.20	38,38,38,38	0
56	MG	1A	4051	1/1	0.95	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	219	1/1	0.95	0.11	57,57,57,57	0
56	MG	13	106	1/1	0.95	0.14	56,56,56,56	0
56	MG	2a	1770	1/1	0.95	0.17	71,71,71,71	0
56	MG	2A	3029	1/1	0.95	0.11	52,52,52,52	0
56	MG	2A	3636	1/1	0.95	0.13	68,68,68,68	0
56	MG	15	101	1/1	0.95	0.17	32,32,32,32	0
56	MG	15	102	1/1	0.95	0.18	26,26,26,26	0
56	MG	2A	3034	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3753	1/1	0.95	0.22	34,34,34,34	0
56	MG	1B	221	1/1	0.95	0.19	39,39,39,39	0
56	MG	2A	3397	1/1	0.95	0.19	47,47,47,47	0
56	MG	1A	3448	1/1	0.95	0.14	64,64,64,64	0
56	MG	16	102	1/1	0.95	0.35	54,54,54,54	0
56	MG	2A	3400	1/1	0.95	0.82	48,48,48,48	0
56	MG	2a	1783	1/1	0.95	0.27	72,72,72,72	0
56	MG	1A	4054	1/1	0.95	0.15	46,46,46,46	0
56	MG	1A	4055	1/1	0.95	0.39	52,52,52,52	0
56	MG	2a	1786	1/1	0.95	0.15	60,60,60,60	0
56	MG	1a	1753	1/1	0.95	0.12	62,62,62,62	0
56	MG	2A	3223	1/1	0.95	0.08	65,65,65,65	0
56	MG	2A	3656	1/1	0.95	0.10	72,72,72,72	0
56	MG	2A	3658	1/1	0.95	0.19	63,63,63,63	0
56	MG	1A	3009	1/1	0.95	0.12	29,29,29,29	0
56	MG	1B	226	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3123	1/1	0.95	0.48	31,31,31,31	0
56	MG	1A	3501	1/1	0.95	0.15	24,24,24,24	0
56	MG	2B	216	1/1	0.95	0.15	66,66,66,66	0
56	MG	2a	1798	1/1	0.95	0.10	64,64,64,64	0
56	MG	2a	1799	1/1	0.95	0.16	71,71,71,71	0
56	MG	1A	3761	1/1	0.95	0.11	49,49,49,49	0
56	MG	2A	3412	1/1	0.95	0.25	60,60,60,60	0
56	MG	2A	3413	1/1	0.95	0.38	60,60,60,60	0
56	MG	1B	230	1/1	0.95	0.14	39,39,39,39	0
56	MG	1A	3007	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3186	1/1	0.95	0.18	38,38,38,38	0
56	MG	2A	3055	1/1	0.95	0.19	54,54,54,54	0
56	MG	1A	3068	1/1	0.95	0.20	36,36,36,36	0
56	MG	1a	1606	1/1	0.95	0.14	52,52,52,52	0
56	MG	2a	1814	1/1	0.95	0.18	62,62,62,62	0
56	MG	1A	3766	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3589	1/1	0.95	0.22	21,21,21,21	0
56	MG	1A	3315	1/1	0.95	0.23	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	3211	1/1	0.95	0.15	58,58,58,58	0
56	MG	2A	3063	1/1	0.95	0.41	63,63,63,63	0
56	MG	1A	3668	1/1	0.95	0.17	17,17,17,17	0
56	MG	2E	306	1/1	0.95	0.15	54,54,54,54	0
56	MG	1D	307	1/1	0.95	0.54	45,45,45,45	0
56	MG	1A	3593	1/1	0.95	0.15	38,38,38,38	0
56	MG	1A	3348	1/1	0.95	0.29	40,40,40,40	0
56	MG	2F	304	1/1	0.95	0.47	50,50,50,50	0
56	MG	1a	1773	1/1	0.95	0.08	63,63,63,63	0
56	MG	1A	3864	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3288	1/1	0.95	0.12	55,55,55,55	0
56	MG	1a	1777	1/1	0.95	0.17	62,62,62,62	0
56	MG	1A	4076	1/1	0.95	0.13	46,46,46,46	0
56	MG	1a	1619	1/1	0.95	0.13	50,50,50,50	0
56	MG	1A	3598	1/1	0.95	0.11	17,17,17,17	0
56	MG	1E	305	1/1	0.95	0.51	39,39,39,39	0
56	MG	1A	3514	1/1	0.95	0.18	29,29,29,29	0
56	MG	2R	203	1/1	0.95	0.14	43,43,43,43	0
56	MG	2A	3696	1/1	0.95	0.13	58,58,58,58	0
56	MG	1A	3778	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3319	1/1	0.95	0.54	33,33,33,33	0
56	MG	1A	3681	1/1	0.95	0.18	26,26,26,26	0
56	MG	1E	313	1/1	0.95	0.34	38,38,38,38	0
56	MG	2A	3454	1/1	0.95	0.22	57,57,57,57	0
56	MG	2W	202	1/1	0.95	0.29	56,56,56,56	0
56	MG	1a	1628	1/1	0.95	0.18	51,51,51,51	0
56	MG	1A	3517	1/1	0.95	0.12	24,24,24,24	0
56	MG	2A	3088	1/1	0.95	0.06	65,65,65,65	0
56	MG	1F	305	1/1	0.95	0.08	36,36,36,36	0
56	MG	1a	1631	1/1	0.95	0.26	48,48,48,48	0
56	MG	1A	3683	1/1	0.95	0.12	38,38,38,38	0
56	MG	2A	3266	1/1	0.95	0.20	61,61,61,61	0
56	MG	21	101	1/1	0.95	1.33	56,56,56,56	0
56	MG	21	102	1/1	0.95	0.16	55,55,55,55	0
56	MG	23	101	1/1	0.95	0.42	59,59,59,59	0
56	MG	2A	3267	1/1	0.95	0.35	60,60,60,60	0
56	MG	25	101	1/1	0.95	0.30	55,55,55,55	0
56	MG	1F	307	1/1	0.95	0.43	33,33,33,33	0
56	MG	1a	1635	1/1	0.95	0.10	65,65,65,65	0
56	MG	1A	4084	1/1	0.95	0.47	47,47,47,47	0
56	MG	2A	3472	1/1	0.95	0.26	50,50,50,50	0
56	MG	1A	3521	1/1	0.95	0.35	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	1F	310	1/1	0.95	0.33	38,38,38,38	0
56	MG	1A	4086	1/1	0.95	0.45	48,48,48,48	0
56	MG	1A	3043	1/1	0.95	0.23	42,42,42,42	0
56	MG	1A	3420	1/1	0.95	0.58	45,45,45,45	0
56	MG	1A	3789	1/1	0.95	0.09	22,22,22,22	0
56	MG	1A	4091	1/1	0.95	0.14	50,50,50,50	0
56	MG	1A	3691	1/1	0.95	0.17	22,22,22,22	0
56	MG	2A	3484	1/1	0.95	0.19	40,40,40,40	0
56	MG	2x	104	1/1	0.95	0.14	79,79,79,79	0
56	MG	2A	3726	1/1	0.95	0.17	40,40,40,40	0
56	MG	1A	3981	1/1	0.95	0.23	33,33,33,33	0
56	MG	1A	3236	1/1	0.95	0.36	36,36,36,36	0
56	MG	2A	3111	1/1	0.95	0.14	73,73,73,73	0
56	MG	2A	3730	1/1	0.95	0.17	57,57,57,57	0
56	MG	2A	3489	1/1	0.95	0.16	53,53,53,53	0
56	MG	1A	3387	1/1	0.95	0.12	39,39,39,39	0
56	MG	2a	1610	1/1	0.95	0.10	65,65,65,65	0
56	MG	1A	3237	1/1	0.95	0.42	35,35,35,35	0
56	MG	1a	1654	1/1	0.95	0.29	58,58,58,58	0
56	MG	1A	3389	1/1	0.95	0.54	61,61,61,61	0
56	MG	1A	4099	1/1	0.95	0.16	35,35,35,35	0
57	ZN	26	102	1/1	0.95	0.11	73,73,73,73	0
56	MG	1A	3471	1/1	0.95	0.13	44,44,44,44	0
56	MG	2A	3496	1/1	0.95	0.10	43,43,43,43	0
56	MG	1w	103	1/1	0.96	0.08	68,68,68,68	0
56	MG	1A	3166	1/1	0.96	0.10	34,34,34,34	0
56	MG	1A	3516	1/1	0.96	0.20	29,29,29,29	0
56	MG	1A	3788	1/1	0.96	0.10	22,22,22,22	0
56	MG	1A	3886	1/1	0.96	0.16	28,28,28,28	0
56	MG	1A	3887	1/1	0.96	0.31	59,59,59,59	0
56	MG	1W	204	1/1	0.96	0.17	37,37,37,37	0
56	MG	1A	3108	1/1	0.96	0.42	36,36,36,36	0
56	MG	1A	3602	1/1	0.96	0.16	45,45,45,45	0
56	MG	1A	3890	1/1	0.96	0.19	55,55,55,55	0
56	MG	1A	4008	1/1	0.96	0.16	17,17,17,17	0
56	MG	1a	1710	1/1	0.96	0.12	45,45,45,45	0
56	MG	2A	3794	1/1	0.96	0.20	52,52,52,52	0
56	MG	1A	3296	1/1	0.96	0.15	49,49,49,49	0
56	MG	2A	3566	1/1	0.96	0.08	49,49,49,49	0
56	MG	2A	3348	1/1	0.96	0.07	65,65,65,65	0
56	MG	1x	108	1/1	0.96	0.11	62,62,62,62	0
56	MG	1a	1714	1/1	0.96	0.16	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	3465	1/1	0.96	0.25	45,45,45,45	0
56	MG	2A	3572	1/1	0.96	0.46	65,65,65,65	0
56	MG	1A	3011	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3088	1/1	0.96	0.13	25,25,25,25	0
56	MG	2A	3575	1/1	0.96	0.11	49,49,49,49	0
56	MG	1A	3196	1/1	0.96	0.46	42,42,42,42	0
56	MG	1y	101	1/1	0.96	0.53	42,42,42,42	0
56	MG	2a	1669	1/1	0.96	0.22	70,70,70,70	0
56	MG	2A	3579	1/1	0.96	0.12	65,65,65,65	0
56	MG	2A	3361	1/1	0.96	0.18	47,47,47,47	0
56	MG	2A	3362	1/1	0.96	0.39	46,46,46,46	0
56	MG	1B	201	1/1	0.96	0.10	39,39,39,39	0
56	MG	2A	3364	1/1	0.96	0.33	48,48,48,48	0
56	MG	1A	4016	1/1	0.96	0.11	40,40,40,40	0
56	MG	1A	3608	1/1	0.96	0.10	55,55,55,55	0
56	MG	10	101	1/1	0.96	0.26	47,47,47,47	0
56	MG	1A	3090	1/1	0.96	0.62	38,38,38,38	0
56	MG	1A	3302	1/1	0.96	0.69	49,49,49,49	0
56	MG	1A	3033	1/1	0.96	0.27	27,27,27,27	0
56	MG	1A	4022	1/1	0.96	0.18	45,45,45,45	0
56	MG	1A	4024	1/1	0.96	0.25	35,35,35,35	0
56	MG	1A	3703	1/1	0.96	0.48	30,30,30,30	0
56	MG	1A	3536	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	4028	1/1	0.96	0.55	38,38,38,38	0
56	MG	1A	3113	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	4031	1/1	0.96	0.17	21,21,21,21	0
56	MG	2A	3598	1/1	0.96	0.18	75,75,75,75	0
56	MG	2A	3017	1/1	0.96	0.12	34,34,34,34	0
56	MG	12	102	1/1	0.96	0.18	48,48,48,48	0
56	MG	1A	3200	1/1	0.96	0.23	25,25,25,25	0
56	MG	2a	1695	1/1	0.96	0.16	58,58,58,58	0
56	MG	2A	3602	1/1	0.96	0.21	61,61,61,61	0
56	MG	2A	3022	1/1	0.96	0.20	50,50,50,50	0
56	MG	1A	3060	1/1	0.96	0.32	24,24,24,24	0
56	MG	2A	3605	1/1	0.96	0.27	69,69,69,69	0
56	MG	1A	3345	1/1	0.96	0.13	45,45,45,45	0
56	MG	1A	3386	1/1	0.96	0.24	48,48,48,48	0
56	MG	2A	3836	1/1	0.96	0.10	59,59,59,59	0
56	MG	2A	3386	1/1	0.96	0.14	41,41,41,41	0
56	MG	1A	3622	1/1	0.96	0.13	46,46,46,46	0
56	MG	1A	3143	1/1	0.96	0.73	39,39,39,39	0
56	MG	1A	3546	1/1	0.96	0.46	55,55,55,55	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	0.96	0.65	30,30,30,30	0
56	MG	2A	3842	1/1	0.96	0.06	64,64,64,64	0
56	MG	1A	3061	1/1	0.96	0.54	33,33,33,33	0
56	MG	2A	3615	1/1	0.96	0.17	48,48,48,48	0
56	MG	1A	3721	1/1	0.96	0.16	32,32,32,32	0
56	MG	1A	3021	1/1	0.96	0.11	17,17,17,17	0
56	MG	2a	1714	1/1	0.96	0.13	77,77,77,77	0
56	MG	17	104	1/1	0.96	0.20	55,55,55,55	0
56	MG	2A	3037	1/1	0.96	0.19	75,75,75,75	0
56	MG	2A	3850	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	4047	1/1	0.96	0.11	37,37,37,37	0
56	MG	1A	4048	1/1	0.96	0.11	28,28,28,28	0
56	MG	1a	1752	1/1	0.96	0.09	41,41,41,41	0
56	MG	2A	3625	1/1	0.96	0.17	60,60,60,60	0
56	MG	1A	3631	1/1	0.96	0.13	52,52,52,52	0
56	MG	2A	3403	1/1	0.96	0.26	56,56,56,56	0
56	MG	2A	3404	1/1	0.96	0.59	72,72,72,72	0
56	MG	1a	1754	1/1	0.96	0.05	56,56,56,56	0
56	MG	1A	3820	1/1	0.96	0.20	61,61,61,61	0
56	MG	18	106	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3633	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3729	1/1	0.96	0.13	57,57,57,57	0
56	MG	2A	3048	1/1	0.96	0.17	56,56,56,56	0
56	MG	1A	3730	1/1	0.96	0.13	35,35,35,35	0
56	MG	1a	1602	1/1	0.96	0.16	63,63,63,63	0
56	MG	2A	3051	1/1	0.96	0.23	61,61,61,61	0
56	MG	1B	234	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3148	1/1	0.96	0.18	30,30,30,30	0
56	MG	2A	3641	1/1	0.96	0.27	31,31,31,31	0
56	MG	2A	3642	1/1	0.96	0.27	76,76,76,76	0
56	MG	2A	3871	1/1	0.96	0.13	51,51,51,51	0
56	MG	1B	236	1/1	0.96	0.16	49,49,49,49	0
56	MG	1A	3932	1/1	0.96	0.08	60,60,60,60	0
56	MG	2A	3874	1/1	0.96	0.12	71,71,71,71	0
56	MG	1A	3828	1/1	0.96	0.12	45,45,45,45	0
56	MG	1D	303	1/1	0.96	0.13	23,23,23,23	0
56	MG	1A	3635	1/1	0.96	0.04	43,43,43,43	0
56	MG	1A	3636	1/1	0.96	0.15	50,50,50,50	0
56	MG	1A	4060	1/1	0.96	0.18	39,39,39,39	0
56	MG	1A	3553	1/1	0.96	0.21	29,29,29,29	0
56	MG	2A	3428	1/1	0.96	0.51	51,51,51,51	0
56	MG	1A	3242	1/1	0.96	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3097	1/1	0.96	0.45	36,36,36,36	0
56	MG	2A	3431	1/1	0.96	0.36	57,57,57,57	0
56	MG	2a	1755	1/1	0.96	0.12	56,56,56,56	0
56	MG	2A	3432	1/1	0.96	0.11	28,28,28,28	0
56	MG	1A	3835	1/1	0.96	0.15	49,49,49,49	0
56	MG	2A	3661	1/1	0.96	0.25	51,51,51,51	0
56	MG	2A	3434	1/1	0.96	0.29	36,36,36,36	0
56	MG	1A	4066	1/1	0.96	0.15	54,54,54,54	0
56	MG	2A	3068	1/1	0.96	0.28	51,51,51,51	0
56	MG	2B	208	1/1	0.96	0.14	65,65,65,65	0
56	MG	1A	3394	1/1	0.96	0.28	43,43,43,43	0
56	MG	2A	3070	1/1	0.96	0.14	48,48,48,48	0
56	MG	2A	3071	1/1	0.96	0.20	30,30,30,30	0
56	MG	1E	304	1/1	0.96	0.25	29,29,29,29	0
56	MG	1A	3118	1/1	0.96	0.23	31,31,31,31	0
56	MG	1A	4069	1/1	0.96	0.17	49,49,49,49	0
56	MG	1a	1622	1/1	0.96	0.24	62,62,62,62	0
56	MG	1A	3077	1/1	0.96	0.20	19,19,19,19	0
56	MG	1a	1782	1/1	0.96	0.12	70,70,70,70	0
56	MG	1A	3560	1/1	0.96	0.06	38,38,38,38	0
56	MG	2A	3676	1/1	0.96	0.15	60,60,60,60	0
56	MG	2A	3449	1/1	0.96	0.24	58,58,58,58	0
56	MG	2A	3257	1/1	0.96	0.32	74,74,74,74	0
56	MG	1E	311	1/1	0.96	0.19	18,18,18,18	0
56	MG	2A	3080	1/1	0.96	0.30	62,62,62,62	0
56	MG	2A	3453	1/1	0.96	0.29	60,60,60,60	0
56	MG	1A	3212	1/1	0.96	0.96	49,49,49,49	0
56	MG	1A	3281	1/1	0.96	0.34	45,45,45,45	0
56	MG	1F	302	1/1	0.96	0.46	33,33,33,33	0
56	MG	2A	3458	1/1	0.96	0.17	49,49,49,49	0
56	MG	2A	3459	1/1	0.96	0.11	63,63,63,63	0
56	MG	1F	303	1/1	0.96	0.13	30,30,30,30	0
56	MG	1a	1790	1/1	0.96	0.10	51,51,51,51	0
56	MG	2A	3463	1/1	0.96	0.24	43,43,43,43	0
56	MG	1A	3843	1/1	0.96	0.13	44,44,44,44	0
56	MG	1A	3042	1/1	0.96	0.20	37,37,37,37	0
56	MG	1A	3747	1/1	0.96	0.21	17,17,17,17	0
56	MG	1A	3035	1/1	0.96	0.33	18,18,18,18	0
56	MG	2a	1794	1/1	0.96	0.06	74,74,74,74	0
56	MG	2A	3468	1/1	0.96	0.12	32,32,32,32	0
56	MG	1A	3565	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3321	1/1	0.96	0.67	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3093	1/1	0.96	0.11	34,34,34,34	0
56	MG	1A	3752	1/1	0.96	0.16	25,25,25,25	0
56	MG	1A	3360	1/1	0.96	0.12	45,45,45,45	0
56	MG	2A	3703	1/1	0.96	0.33	83,83,83,83	0
56	MG	1a	1641	1/1	0.96	0.12	57,57,57,57	0
56	MG	1a	1642	1/1	0.96	0.14	48,48,48,48	0
56	MG	1a	1643	1/1	0.96	0.19	65,65,65,65	0
56	MG	2A	3707	1/1	0.96	0.17	68,68,68,68	0
56	MG	1A	3101	1/1	0.96	0.20	47,47,47,47	0
56	MG	2A	3479	1/1	0.96	0.19	51,51,51,51	0
56	MG	2U	202	1/1	0.96	0.28	62,62,62,62	0
56	MG	2a	1812	1/1	0.96	0.09	76,76,76,76	0
56	MG	1A	3572	1/1	0.96	0.16	20,20,20,20	0
56	MG	1A	3757	1/1	0.96	0.15	48,48,48,48	0
56	MG	1A	3216	1/1	0.96	0.19	29,29,29,29	0
56	MG	2A	3483	1/1	0.96	0.21	56,56,56,56	0
56	MG	1A	3575	1/1	0.96	0.13	46,46,46,46	0
56	MG	2A	3107	1/1	0.96	0.38	51,51,51,51	0
56	MG	1A	3964	1/1	0.96	0.15	22,22,22,22	0
56	MG	2Y	201	1/1	0.96	0.30	55,55,55,55	0
56	MG	2A	3487	1/1	0.96	0.14	50,50,50,50	0
56	MG	1A	3760	1/1	0.96	0.18	47,47,47,47	0
56	MG	1A	3966	1/1	0.96	0.17	15,15,15,15	0
56	MG	1a	1813	1/1	0.96	0.14	62,62,62,62	0
56	MG	1A	3286	1/1	0.96	0.50	26,26,26,26	0
56	MG	2A	3114	1/1	0.96	0.11	55,55,55,55	0
56	MG	1N	204	1/1	0.96	0.74	45,45,45,45	0
56	MG	1A	4092	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3326	1/1	0.96	0.30	33,33,33,33	0
56	MG	25	102	1/1	0.96	0.55	46,46,46,46	0
56	MG	1A	3969	1/1	0.96	0.12	43,43,43,43	0
56	MG	1a	1658	1/1	0.96	0.16	54,54,54,54	0
56	MG	1O	202	1/1	0.96	0.88	53,53,53,53	0
56	MG	1A	3036	1/1	0.96	0.40	32,32,32,32	0
56	MG	1A	3971	1/1	0.96	0.12	32,32,32,32	0
56	MG	2A	3123	1/1	0.96	0.52	52,52,52,52	0
56	MG	2A	3124	1/1	0.96	0.07	78,78,78,78	0
56	MG	1P	203	1/1	0.96	0.17	31,31,31,31	0
56	MG	1A	3764	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3046	1/1	0.96	0.12	26,26,26,26	0
56	MG	2A	3130	1/1	0.96	0.39	40,40,40,40	0
56	MG	2A	3132	1/1	0.96	0.30	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1665	1/1	0.96	0.15	68,68,68,68	0
56	MG	1A	3037	1/1	0.96	0.73	40,40,40,40	0
56	MG	2l	201	1/1	0.96	0.93	77,77,77,77	0
56	MG	2A	3511	1/1	0.96	0.45	58,58,58,58	0
56	MG	2A	3513	1/1	0.96	0.09	36,36,36,36	0
56	MG	1Q	202	1/1	0.96	0.19	56,56,56,56	0
56	MG	1A	3583	1/1	0.96	0.19	26,26,26,26	0
56	MG	1A	3504	1/1	0.96	0.11	49,49,49,49	0
56	MG	2A	3517	1/1	0.96	0.32	54,54,54,54	0
56	MG	1A	4102	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3505	1/1	0.96	0.15	32,32,32,32	0
56	MG	1A	3586	1/1	0.96	0.17	16,16,16,16	0
56	MG	1R	201	1/1	0.96	0.52	45,45,45,45	0
56	MG	2A	3522	1/1	0.96	0.20	63,63,63,63	0
56	MG	2A	3754	1/1	0.96	0.11	70,70,70,70	0
56	MG	1A	3410	1/1	0.96	0.20	38,38,38,38	0
56	MG	1A	4108	1/1	0.96	0.27	34,34,34,34	0
56	MG	1A	3454	1/1	0.96	0.39	36,36,36,36	0
56	MG	2a	1619	1/1	0.96	0.35	56,56,56,56	0
56	MG	1A	3984	1/1	0.96	0.16	43,43,43,43	0
56	MG	1a	1680	1/1	0.96	0.27	56,56,56,56	0
56	MG	1A	3672	1/1	0.96	0.05	50,50,50,50	0
56	MG	1b	302	1/1	0.96	0.08	71,71,71,71	0
56	MG	1A	3674	1/1	0.96	0.16	21,21,21,21	0
56	MG	1T	202	1/1	0.96	0.14	52,52,52,52	0
56	MG	1A	3105	1/1	0.96	0.70	35,35,35,35	0
56	MG	2a	1627	1/1	0.96	0.15	52,52,52,52	0
56	MG	1A	3131	1/1	0.96	0.10	43,43,43,43	0
56	MG	2A	3535	1/1	0.96	0.14	43,43,43,43	0
56	MG	1A	3510	1/1	0.96	0.15	17,17,17,17	0
56	MG	1a	1689	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3332	1/1	0.96	0.75	50,50,50,50	0
56	MG	1A	3513	1/1	0.96	0.18	27,27,27,27	0
56	MG	2A	3329	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3543	1/1	0.96	0.44	69,69,69,69	0
56	MG	2y	107	1/1	0.96	0.06	77,77,77,77	0
57	ZN	1Y	205	1/1	0.96	0.15	63,63,63,63	0
56	MG	2A	3544	1/1	0.96	0.20	63,63,63,63	0
57	ZN	1n	102	1/1	0.96	0.15	69,69,69,69	0
56	MG	1A	3596	1/1	0.96	0.17	26,26,26,26	0
56	MG	1A	3879	1/1	0.96	0.08	71,71,71,71	0
56	MG	1V	201	1/1	0.96	0.24	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	Y7K	1a	1842	33/33	0.96	0.23	51,58,66,70	0
56	MG	1A	3459	1/1	0.96	0.36	34,34,34,34	0
60	K	1x	101	1/1	0.96	0.15	59,59,59,59	0
56	MG	1A	3882	1/1	0.96	0.14	26,26,26,26	0
56	MG	2A	3016	1/1	0.97	0.13	54,54,54,54	0
56	MG	1A	4088	1/1	0.97	0.09	57,57,57,57	0
56	MG	2A	3018	1/1	0.97	0.31	48,48,48,48	0
56	MG	1A	3982	1/1	0.97	0.30	40,40,40,40	0
56	MG	1A	3093	1/1	0.97	0.17	36,36,36,36	0
56	MG	1a	1613	1/1	0.97	0.11	65,65,65,65	0
56	MG	1A	3647	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3267	1/1	0.97	0.21	53,53,53,53	0
56	MG	1A	3803	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3987	1/1	0.97	0.22	57,57,57,57	0
56	MG	1A	3649	1/1	0.97	0.14	20,20,20,20	0
56	MG	1F	312	1/1	0.97	0.10	44,44,44,44	0
56	MG	1A	3727	1/1	0.97	0.20	43,43,43,43	0
56	MG	2A	3031	1/1	0.97	0.12	36,36,36,36	0
56	MG	2B	204	1/1	0.97	0.31	77,77,77,77	0
56	MG	1A	3235	1/1	0.97	0.22	29,29,29,29	0
56	MG	2A	3033	1/1	0.97	0.47	43,43,43,43	0
56	MG	2A	3352	1/1	0.97	0.76	62,62,62,62	0
56	MG	1A	3532	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3441	1/1	0.97	0.49	34,34,34,34	0
56	MG	2A	3355	1/1	0.97	0.32	43,43,43,43	0
56	MG	1G	204	1/1	0.97	0.26	46,46,46,46	0
56	MG	2A	3358	1/1	0.97	0.19	55,55,55,55	0
56	MG	1A	3811	1/1	0.97	0.14	27,27,27,27	0
56	MG	2a	1719	1/1	0.97	0.10	64,64,64,64	0
56	MG	2A	3717	1/1	0.97	0.29	60,60,60,60	0
56	MG	1A	3301	1/1	0.97	0.41	46,46,46,46	0
56	MG	1A	3591	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	3017	1/1	0.97	0.24	64,64,64,64	0
56	MG	1A	4104	1/1	0.97	0.09	17,17,17,17	0
56	MG	1A	3815	1/1	0.97	0.21	56,56,56,56	0
56	MG	1A	3999	1/1	0.97	0.19	36,36,36,36	0
56	MG	1A	3537	1/1	0.97	0.20	11,11,11,11	0
56	MG	2A	3368	1/1	0.97	0.12	53,53,53,53	0
56	MG	2D	303	1/1	0.97	0.14	37,37,37,37	0
56	MG	2A	3206	1/1	0.97	0.37	66,66,66,66	0
56	MG	1A	3119	1/1	0.97	0.15	15,15,15,15	0
56	MG	1a	1634	1/1	0.97	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3238	1/1	0.97	0.19	23,23,23,23	0
56	MG	2A	3549	1/1	0.97	0.20	31,31,31,31	0
56	MG	1A	4003	1/1	0.97	0.11	27,27,27,27	0
56	MG	1a	1637	1/1	0.97	0.22	43,43,43,43	0
56	MG	1A	3239	1/1	0.97	0.37	28,28,28,28	0
56	MG	2a	1739	1/1	0.97	0.15	57,57,57,57	0
56	MG	1a	1639	1/1	0.97	0.16	58,58,58,58	0
56	MG	1O	205	1/1	0.97	0.31	64,64,64,64	0
56	MG	1O	206	1/1	0.97	0.14	50,50,50,50	0
56	MG	1P	201	1/1	0.97	0.15	28,28,28,28	0
56	MG	2A	3738	1/1	0.97	0.13	60,60,60,60	0
56	MG	1P	202	1/1	0.97	0.35	30,30,30,30	0
56	MG	1A	3908	1/1	0.97	0.09	39,39,39,39	0
56	MG	1A	3106	1/1	0.97	0.44	32,32,32,32	0
56	MG	1A	3910	1/1	0.97	0.13	38,38,38,38	0
56	MG	2O	201	1/1	0.97	0.08	72,72,72,72	0
56	MG	1A	3542	1/1	0.97	0.15	39,39,39,39	0
56	MG	1A	3141	1/1	0.97	0.08	56,56,56,56	0
56	MG	1A	4010	1/1	0.97	0.09	25,25,25,25	0
56	MG	2Q	201	1/1	0.97	0.06	59,59,59,59	0
56	MG	2A	3387	1/1	0.97	0.07	61,61,61,61	0
56	MG	1A	3742	1/1	0.97	0.13	55,55,55,55	0
56	MG	1A	3544	1/1	0.97	0.10	28,28,28,28	0
56	MG	1A	4121	1/1	0.97	0.08	53,53,53,53	0
56	MG	1A	3916	1/1	0.97	0.08	50,50,50,50	0
56	MG	2A	3570	1/1	0.97	0.19	50,50,50,50	0
56	MG	1a	1796	1/1	0.97	0.15	64,64,64,64	0
56	MG	2U	201	1/1	0.97	0.27	55,55,55,55	0
56	MG	1A	4123	1/1	0.97	0.41	59,59,59,59	0
56	MG	1A	3744	1/1	0.97	0.17	45,45,45,45	0
56	MG	1A	4125	1/1	0.97	0.23	49,49,49,49	0
56	MG	1A	4126	1/1	0.97	0.77	34,34,34,34	0
56	MG	2A	3576	1/1	0.97	0.20	71,71,71,71	0
56	MG	1A	3107	1/1	0.97	0.70	38,38,38,38	0
56	MG	1A	3122	1/1	0.97	0.23	26,26,26,26	0
56	MG	1A	4018	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3547	1/1	0.97	0.12	28,28,28,28	0
56	MG	1A	3669	1/1	0.97	0.16	16,16,16,16	0
56	MG	1A	3922	1/1	0.97	0.11	44,44,44,44	0
56	MG	1U	202	1/1	0.97	0.24	28,28,28,28	0
56	MG	1A	3548	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	4023	1/1	0.97	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1811	1/1	0.97	0.12	57,57,57,57	0
56	MG	2A	3084	1/1	0.97	0.59	57,57,57,57	0
56	MG	2A	3588	1/1	0.97	0.33	44,44,44,44	0
56	MG	1U	205	1/1	0.97	0.10	29,29,29,29	0
56	MG	1A	3169	1/1	0.97	0.17	32,32,32,32	0
56	MG	1A	3218	1/1	0.97	0.15	30,30,30,30	0
56	MG	1A	3673	1/1	0.97	0.09	24,24,24,24	0
56	MG	2A	3416	1/1	0.97	0.45	46,46,46,46	0
56	MG	1A	3928	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3030	1/1	0.97	0.20	22,22,22,22	0
56	MG	2A	3779	1/1	0.97	0.12	66,66,66,66	0
56	MG	1A	4030	1/1	0.97	0.18	23,23,23,23	0
56	MG	1A	3611	1/1	0.97	0.16	59,59,59,59	0
56	MG	1A	3383	1/1	0.97	0.12	27,27,27,27	0
56	MG	1a	1678	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3841	1/1	0.97	0.15	58,58,58,58	0
56	MG	1A	3082	1/1	0.97	0.40	42,42,42,42	0
56	MG	2A	3786	1/1	0.97	0.17	51,51,51,51	0
56	MG	1A	3678	1/1	0.97	0.14	18,18,18,18	0
56	MG	1A	3457	1/1	0.97	0.39	31,31,31,31	0
56	MG	2A	3099	1/1	0.97	0.07	46,46,46,46	0
56	MG	1W	205	1/1	0.97	0.28	36,36,36,36	0
56	MG	2a	1802	1/1	0.97	0.18	71,71,71,71	0
56	MG	1A	3680	1/1	0.97	0.15	44,44,44,44	0
56	MG	1a	1685	1/1	0.97	0.10	54,54,54,54	0
56	MG	1W	207	1/1	0.97	0.23	38,38,38,38	0
56	MG	1a	1687	1/1	0.97	0.15	65,65,65,65	0
56	MG	1a	1831	1/1	0.97	0.12	50,50,50,50	0
56	MG	1A	3146	1/1	0.97	0.51	32,32,32,32	0
56	MG	2A	3437	1/1	0.97	0.06	58,58,58,58	0
56	MG	2A	3109	1/1	0.97	0.26	58,58,58,58	0
56	MG	1A	4039	1/1	0.97	0.11	54,54,54,54	0
56	MG	1A	4040	1/1	0.97	0.11	57,57,57,57	0
56	MG	2A	3617	1/1	0.97	0.11	65,65,65,65	0
56	MG	1A	3617	1/1	0.97	0.18	23,23,23,23	0
56	MG	1A	3940	1/1	0.97	0.25	27,27,27,27	0
56	MG	1A	3031	1/1	0.97	0.38	26,26,26,26	0
56	MG	1B	216	1/1	0.97	0.30	51,51,51,51	0
56	MG	1A	3149	1/1	0.97	0.17	18,18,18,18	0
56	MG	1A	3317	1/1	0.97	0.17	36,36,36,36	0
56	MG	2A	3808	1/1	0.97	0.07	54,54,54,54	0
56	MG	1A	3687	1/1	0.97	0.21	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	4049	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	3022	1/1	0.97	0.10	32,32,32,32	0
56	MG	1a	1701	1/1	0.97	0.11	33,33,33,33	0
56	MG	1A	3946	1/1	0.97	0.18	23,23,23,23	0
56	MG	1A	3690	1/1	0.97	0.14	16,16,16,16	0
56	MG	1A	3010	1/1	0.97	0.12	28,28,28,28	0
56	MG	1l	202	1/1	0.97	0.14	56,56,56,56	0
56	MG	2A	3127	1/1	0.97	0.20	45,45,45,45	0
56	MG	2a	1832	1/1	0.97	0.33	50,50,50,50	0
56	MG	2a	1833	1/1	0.97	0.22	67,67,67,67	0
56	MG	1A	3623	1/1	0.97	0.27	51,51,51,51	0
56	MG	2A	3457	1/1	0.97	0.11	47,47,47,47	0
56	MG	1A	3153	1/1	0.97	0.25	38,38,38,38	0
56	MG	1A	3154	1/1	0.97	0.18	65,65,65,65	0
56	MG	2A	3131	1/1	0.97	0.14	41,41,41,41	0
56	MG	1A	3858	1/1	0.97	0.23	41,41,41,41	0
56	MG	1A	3775	1/1	0.97	0.28	36,36,36,36	0
56	MG	1a	1711	1/1	0.97	0.17	47,47,47,47	0
56	MG	2A	3644	1/1	0.97	0.16	30,30,30,30	0
56	MG	1a	1712	1/1	0.97	0.11	55,55,55,55	0
56	MG	1A	3015	1/1	0.97	0.23	26,26,26,26	0
56	MG	2a	1646	1/1	0.97	0.12	82,82,82,82	0
56	MG	1A	3289	1/1	0.97	0.18	38,38,38,38	0
56	MG	1A	3290	1/1	0.97	0.32	67,67,67,67	0
56	MG	1A	3863	1/1	0.97	0.27	25,25,25,25	0
56	MG	1A	4063	1/1	0.97	0.20	48,48,48,48	0
56	MG	1A	3512	1/1	0.97	0.17	11,11,11,11	0
56	MG	13	105	1/1	0.97	0.09	54,54,54,54	0
56	MG	2A	3473	1/1	0.97	0.10	71,71,71,71	0
56	MG	1A	3569	1/1	0.97	0.13	20,20,20,20	0
56	MG	1A	3960	1/1	0.97	0.19	43,43,43,43	0
56	MG	2A	3657	1/1	0.97	0.16	61,61,61,61	0
56	MG	1A	3700	1/1	0.97	0.11	18,18,18,18	0
56	MG	1A	3962	1/1	0.97	0.14	11,11,11,11	0
56	MG	1A	3701	1/1	0.97	0.12	34,34,34,34	0
56	MG	1a	1725	1/1	0.97	0.08	57,57,57,57	0
56	MG	1A	3259	1/1	0.97	0.13	55,55,55,55	0
56	MG	2A	3152	1/1	0.97	0.17	39,39,39,39	0
56	MG	1A	3472	1/1	0.97	0.11	41,41,41,41	0
56	MG	1A	3786	1/1	0.97	0.12	35,35,35,35	0
56	MG	1D	310	1/1	0.97	0.13	53,53,53,53	0
56	MG	1x	111	1/1	0.97	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1x	112	1/1	0.97	0.13	62,62,62,62	0
56	MG	1A	3064	1/1	0.97	0.30	39,39,39,39	0
56	MG	18	102	1/1	0.97	0.67	41,41,41,41	0
56	MG	1A	3205	1/1	0.97	0.29	43,43,43,43	0
56	MG	1A	3132	1/1	0.97	0.32	31,31,31,31	0
56	MG	2a	1672	1/1	0.97	0.12	64,64,64,64	0
56	MG	1A	3707	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3520	1/1	0.97	0.15	49,49,49,49	0
56	MG	2A	3164	1/1	0.97	0.20	65,65,65,65	0
56	MG	1A	3027	1/1	0.97	0.51	24,24,24,24	0
56	MG	1a	1738	1/1	0.97	0.14	51,51,51,51	0
56	MG	1A	3973	1/1	0.97	0.16	54,54,54,54	0
56	MG	2a	1679	1/1	0.97	0.18	42,42,42,42	0
56	MG	1A	3974	1/1	0.97	0.18	51,51,51,51	0
56	MG	2A	3006	1/1	0.97	0.13	42,42,42,42	0
56	MG	1A	3712	1/1	0.97	0.18	45,45,45,45	0
56	MG	2A	3684	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	3713	1/1	0.97	0.48	31,31,31,31	0
56	MG	1A	3522	1/1	0.97	0.17	18,18,18,18	0
56	MG	1A	3264	1/1	0.97	0.43	33,33,33,33	0
56	MG	2A	3011	1/1	0.97	0.23	47,47,47,47	0
56	MG	2A	3689	1/1	0.97	0.15	61,61,61,61	0
57	ZN	2n	501	1/1	0.97	0.05	109,109,109,109	0
56	MG	1A	3001	1/1	0.97	0.09	36,36,36,36	0
56	MG	1E	314	1/1	0.97	0.16	56,56,56,56	0
56	MG	1A	3644	1/1	0.97	0.10	33,33,33,33	0
56	MG	1A	3526	1/1	0.97	0.11	15,15,15,15	0
56	MG	2A	3359	1/1	0.98	0.29	53,53,53,53	0
56	MG	1U	201	1/1	0.98	0.20	26,26,26,26	0
56	MG	2A	3139	1/1	0.98	0.14	34,34,34,34	0
56	MG	1A	3580	1/1	0.98	0.20	22,22,22,22	0
56	MG	1A	3137	1/1	0.98	0.32	31,31,31,31	0
56	MG	2A	3142	1/1	0.98	0.32	60,60,60,60	0
56	MG	1A	3805	1/1	0.98	0.14	40,40,40,40	0
56	MG	1A	3632	1/1	0.98	0.11	48,48,48,48	0
56	MG	1A	3498	1/1	0.98	0.17	22,22,22,22	0
56	MG	1A	3685	1/1	0.98	0.18	17,17,17,17	0
56	MG	1U	208	1/1	0.98	0.50	36,36,36,36	0
56	MG	1D	304	1/1	0.98	0.46	28,28,28,28	0
56	MG	1U	210	1/1	0.98	0.53	46,46,46,46	0
56	MG	2a	1766	1/1	0.98	0.18	73,73,73,73	0
56	MG	1A	3089	1/1	0.98	0.51	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3012	1/1	0.98	0.10	31,31,31,31	0
56	MG	2A	3613	1/1	0.98	0.14	60,60,60,60	0
56	MG	2A	3741	1/1	0.98	0.27	31,31,31,31	0
56	MG	1A	3091	1/1	0.98	0.19	28,28,28,28	0
56	MG	2a	1772	1/1	0.98	0.12	54,54,54,54	0
56	MG	1V	204	1/1	0.98	0.28	31,31,31,31	0
56	MG	1D	308	1/1	0.98	0.36	32,32,32,32	0
56	MG	1A	4105	1/1	0.98	0.14	47,47,47,47	0
56	MG	1A	3689	1/1	0.98	0.11	48,48,48,48	0
56	MG	2a	1640	1/1	0.98	0.09	74,74,74,74	0
56	MG	1A	3750	1/1	0.98	0.15	58,58,58,58	0
56	MG	1A	3003	1/1	0.98	0.10	24,24,24,24	0
56	MG	1W	203	1/1	0.98	0.32	35,35,35,35	0
56	MG	2A	3622	1/1	0.98	0.09	65,65,65,65	0
56	MG	2A	3052	1/1	0.98	0.25	53,53,53,53	0
56	MG	1A	3254	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3255	1/1	0.98	0.17	35,35,35,35	0
56	MG	1a	1735	1/1	0.98	0.04	48,48,48,48	0
56	MG	1A	3051	1/1	0.98	0.13	25,25,25,25	0
56	MG	1A	3473	1/1	0.98	0.38	38,38,38,38	0
56	MG	2A	3757	1/1	0.98	0.12	69,69,69,69	0
56	MG	2B	203	1/1	0.98	0.33	73,73,73,73	0
56	MG	1A	3756	1/1	0.98	0.11	36,36,36,36	0
56	MG	1a	1837	1/1	0.98	0.18	48,48,48,48	0
56	MG	1A	3821	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3061	1/1	0.98	0.30	49,49,49,49	0
56	MG	1E	307	1/1	0.98	0.11	44,44,44,44	0
56	MG	2A	3512	1/1	0.98	0.19	39,39,39,39	0
56	MG	2A	3394	1/1	0.98	0.18	28,28,28,28	0
56	MG	1A	3208	1/1	0.98	0.40	40,40,40,40	0
56	MG	2A	3637	1/1	0.98	0.11	47,47,47,47	0
56	MG	2a	1800	1/1	0.98	0.31	65,65,65,65	0
56	MG	1A	3823	1/1	0.98	0.11	30,30,30,30	0
56	MG	1a	1743	1/1	0.98	0.14	56,56,56,56	0
56	MG	1A	3444	1/1	0.98	0.35	38,38,38,38	0
56	MG	1A	3825	1/1	0.98	0.14	43,43,43,43	0
56	MG	1e	202	1/1	0.98	0.41	61,61,61,61	0
56	MG	2a	1806	1/1	0.98	0.09	71,71,71,71	0
56	MG	2A	3643	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	3893	1/1	0.98	0.14	42,42,42,42	0
56	MG	1A	4044	1/1	0.98	0.08	32,32,32,32	0
56	MG	2A	3646	1/1	0.98	0.11	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1F	301	1/1	0.98	0.41	37,37,37,37	0
56	MG	1A	3163	1/1	0.98	0.32	32,32,32,32	0
56	MG	1A	3079	1/1	0.98	0.29	38,38,38,38	0
56	MG	1A	3023	1/1	0.98	0.13	20,20,20,20	0
56	MG	1A	3897	1/1	0.98	0.16	18,18,18,18	0
56	MG	1a	1657	1/1	0.98	0.17	65,65,65,65	0
56	MG	1A	3081	1/1	0.98	0.16	23,23,23,23	0
56	MG	2A	3529	1/1	0.98	0.19	56,56,56,56	0
56	MG	1A	3830	1/1	0.98	0.14	22,22,22,22	0
56	MG	1A	3024	1/1	0.98	0.11	39,39,39,39	0
56	MG	1A	3147	1/1	0.98	0.50	28,28,28,28	0
56	MG	10	108	1/1	0.98	0.13	57,57,57,57	0
56	MG	1A	3600	1/1	0.98	0.15	27,27,27,27	0
56	MG	1A	3651	1/1	0.98	0.15	46,46,46,46	0
56	MG	1A	3905	1/1	0.98	0.08	27,27,27,27	0
56	MG	1A	3554	1/1	0.98	0.13	29,29,29,29	0
56	MG	2A	3538	1/1	0.98	0.12	71,71,71,71	0
56	MG	2A	3539	1/1	0.98	0.15	55,55,55,55	0
56	MG	1A	3907	1/1	0.98	0.15	23,23,23,23	0
56	MG	2A	3421	1/1	0.98	0.05	59,59,59,59	0
56	MG	1A	3369	1/1	0.98	0.24	32,32,32,32	0
56	MG	1A	3192	1/1	0.98	0.29	38,38,38,38	0
56	MG	13	103	1/1	0.98	0.17	32,32,32,32	0
56	MG	1A	3062	1/1	0.98	0.11	11,11,11,11	0
56	MG	1A	3911	1/1	0.98	0.18	28,28,28,28	0
56	MG	1A	3518	1/1	0.98	0.18	27,27,27,27	0
56	MG	2A	3548	1/1	0.98	0.16	55,55,55,55	0
56	MG	2A	3674	1/1	0.98	0.22	61,61,61,61	0
56	MG	1A	3711	1/1	0.98	0.17	25,25,25,25	0
56	MG	2A	3550	1/1	0.98	0.22	47,47,47,47	0
56	MG	1A	3519	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3129	1/1	0.98	0.11	27,27,27,27	0
56	MG	1A	3714	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	3241	1/1	0.98	0.26	39,39,39,39	0
56	MG	1A	3150	1/1	0.98	0.08	33,33,33,33	0
56	MG	2A	3682	1/1	0.98	0.12	57,57,57,57	0
56	MG	17	101	1/1	0.98	0.16	27,27,27,27	0
56	MG	2a	1709	1/1	0.98	0.16	63,63,63,63	0
56	MG	17	102	1/1	0.98	0.16	29,29,29,29	0
56	MG	1A	3610	1/1	0.98	0.10	17,17,17,17	0
56	MG	1A	3523	1/1	0.98	0.12	44,44,44,44	0
56	MG	1A	3040	1/1	0.98	0.32	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3104	1/1	0.98	0.18	41,41,41,41	0
56	MG	1A	3014	1/1	0.98	0.21	27,27,27,27	0
56	MG	2A	3106	1/1	0.98	0.05	64,64,64,64	0
56	MG	1A	3074	1/1	0.98	0.25	41,41,41,41	0
56	MG	1B	211	1/1	0.98	0.20	40,40,40,40	0
56	MG	1a	1785	1/1	0.98	0.11	32,32,32,32	0
56	MG	1A	3615	1/1	0.98	0.12	53,53,53,53	0
56	MG	1A	3998	1/1	0.98	0.29	57,57,57,57	0
56	MG	1A	3785	1/1	0.98	0.13	51,51,51,51	0
56	MG	1A	3724	1/1	0.98	0.24	44,44,44,44	0
56	MG	1a	1693	1/1	0.98	0.12	39,39,39,39	0
56	MG	1A	3927	1/1	0.98	0.11	21,21,21,21	0
56	MG	1A	3667	1/1	0.98	0.09	47,47,47,47	0
56	MG	1A	3726	1/1	0.98	0.09	56,56,56,56	0
56	MG	1A	3134	1/1	0.98	0.32	42,42,42,42	0
56	MG	2a	1729	1/1	0.98	0.20	68,68,68,68	0
56	MG	1A	3087	1/1	0.98	0.20	37,37,37,37	0
56	MG	1A	3529	1/1	0.98	0.13	50,50,50,50	0
56	MG	1A	3571	1/1	0.98	0.15	25,25,25,25	0
56	MG	1A	3493	1/1	0.98	0.29	31,31,31,31	0
56	MG	1A	3573	1/1	0.98	0.11	27,27,27,27	0
56	MG	1A	3531	1/1	0.98	0.13	22,22,22,22	0
56	MG	2A	3125	1/1	0.98	0.20	34,34,34,34	0
56	MG	2A	3462	1/1	0.98	0.23	46,46,46,46	0
56	MG	1a	1704	1/1	0.98	0.12	61,61,61,61	0
56	MG	1A	4011	1/1	0.98	0.12	29,29,29,29	0
56	MG	2A	3021	1/1	0.98	0.29	51,51,51,51	0
56	MG	1A	3462	1/1	0.98	0.18	28,28,28,28	0
56	MG	1A	3463	1/1	0.98	0.75	40,40,40,40	0
56	MG	2A	3024	1/1	0.98	0.60	46,46,46,46	0
56	MG	1A	3625	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	3065	1/1	0.98	0.21	26,26,26,26	0
56	MG	1A	3738	1/1	0.98	0.21	39,39,39,39	0
57	ZN	25	106	1/1	0.98	0.19	59,59,59,59	0
56	MG	2A	3849	1/1	0.98	0.12	44,44,44,44	0
57	ZN	29	501	1/1	0.98	0.06	76,76,76,76	0
56	MG	1A	3578	1/1	0.98	0.18	22,22,22,22	0
56	MG	1a	1809	1/1	0.98	0.10	63,63,63,63	0
56	MG	1A	3535	1/1	0.98	0.15	52,52,52,52	0
56	MG	2A	3357	1/1	0.98	0.31	42,42,42,42	0
56	MG	2A	3247	1/1	0.98	0.09	67,67,67,67	0
56	MG	1A	3053	1/1	0.99	0.11	35,35,35,35	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	0.99	0.07	35,35,35,35	0
56	MG	1A	3627	1/1	0.99	0.15	21,21,21,21	0
56	MG	1A	3939	1/1	0.99	0.16	30,30,30,30	0
56	MG	2A	3414	1/1	0.99	0.14	49,49,49,49	0
56	MG	2A	3415	1/1	0.99	0.25	50,50,50,50	0
56	MG	1E	308	1/1	0.99	0.09	47,47,47,47	0
56	MG	2A	3241	1/1	0.99	0.19	49,49,49,49	0
56	MG	1a	1776	1/1	0.99	0.10	48,48,48,48	0
56	MG	2a	1790	1/1	0.99	0.29	65,65,65,65	0
56	MG	1a	1676	1/1	0.99	0.10	45,45,45,45	0
56	MG	1A	4043	1/1	0.99	0.20	20,20,20,20	0
56	MG	1A	3045	1/1	0.99	0.17	26,26,26,26	0
56	MG	1D	302	1/1	0.99	0.23	31,31,31,31	0
56	MG	1Y	204	1/1	0.99	0.39	48,48,48,48	0
56	MG	1A	4026	1/1	0.99	0.12	29,29,29,29	0
56	MG	1A	3709	1/1	0.99	0.10	50,50,50,50	0
56	MG	1A	3172	1/1	0.99	0.12	26,26,26,26	0
56	MG	1A	3722	1/1	0.99	0.26	37,37,37,37	0
56	MG	1A	3880	1/1	0.99	0.09	45,45,45,45	0
56	MG	2a	1692	1/1	0.99	0.07	74,74,74,74	0
56	MG	1A	3810	1/1	0.99	0.13	21,21,21,21	0
56	MG	2F	305	1/1	0.99	0.59	50,50,50,50	0
56	MG	1A	3323	1/1	0.99	0.24	41,41,41,41	0
56	MG	1A	3898	1/1	0.99	0.13	30,30,30,30	0
56	MG	2A	3284	1/1	0.99	0.34	66,66,66,66	0
56	MG	1D	311	1/1	0.99	0.19	45,45,45,45	0
57	ZN	16	103	1/1	0.99	0.15	46,46,46,46	0
57	ZN	19	102	1/1	0.99	0.18	42,42,42,42	0
56	MG	1A	3594	1/1	0.99	0.17	23,23,23,23	0
56	MG	2A	3435	1/1	0.99	0.20	34,34,34,34	0
56	MG	2A	3500	1/1	0.99	0.17	32,32,32,32	0
56	MG	1A	3130	1/1	0.99	0.25	36,36,36,36	0
56	MG	2A	3042	1/1	0.99	0.17	30,30,30,30	0
56	MG	2a	1813	1/1	0.99	0.14	54,54,54,54	0
56	MG	11	101	1/1	0.99	0.58	27,27,27,27	0
56	MG	1A	3774	1/1	0.99	0.28	37,37,37,37	0
56	MG	2R	202	1/1	0.99	0.26	38,38,38,38	0
59	SF4	1d	501	8/8	0.99	0.15	55,69,72,74	0
59	SF4	2d	303	8/8	0.99	0.12	70,78,89,91	0
56	MG	1A	3008	1/1	0.99	0.10	15,15,15,15	0
56	MG	1A	3164	1/1	0.99	0.56	28,28,28,28	0
57	ZN	15	105	1/1	1.00	0.20	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.