Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 07:38 AM EST

PDB ID	:	6O97
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with propylamycin and bound to mRNA and A-, P-, and E-site tRNAs at 2.75A resolution
Authors	:	Matsushita, T.; Sati, G.C.; Kondasinghe, N.; Pirrone, M.G.; Kato, T.; Waduge, P.; Kumar, H.S.; Sanchon, A.C.; Dobosz-Bartoszek, M.; Shcherbakov, D.; Juhas, M.; Hobbie, S.N.; Schrepfer, T.; Chow, C.S.; Polikanov, Y.S.; Schacht, J.; Vasella, A.; Bottger, E.C.; Crich, D.
Deposited on	:	2019-03-13
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 (i) symbol.

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

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

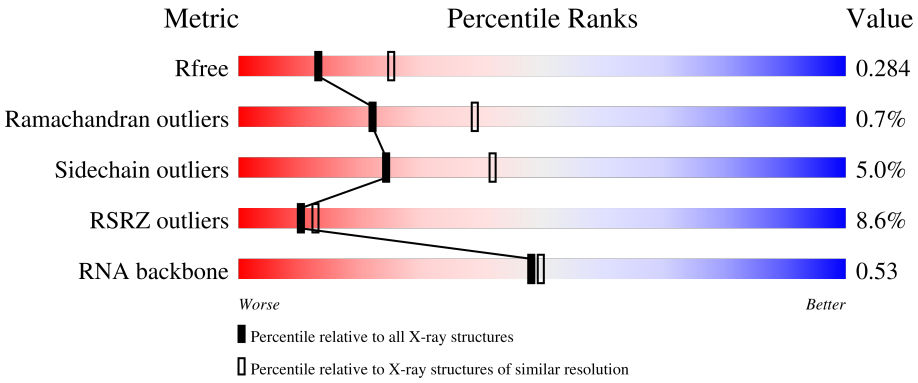
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

1 Overall quality at a glance (i)

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

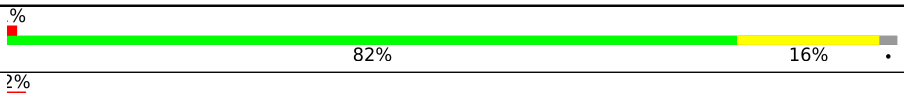
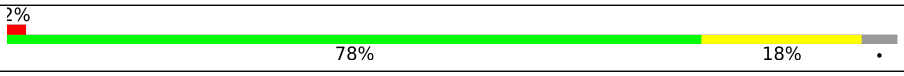
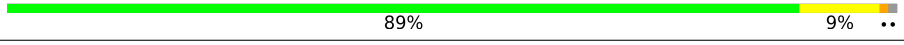
The reported resolution of this entry is 2.75 Å.

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	
1	2A	2915	
2	1B	121	

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Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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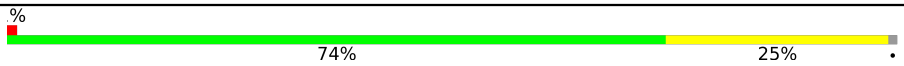
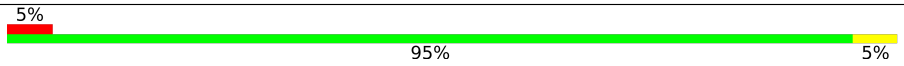
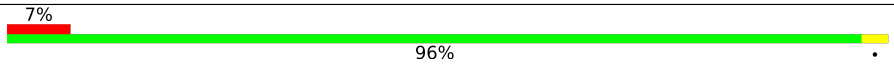
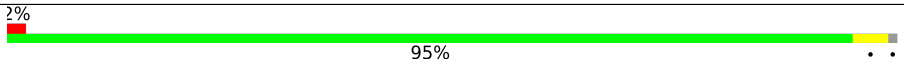
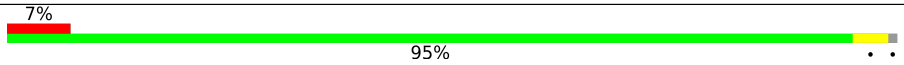
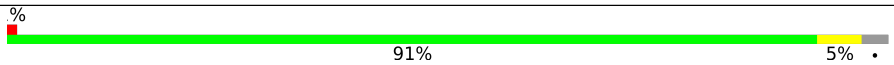
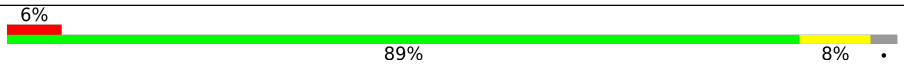
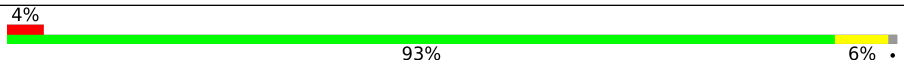
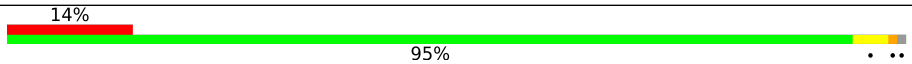
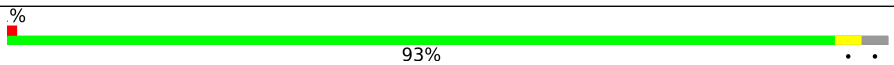
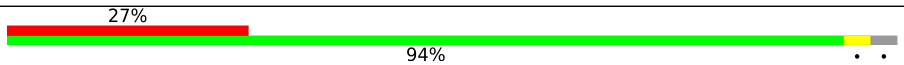
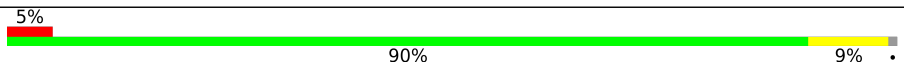
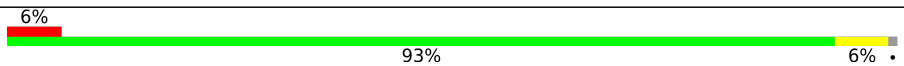
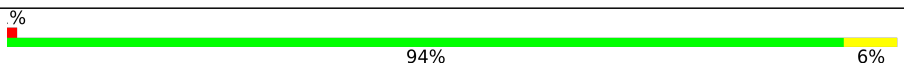
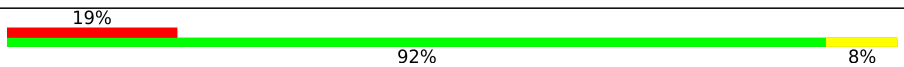
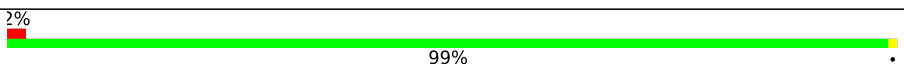
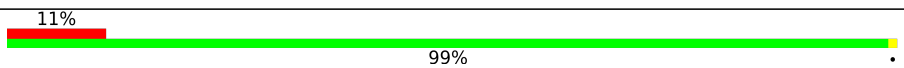
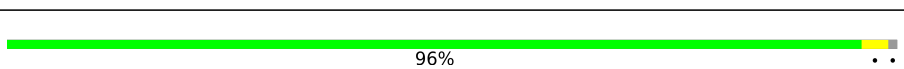
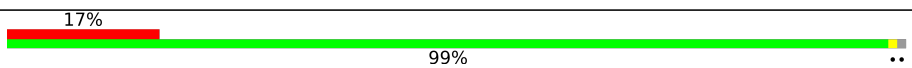
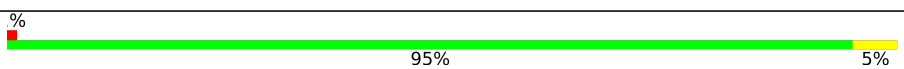
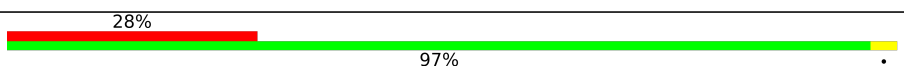
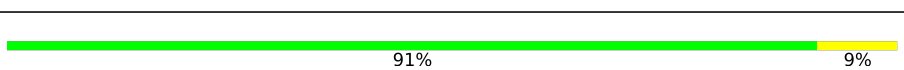
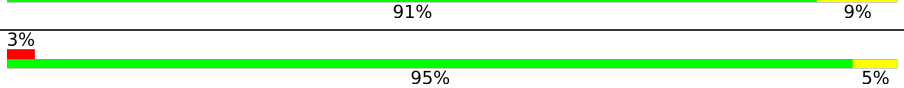
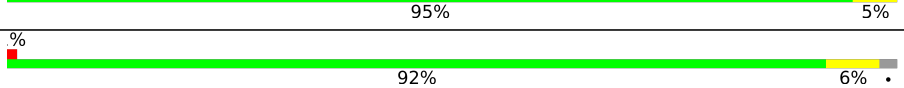
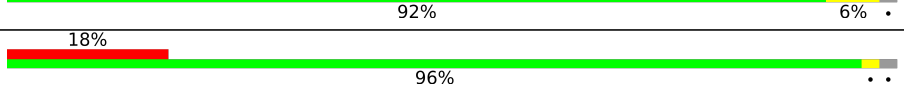
Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	

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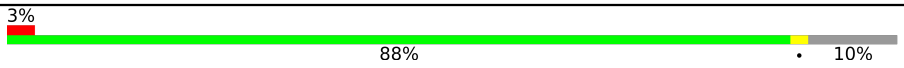
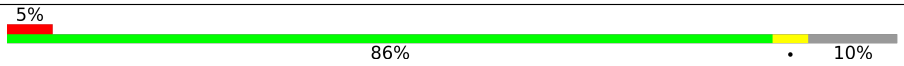
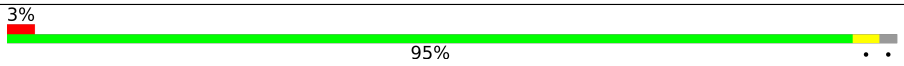
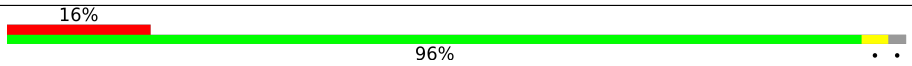
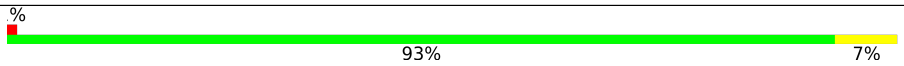
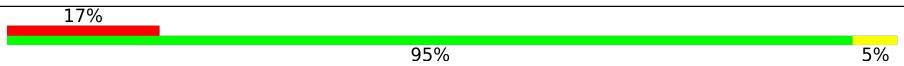
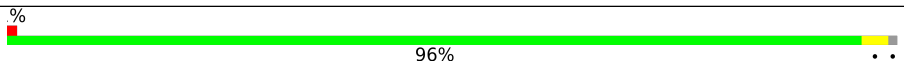
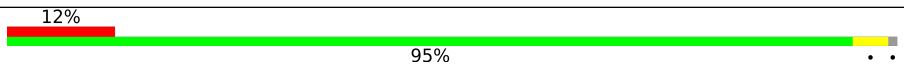
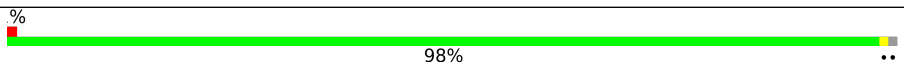
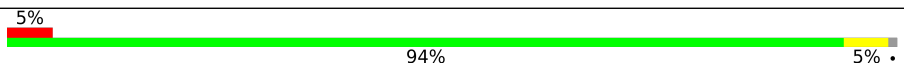
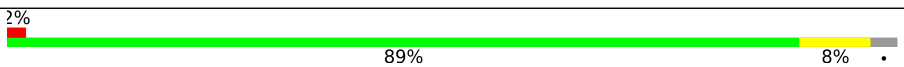
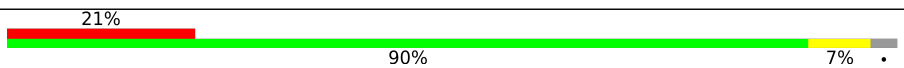
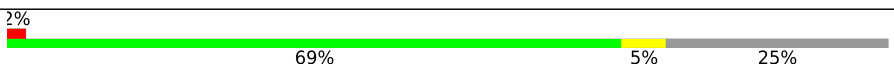
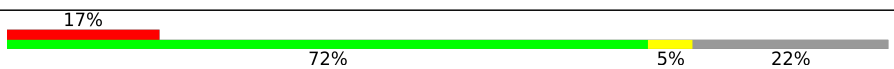
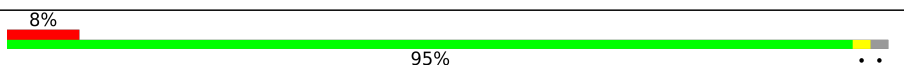
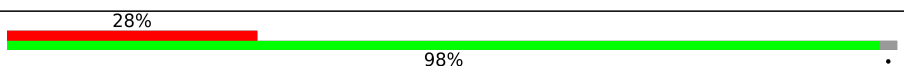
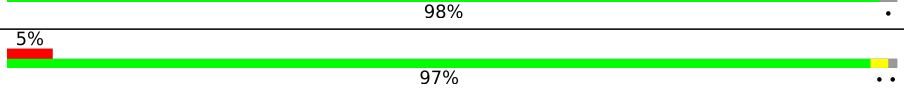
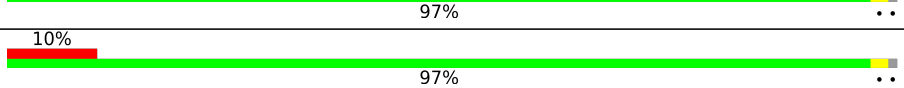
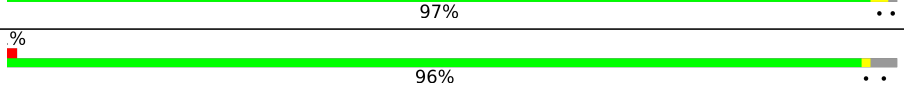
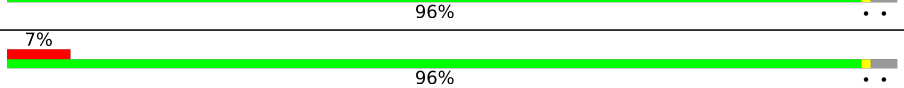
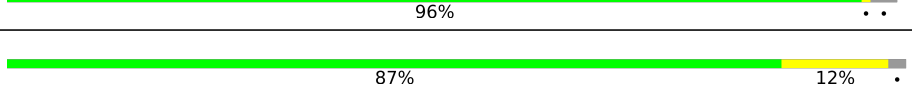
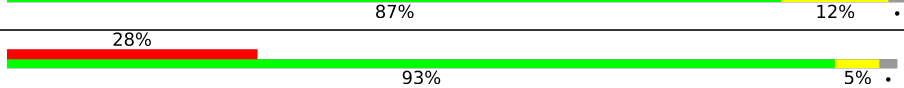
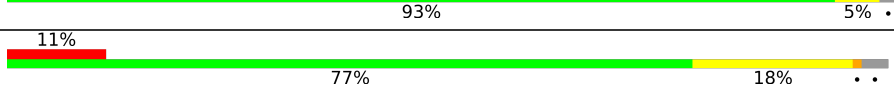
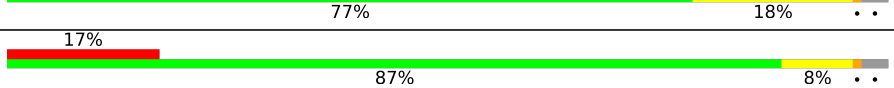
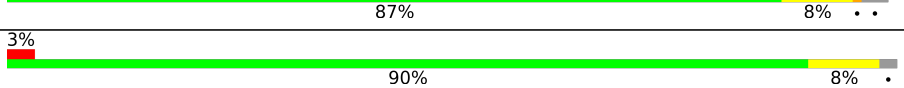
Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	

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Mol	Chain	Length	Quality of chain
27	25	60	8% 93% 5%
28	16	54	89% 9%
28	26	54	19% 93% 6%
29	17	49	10% 88% 10%
29	27	49	16% 90% 8%
30	18	65	5% 89% 9%
30	28	65	40% 95%
31	19	37	97%
31	29	37	30% 97%
32	1a	1521	% 81% 17%
32	2a	1521	3% 79% 18%
33	1b	256	9% 85% 10%
33	2b	256	29% 83% 7% 10%
34	1c	239	8% 83% 14%
34	2c	239	23% 84% 14%
35	1d	209	13% 96%
35	2d	209	17% 96%
36	1e	162	11% 85% 6% 9%
36	2e	162	29% 88% 9%
37	1f	101	2% 97%
37	2f	101	2% 96%
38	1g	156	14% 96%
38	2g	156	18% 97%
39	1h	138	16% 93% 6%
39	2h	138	26% 96%

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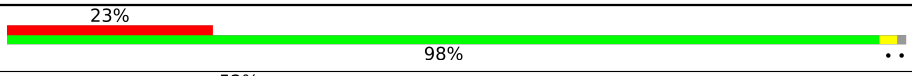
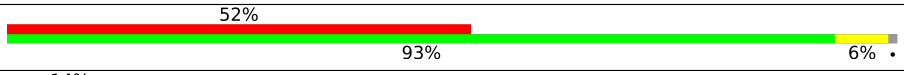
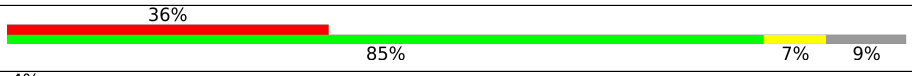
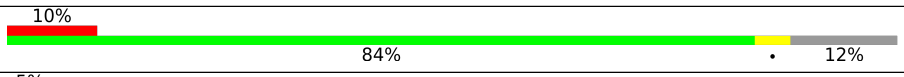
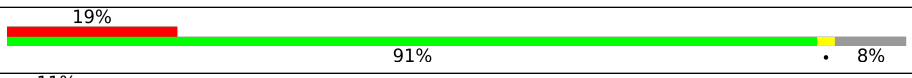
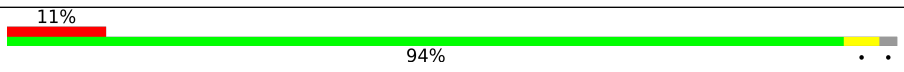
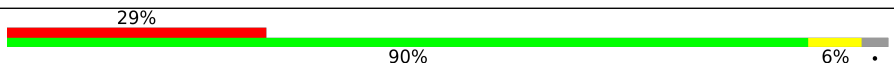
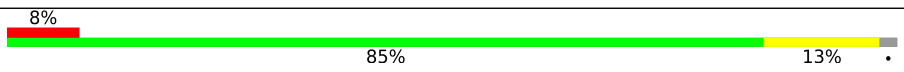
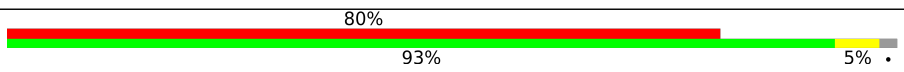
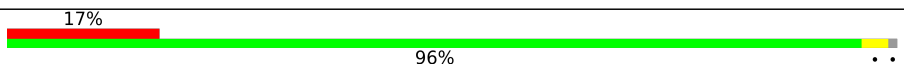
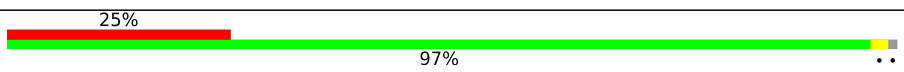
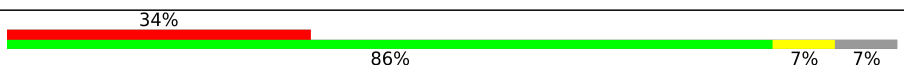
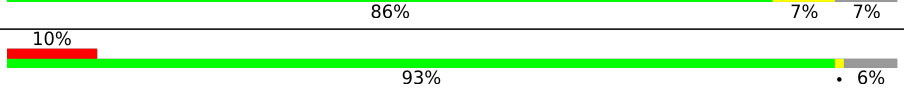
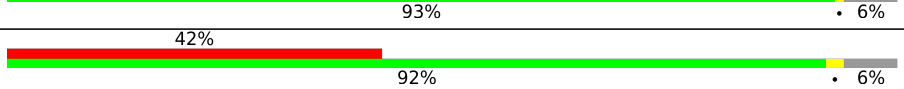
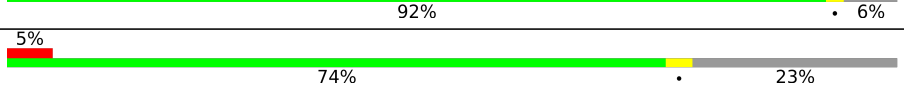
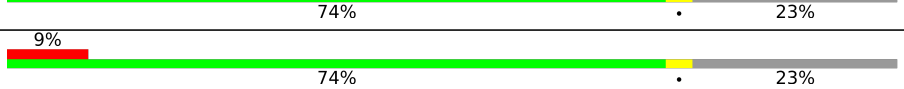
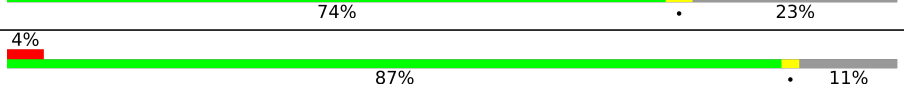
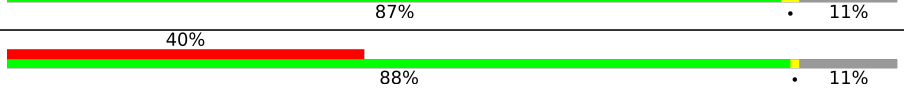
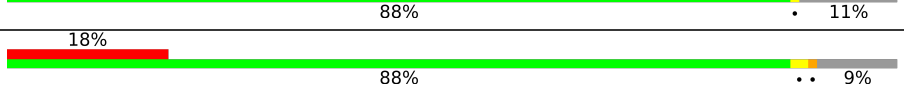
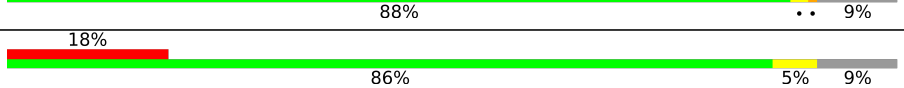
Mol	Chain	Length	Quality of chain
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	

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Mol	Chain	Length	Quality of chain
52	2u	27	56% 85% 15%
53	1v	27	15% 37% 11% 52%
53	2v	27	22% 33% 15% 52%
54	1w	76	20% 57% 34% 5%
54	1y	76	16% 57% 32% 8%
54	2w	76	37% 51% 39% 5%
54	2y	76	18% 54% 37% 5%
55	1x	77	73% 25%
55	2x	77	8% 71% 26%

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	CM0	2y	34	-	-	-	X
56	MG	1A	3354	-	-	-	X
56	MG	1A	3360	-	-	-	X
56	MG	1A	3453	-	-	-	X
56	MG	1A	3525	-	-	-	X
56	MG	1A	3948	-	-	-	X
56	MG	1A	3993	-	-	-	X
56	MG	1A	4017	-	-	-	X
56	MG	1A	4053	-	-	-	X
56	MG	1A	4098	-	-	-	X
56	MG	1E	302	-	-	-	X
56	MG	1a	1603	-	-	-	X
56	MG	1a	1605	-	-	-	X
56	MG	1a	1622	-	-	-	X
56	MG	1l	202	-	-	-	X
56	MG	1v	101	-	-	-	X
56	MG	1y	105	-	-	-	X
56	MG	2A	3177	-	-	-	X
56	MG	2A	3232	-	-	-	X
56	MG	2A	3251	-	-	-	X
56	MG	2A	3288	-	-	-	X
56	MG	2A	3503	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3647	-	-	-	X
56	MG	2A	3854	-	-	-	X
56	MG	2F	303	-	-	-	X
56	MG	2a	3015	-	-	-	X
56	MG	2a	3016	-	-	-	X
56	MG	2a	3027	-	-	-	X
56	MG	2a	3049	-	-	-	X
56	MG	2a	3091	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300702 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			276	124	48	91	13			
53	2v	13	Total	C	N	O	P	0	0	0
			276	124	48	91	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total	C	N	O	P	S	0	0	0
			1568	700	282	512	73	1			
54	1y	73	Total	C	N	O	P	S	0	0	0
			1568	700	282	512	73	1			
54	2w	73	Total	C	N	O	P	S	0	0	0
			1568	700	282	512	73	1			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1568	700	282	512	73	1			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1134	Total	Mg	0	0
			1134	1134		
56	1B	36	Total	Mg	0	0
			36	36		
56	1D	13	Total	Mg	0	0
			13	13		
56	1E	7	Total	Mg	0	0
			7	7		
56	1F	10	Total	Mg	0	0
			10	10		
56	1G	5	Total	Mg	0	0
			5	5		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	7	Total	Mg	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1O	4	Total Mg 4 4	0	0
56	1P	3	Total Mg 3 3	0	0
56	1Q	5	Total Mg 5 5	0	0
56	1R	4	Total Mg 4 4	0	0
56	1S	3	Total Mg 3 3	0	0
56	1T	2	Total Mg 2 2	0	0
56	1U	7	Total Mg 7 7	0	0
56	1V	2	Total Mg 2 2	0	0
56	1W	7	Total Mg 7 7	0	0
56	1X	5	Total Mg 5 5	0	0
56	1Y	5	Total Mg 5 5	0	0
56	1Z	5	Total Mg 5 5	0	0
56	10	5	Total Mg 5 5	0	0
56	11	2	Total Mg 2 2	0	0
56	12	2	Total Mg 2 2	0	0
56	13	1	Total Mg 1 1	0	0
56	14	1	Total Mg 1 1	0	0
56	15	3	Total Mg 3 3	0	0
56	16	2	Total Mg 2 2	0	0
56	17	4	Total Mg 4 4	0	0
56	18	4	Total Mg 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	19	1	Total Mg 1 1	0	0
56	1a	233	Total Mg 233 233	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	1l	3	Total Mg 3 3	0	0
56	1n	1	Total Mg 1 1	0	0
56	1q	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1v	1	Total Mg 1 1	0	0
56	1w	8	Total Mg 8 8	0	0
56	1x	15	Total Mg 15 15	0	0
56	1y	6	Total Mg 6 6	0	0
56	2A	860	Total Mg 860 860	0	0
56	2B	18	Total Mg 18 18	0	0
56	2D	3	Total Mg 3 3	0	0
56	2E	8	Total Mg 8 8	0	0
56	2F	5	Total Mg 5 5	0	0
56	2G	1	Total Mg 1 1	0	0
56	2N	1	Total Mg 1 1	0	0
56	2O	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2P	2	Total Mg 2 2	0	0
56	2Q	5	Total Mg 5 5	0	0
56	2R	3	Total Mg 3 3	0	0
56	2T	4	Total Mg 4 4	0	0
56	2U	4	Total Mg 4 4	0	0
56	2V	2	Total Mg 2 2	0	0
56	2W	1	Total Mg 1 1	0	0
56	2X	1	Total Mg 1 1	0	0
56	2Y	1	Total Mg 1 1	0	0
56	20	2	Total Mg 2 2	0	0
56	21	1	Total Mg 1 1	0	0
56	25	2	Total Mg 2 2	0	0
56	27	1	Total Mg 1 1	0	0
56	28	1	Total Mg 1 1	0	0
56	29	1	Total Mg 1 1	0	0
56	2a	231	Total Mg 231 231	0	0
56	2d	2	Total Mg 2 2	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	2i	1	Total Mg 1 1	0	0
56	2j	2	Total Mg 2 2	0	0

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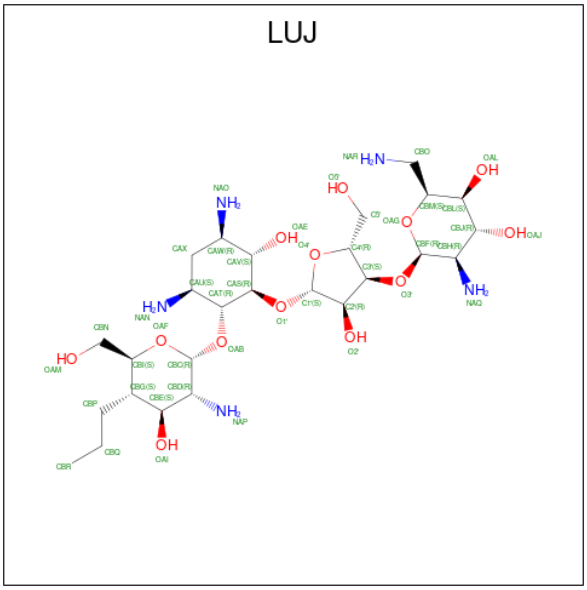
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2k	1	Total Mg 1 1	0	0
56	2l	4	Total Mg 4 4	0	0
56	2q	3	Total Mg 3 3	0	0
56	2r	1	Total Mg 1 1	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	3	Total Mg 3 3	0	0
56	2x	5	Total Mg 5 5	0	0
56	2y	6	Total Mg 6 6	0	0

- Molecule 57 is (1R,2R,3S,4R,6S)-4,6-diamino-2-{[3-O-(2,6-diamino-2,6-dideoxy-beta-L-idopyranosyl)-beta-D-ribofuranosyl]oxy}-3-hydroxyc yclohexyl 2-amino-2,4-dideoxy-4-propyl-alpha-D-glucopyranoside (three-letter code: LUJ) (formula: $C_{26}H_{51}N_5O_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total C N O 42 24 5 13	0	0
57	1A	1	Total C N O 42 24 5 13	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1a	1	Total C N O 44 26 5 13	0	0
57	2A	1	Total C N O 42 24 5 13	0	0
57	2A	1	Total C N O 42 24 5 13	0	0
57	2a	1	Total C N O 44 26 5 13	0	0

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total K 1 1	0	0
58	2A	1	Total K 1 1	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0
59	14	1	Total Zn 1 1	0	0
59	15	1	Total Zn 1 1	0	0
59	16	1	Total Zn 1 1	0	0
59	19	1	Total Zn 1 1	0	0
59	1n	1	Total Zn 1 1	0	0
59	2Y	1	Total Zn 1 1	0	0
59	24	1	Total Zn 1 1	0	0
59	25	1	Total Zn 1 1	0	0
59	26	1	Total Zn 1 1	0	0
59	29	1	Total Zn 1 1	0	0

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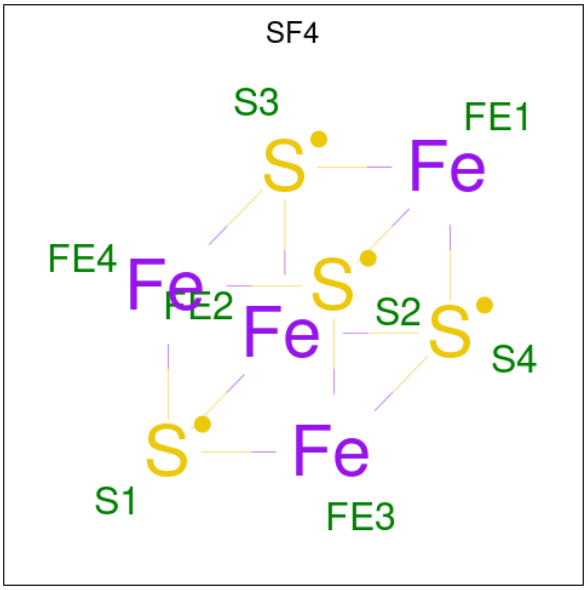
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1d	1	Total Fe S 8 4 4	0	0
60	2d	1	Total Fe S 8 4 4	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2225	Total O 2225 2225	0	0
61	1B	69	Total O 69 69	0	0
61	1D	28	Total O 28 28	0	0
61	1E	27	Total O 27 27	0	0
61	1F	17	Total O 17 17	0	0
61	1G	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1H	1	Total O 1 1	0	0
61	1I	2	Total O 2 2	0	0
61	1N	3	Total O 3 3	0	0
61	1O	7	Total O 7 7	0	0
61	1P	26	Total O 26 26	0	0
61	1Q	12	Total O 12 12	0	0
61	1R	14	Total O 14 14	0	0
61	1S	4	Total O 4 4	0	0
61	1T	7	Total O 7 7	0	0
61	1U	13	Total O 13 13	0	0
61	1V	8	Total O 8 8	0	0
61	1W	9	Total O 9 9	0	0
61	1X	7	Total O 7 7	0	0
61	1Y	4	Total O 4 4	0	0
61	1Z	1	Total O 1 1	0	0
61	10	9	Total O 9 9	0	0
61	11	12	Total O 12 12	0	0
61	12	4	Total O 4 4	0	0
61	13	4	Total O 4 4	0	0
61	14	1	Total O 1 1	0	0
61	15	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	16	2	Total O 2 2	0	0
61	17	8	Total O 8 8	0	0
61	18	13	Total O 13 13	0	0
61	19	1	Total O 1 1	0	0
61	1a	438	Total O 438 438	0	0
61	1b	1	Total O 1 1	0	0
61	1d	1	Total O 1 1	0	0
61	1e	1	Total O 1 1	0	0
61	1g	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	2	Total O 2 2	0	0
61	1n	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	4	Total O 4 4	0	0
61	1w	6	Total O 6 6	0	0
61	1x	17	Total O 17 17	0	0
61	1y	3	Total O 3 3	0	0
61	2A	1163	Total O 1163 1163	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2B	20	Total O 20 20	0	0
61	2D	23	Total O 23 23	0	0
61	2E	10	Total O 10 10	0	0
61	2F	13	Total O 13 13	0	0
61	2I	2	Total O 2 2	0	0
61	2N	1	Total O 1 1	0	0
61	2O	2	Total O 2 2	0	0
61	2P	6	Total O 6 6	0	0
61	2Q	1	Total O 1 1	0	0
61	2R	3	Total O 3 3	0	0
61	2T	2	Total O 2 2	0	0
61	2U	3	Total O 3 3	0	0
61	2V	2	Total O 2 2	0	0
61	2W	1	Total O 1 1	0	0
61	2X	2	Total O 2 2	0	0
61	2Z	1	Total O 1 1	0	0
61	20	3	Total O 3 3	0	0
61	21	9	Total O 9 9	0	0
61	23	1	Total O 1 1	0	0
61	25	3	Total O 3 3	0	0
61	27	3	Total O 3 3	0	0

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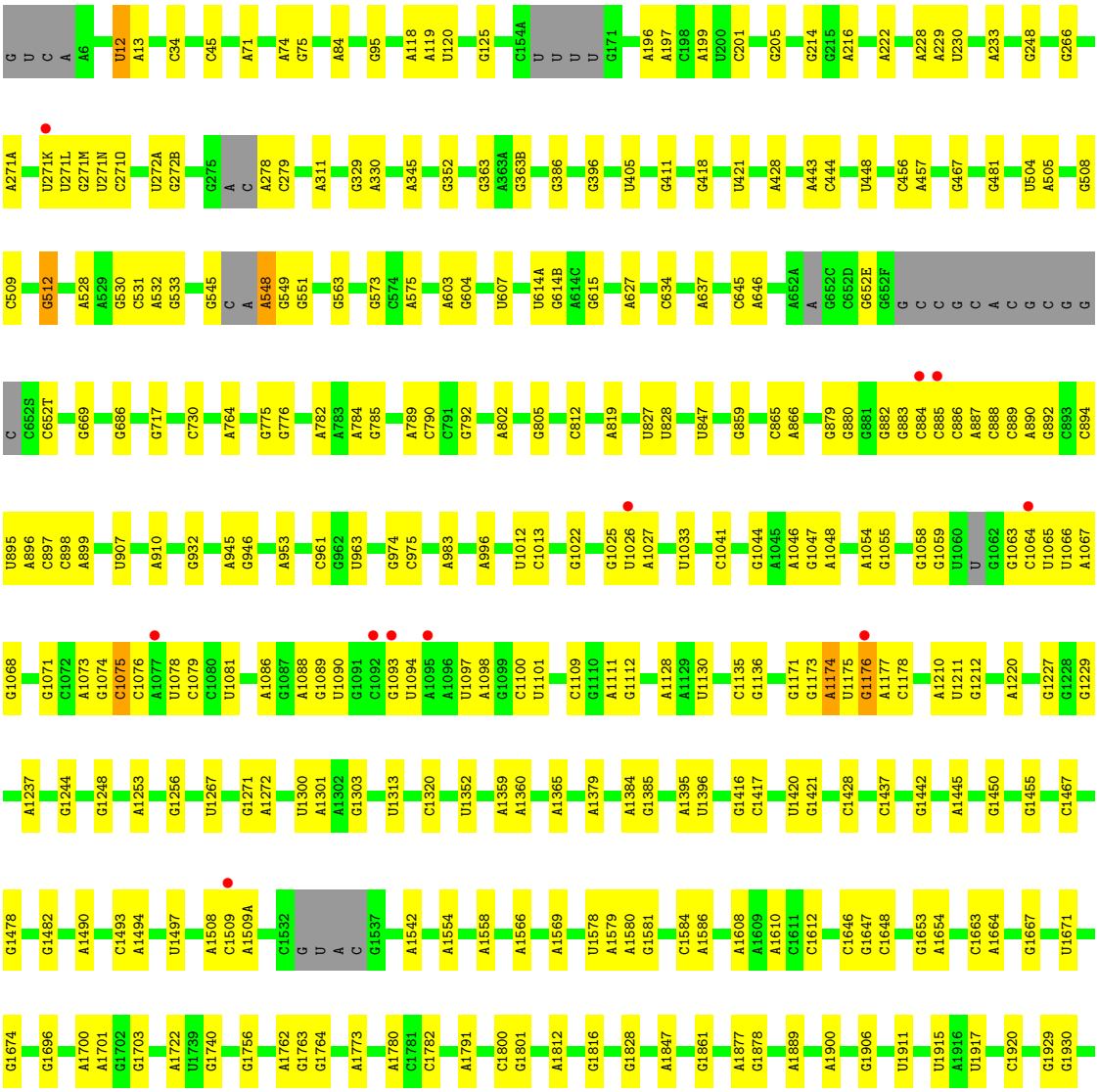
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	28	6	Total O 6 6	0	0
61	2a	322	Total O 322 322	0	0
61	2e	2	Total O 2 2	0	0
61	2f	1	Total O 1 1	0	0
61	2g	2	Total O 2 2	0	0
61	2j	4	Total O 4 4	0	0
61	2l	5	Total O 5 5	0	0
61	2o	2	Total O 2 2	0	0
61	2p	4	Total O 4 4	0	0
61	2q	1	Total O 1 1	0	0
61	2r	1	Total O 1 1	0	0
61	2t	4	Total O 4 4	0	0
61	2u	1	Total O 1 1	0	0
61	2v	3	Total O 3 3	0	0
61	2w	3	Total O 3 3	0	0
61	2x	7	Total O 7 7	0	0
61	2y	9	Total O 9 9	0	0

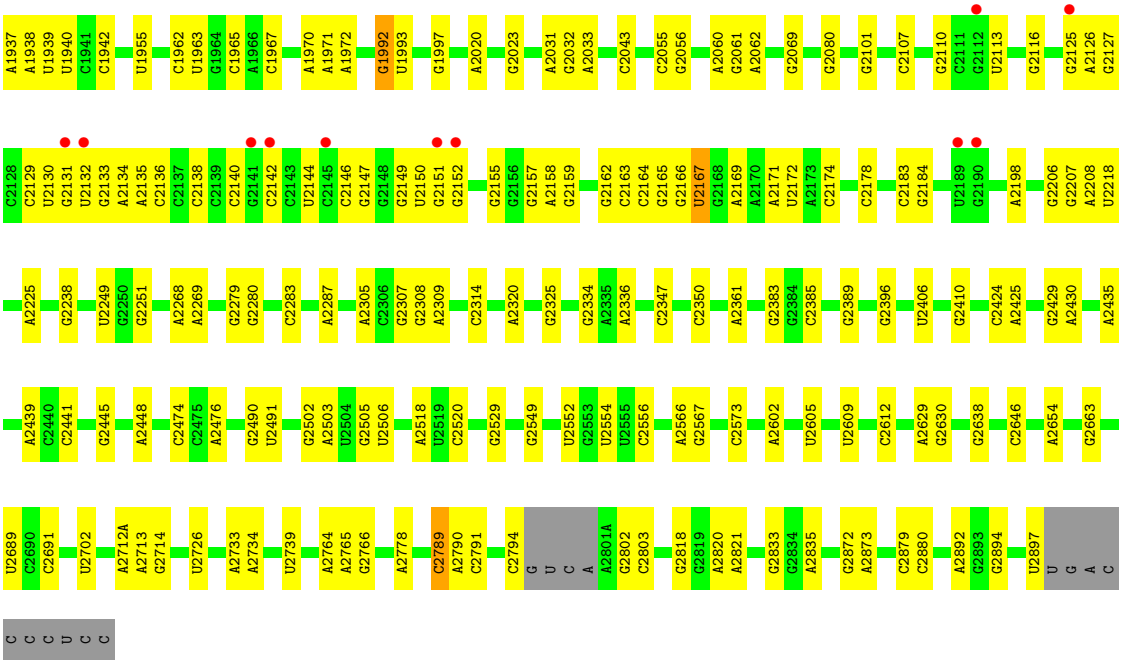
3 Residue-property plots (i)

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

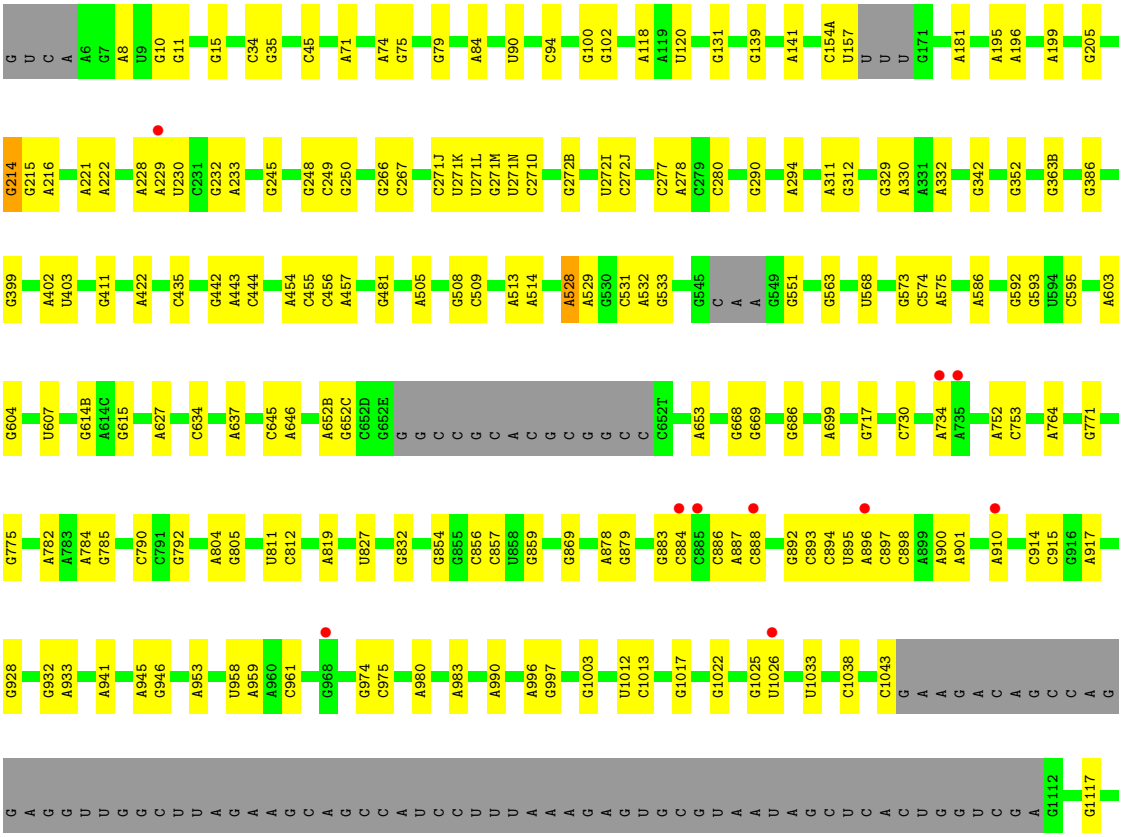
Chain 1A:

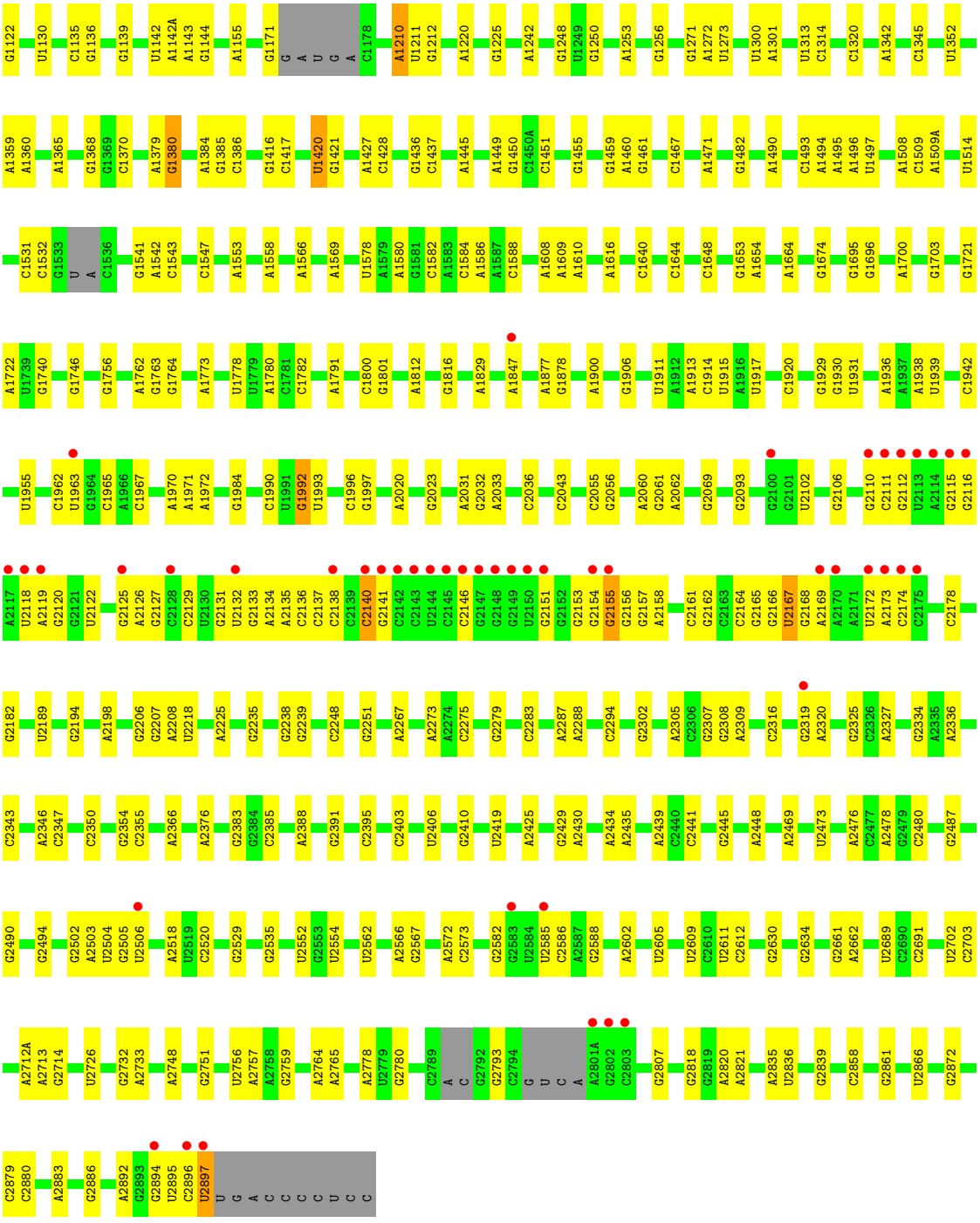




• Molecule 1: 23S Ribosomal RNA

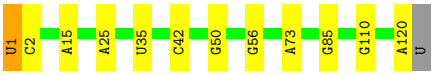
Chain 2A:





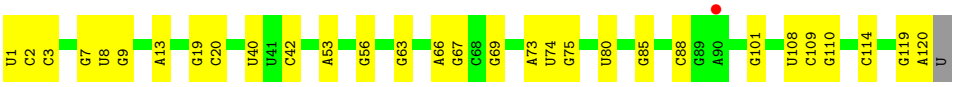
• Molecule 2: 5S Ribosomal RNA

Chain 1B:

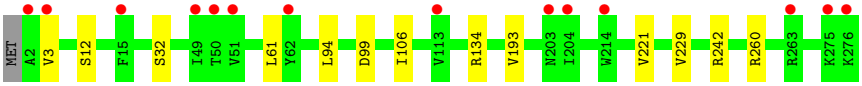


• Molecule 2: 5S Ribosomal RNA

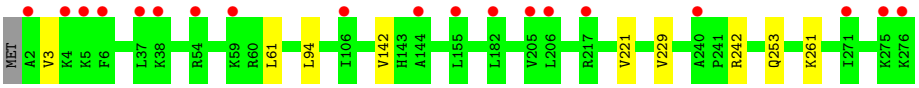
Chain 2B:



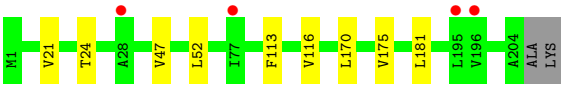
• Molecule 3: 50S ribosomal protein L2



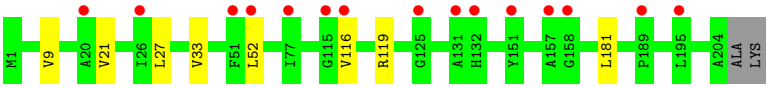
• Molecule 3: 50S ribosomal protein L2



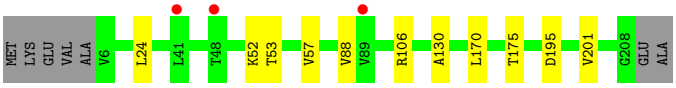
• Molecule 4: 50S ribosomal protein L3



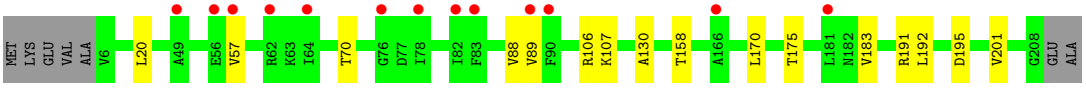
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

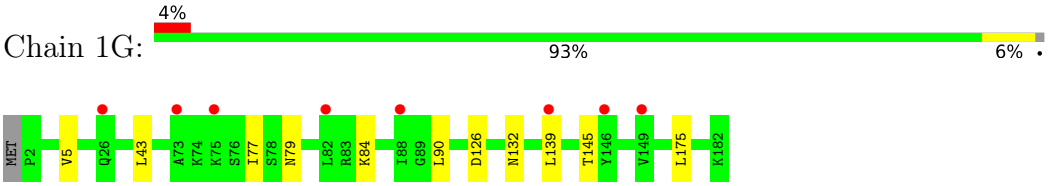


• Molecule 5: 50S ribosomal protein L4



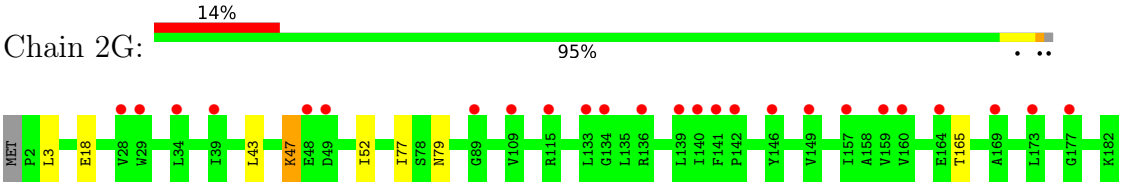
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



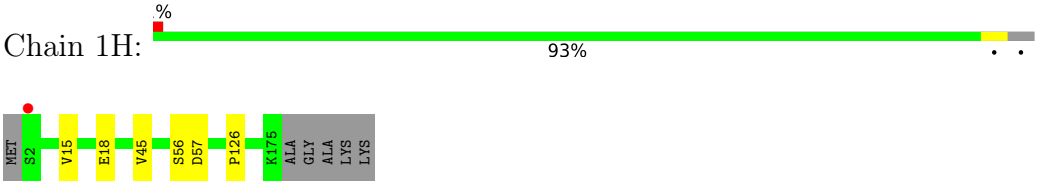
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



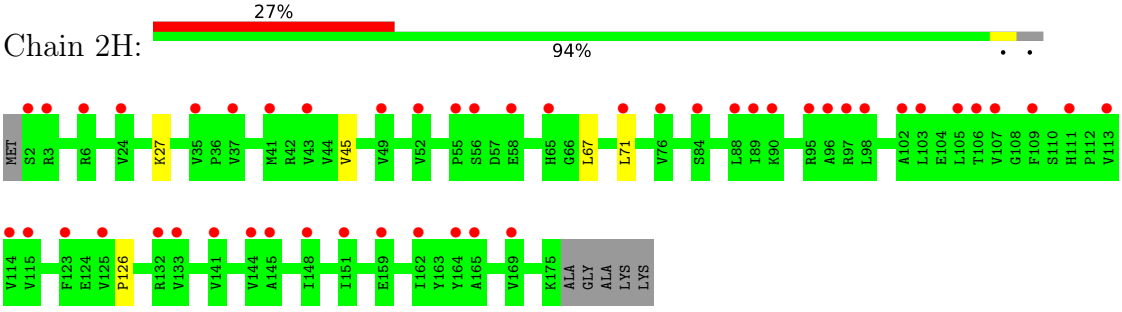
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



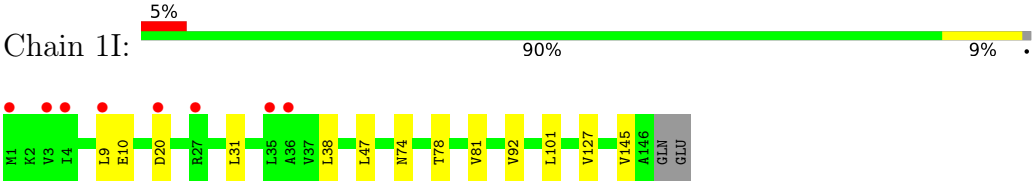
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



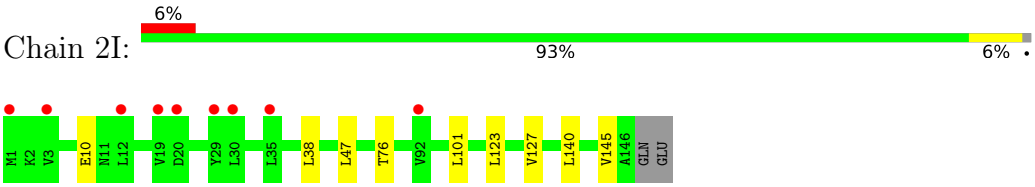
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



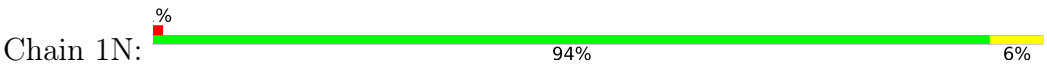
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



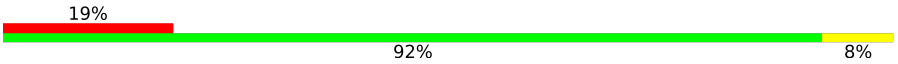
• Molecule 9: 50S ribosomal protein L13

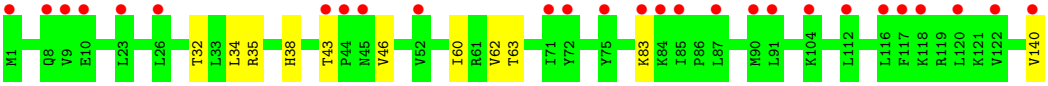
Chain 1N:



• Molecule 9: 50S ribosomal protein L13

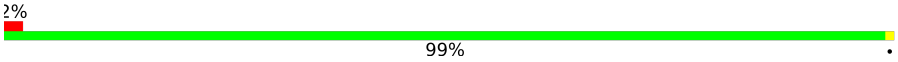
Chain 2N:

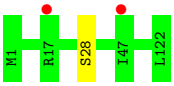




• Molecule 10: 50S ribosomal protein L14

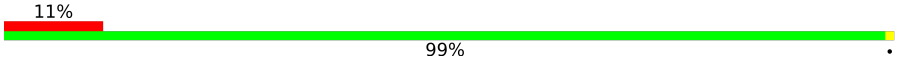
Chain 1O:

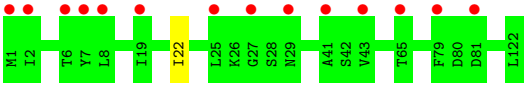




• Molecule 10: 50S ribosomal protein L14

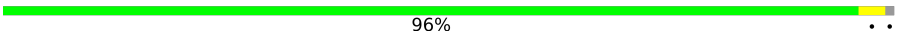
Chain 2O:

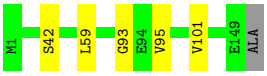




• Molecule 11: 50S ribosomal protein L15

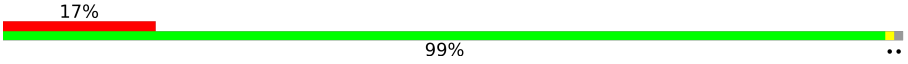
Chain 1P:

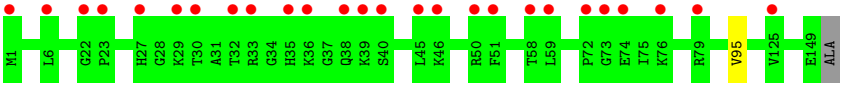




• Molecule 11: 50S ribosomal protein L15

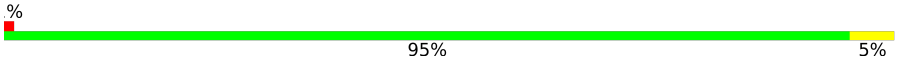
Chain 2P:

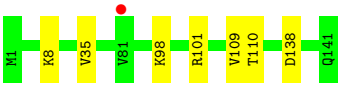




• Molecule 12: 50S ribosomal protein L16

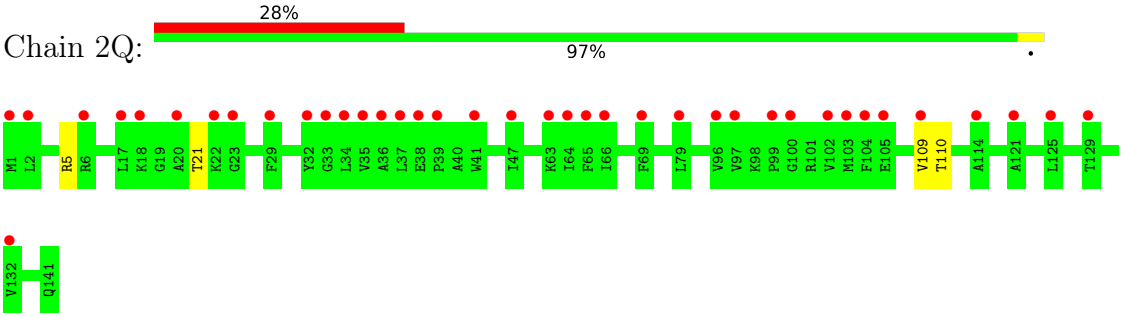
Chain 1Q:





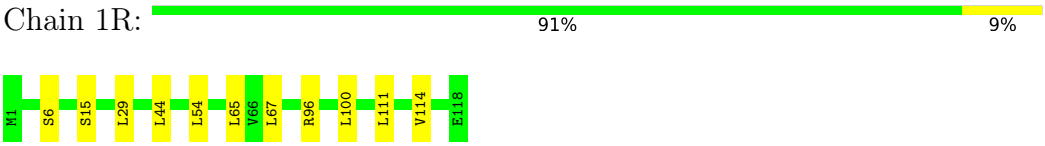
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



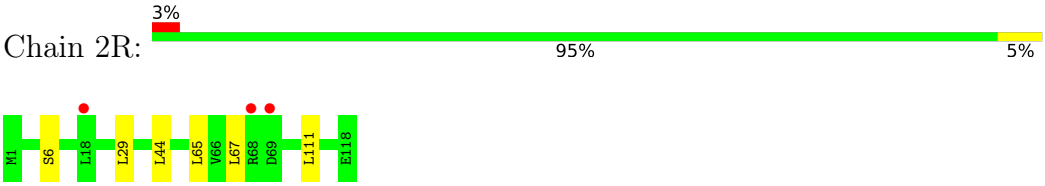
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



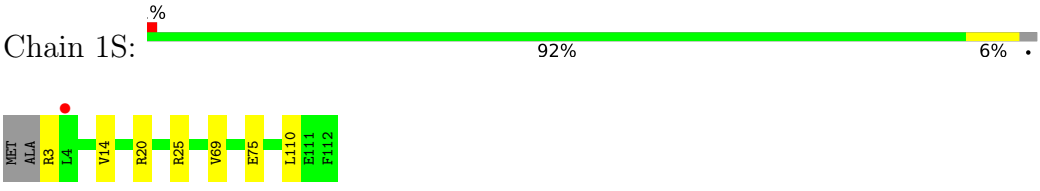
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



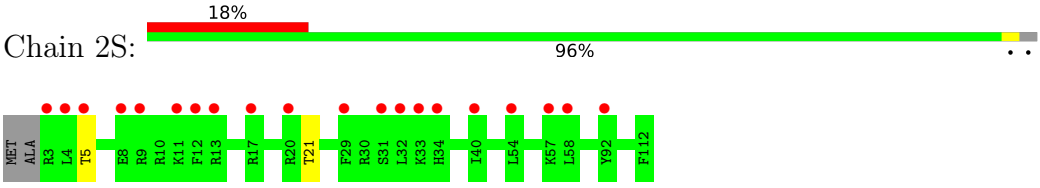
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



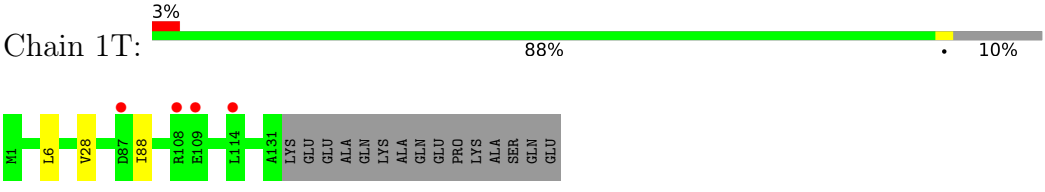
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



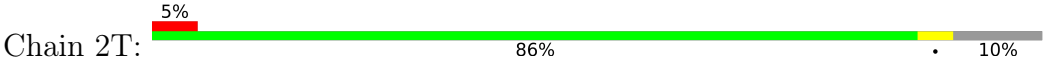
• Molecule 15: 50S ribosomal protein L19

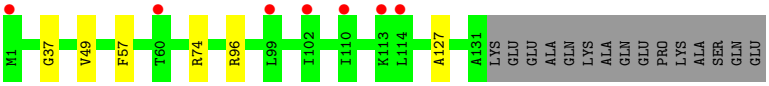
Chain 1T:



• Molecule 15: 50S ribosomal protein L19

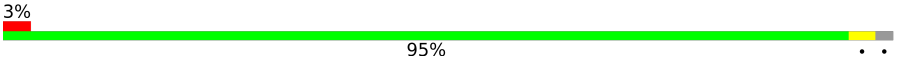
Chain 2T:

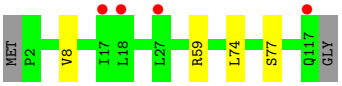




• Molecule 16: 50S ribosomal protein L20

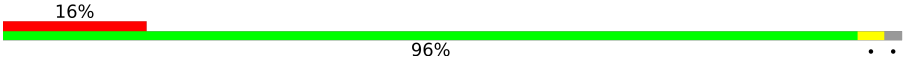
Chain 1U:

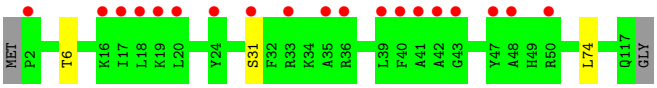




• Molecule 16: 50S ribosomal protein L20

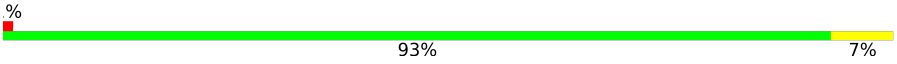
Chain 2U:

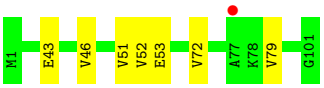




• Molecule 17: 50S ribosomal protein L21

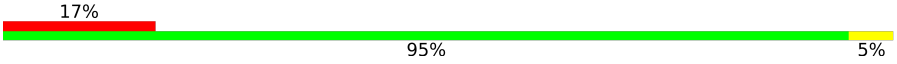
Chain 1V:

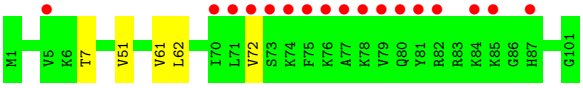




• Molecule 17: 50S ribosomal protein L21

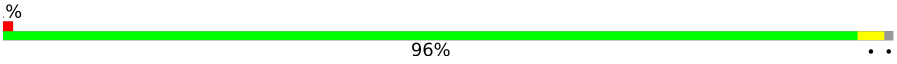
Chain 2V:

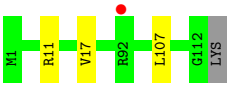




• Molecule 18: 50S ribosomal protein L22

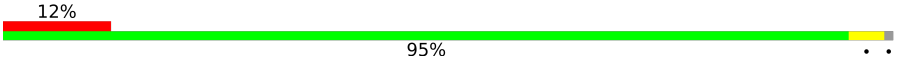
Chain 1W:

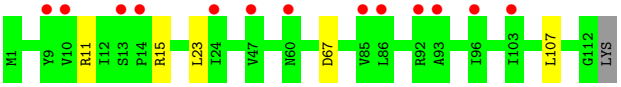




• Molecule 18: 50S ribosomal protein L22

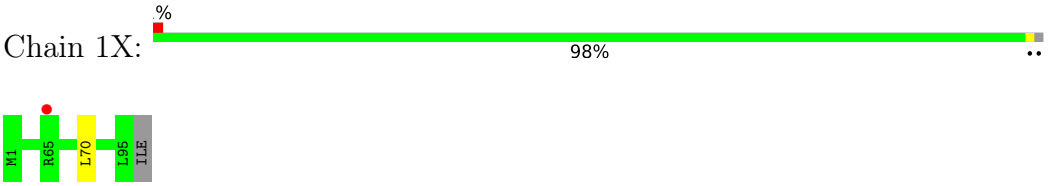
Chain 2W:





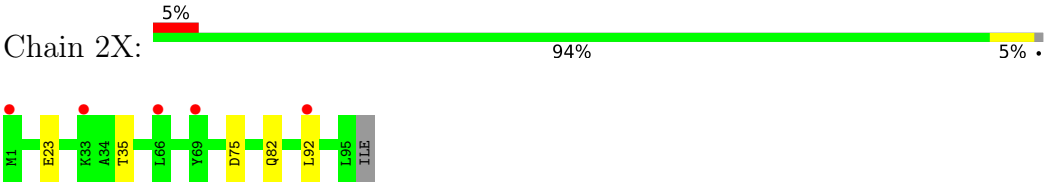
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



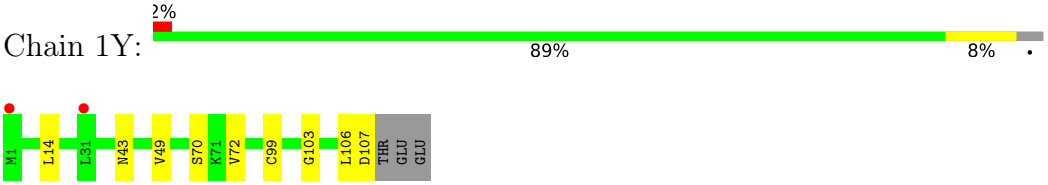
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



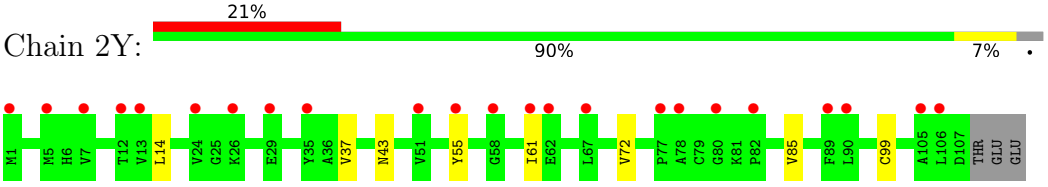
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



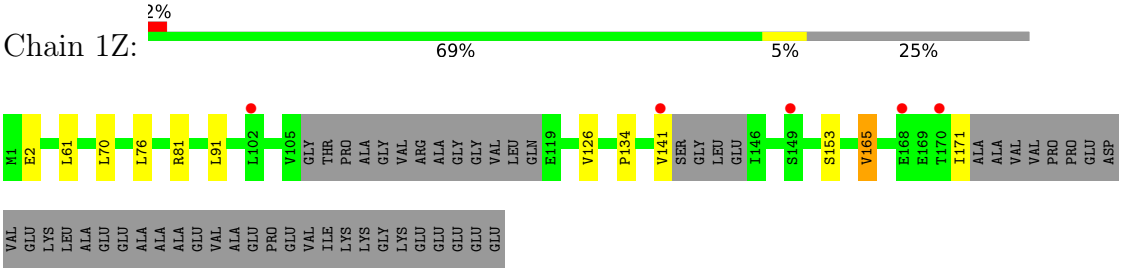
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



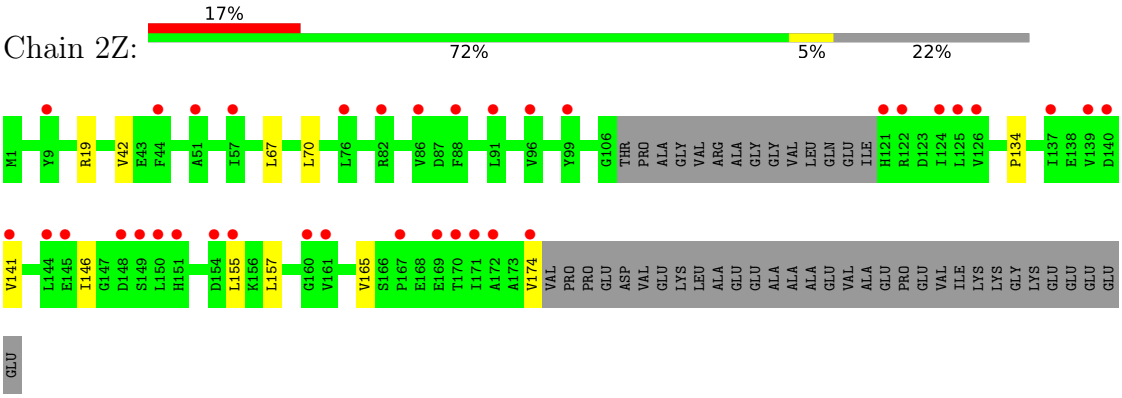
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



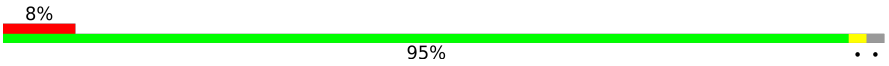
• Molecule 21: 50S ribosomal protein L25

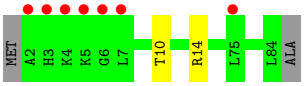
Chain 2Z:



• Molecule 22: 50S ribosomal protein L27

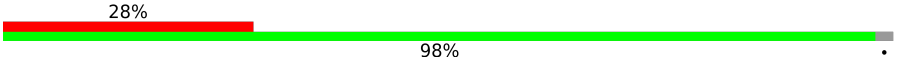
Chain 10:

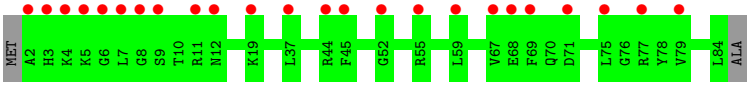




• Molecule 22: 50S ribosomal protein L27

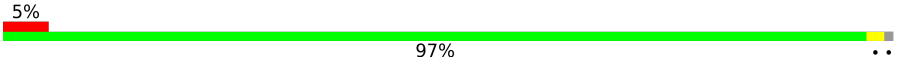
Chain 20:

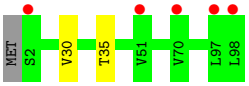




• Molecule 23: 50S ribosomal protein L28

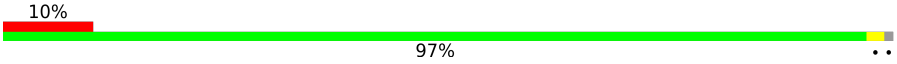
Chain 11:

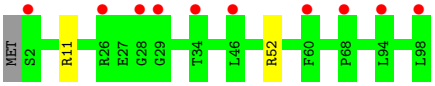




• Molecule 23: 50S ribosomal protein L28

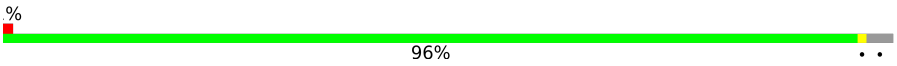
Chain 21:

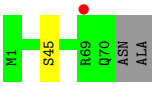




• Molecule 24: 50S ribosomal protein L29

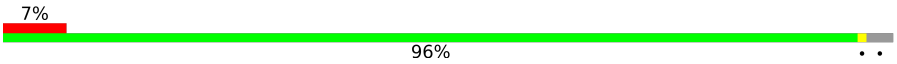
Chain 12:

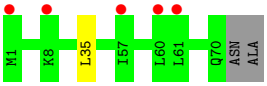




• Molecule 24: 50S ribosomal protein L29

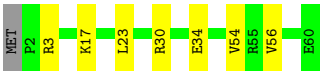
Chain 22:





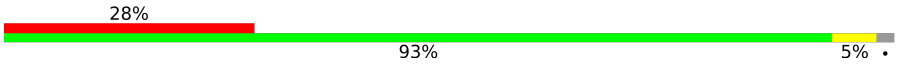
• Molecule 25: 50S ribosomal protein L30

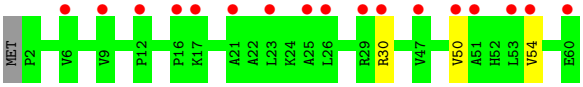
Chain 13:



• Molecule 25: 50S ribosomal protein L30

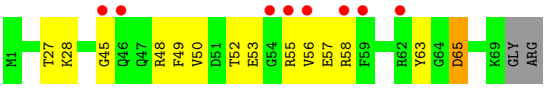
Chain 23:





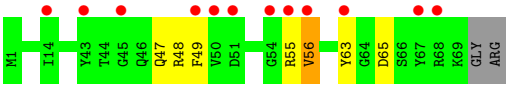
• Molecule 26: 50S ribosomal protein L31

Chain 14:



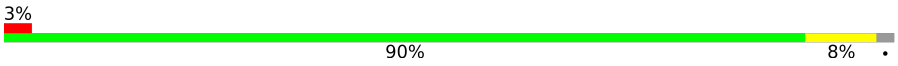
• Molecule 26: 50S ribosomal protein L31

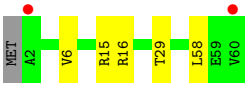
Chain 24:



• Molecule 27: 50S ribosomal protein L32

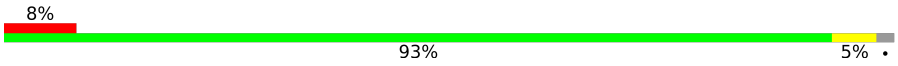
Chain 15:

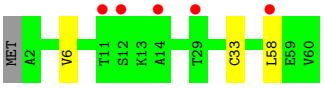




• Molecule 27: 50S ribosomal protein L32

Chain 25:



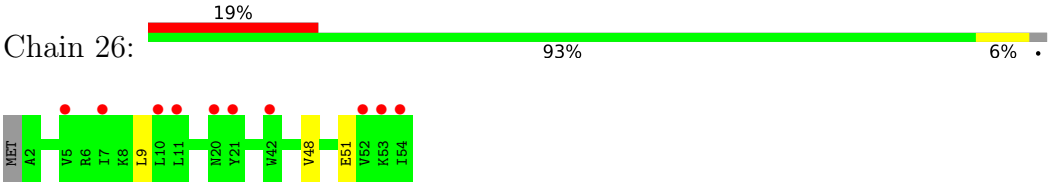


• Molecule 28: 50S ribosomal protein L33

Chain 16:

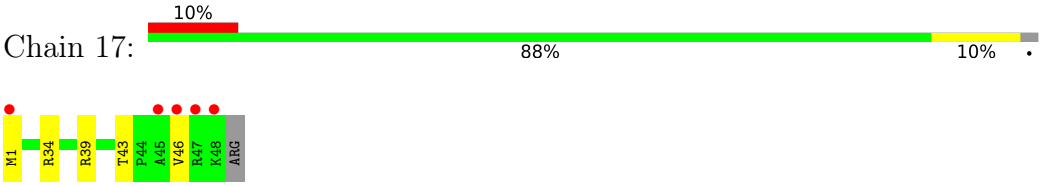
• Molecule 28: 50S ribosomal protein L33

Chain 26:



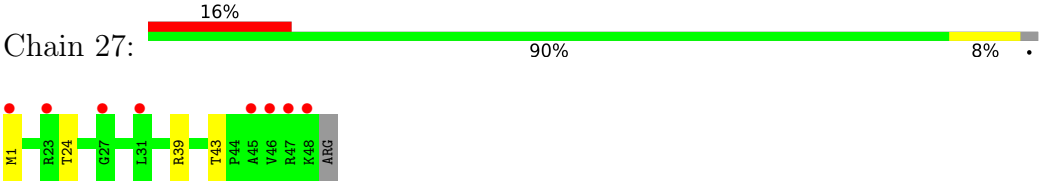
• Molecule 29: 50S ribosomal protein L34

Chain 17:



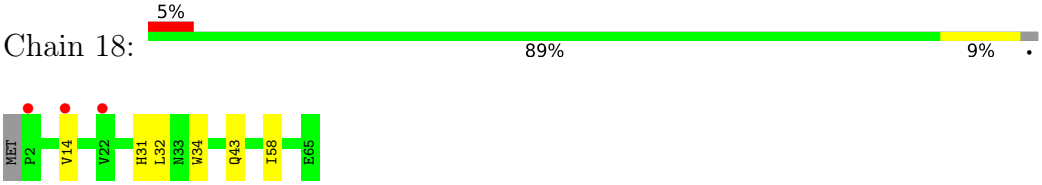
• Molecule 29: 50S ribosomal protein L34

Chain 27:



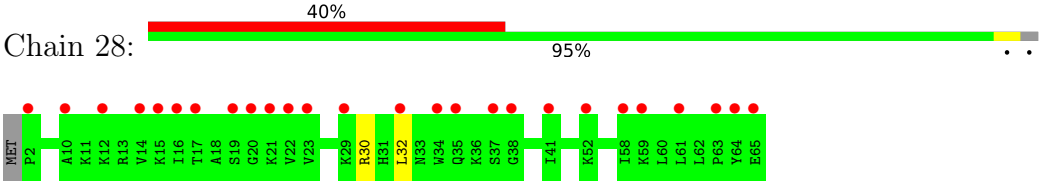
• Molecule 30: 50S ribosomal protein L35

Chain 18:



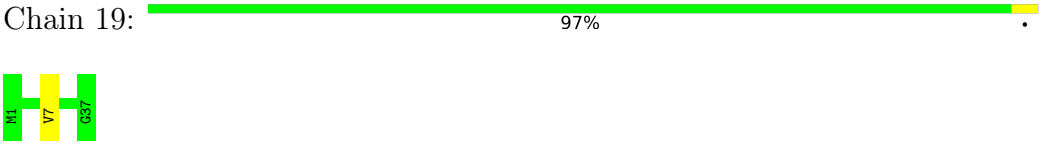
• Molecule 30: 50S ribosomal protein L35

Chain 28:



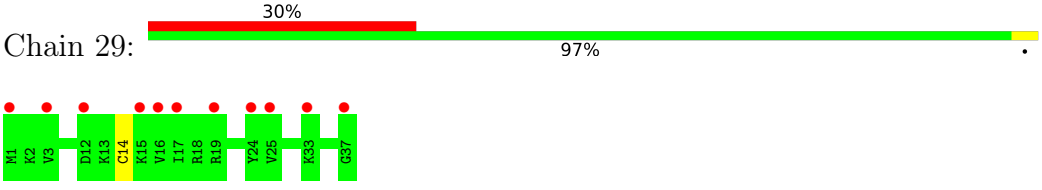
• Molecule 31: 50S ribosomal protein L36

Chain 19:



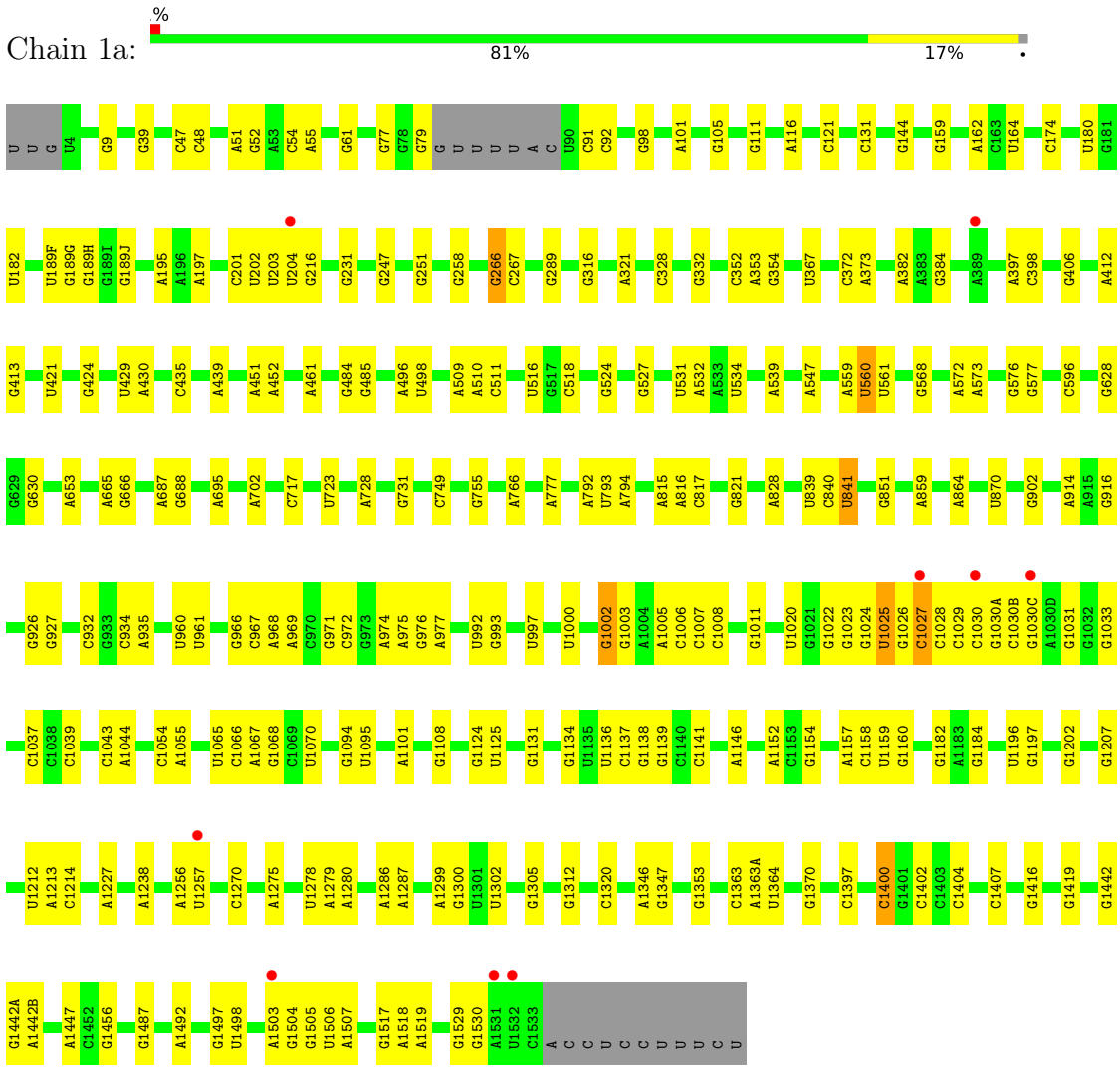
• Molecule 31: 50S ribosomal protein L36

Chain 29:



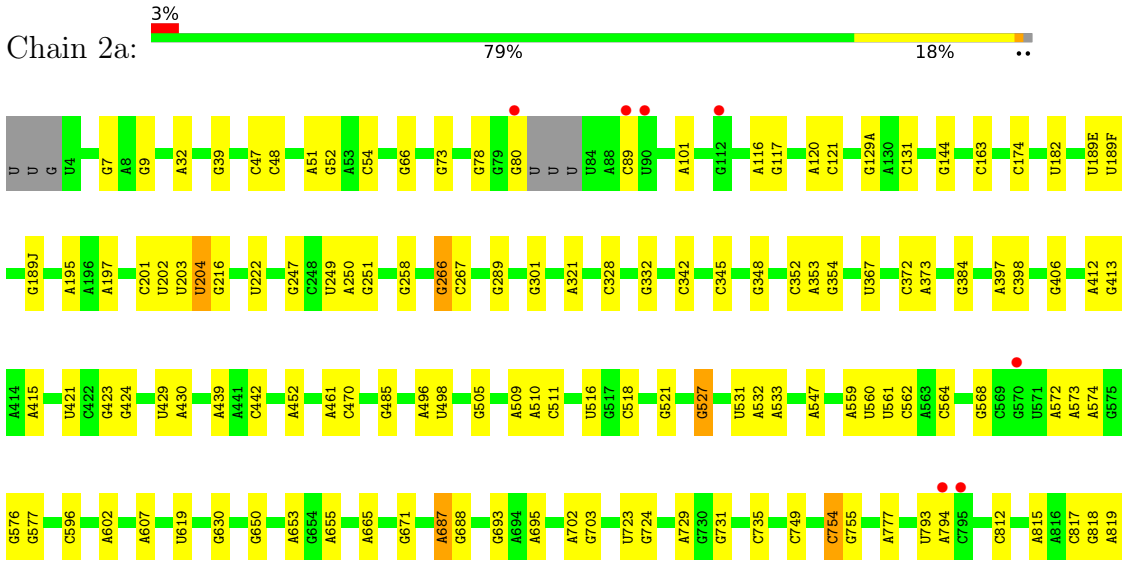
• Molecule 32: 16S Ribosomal RNA

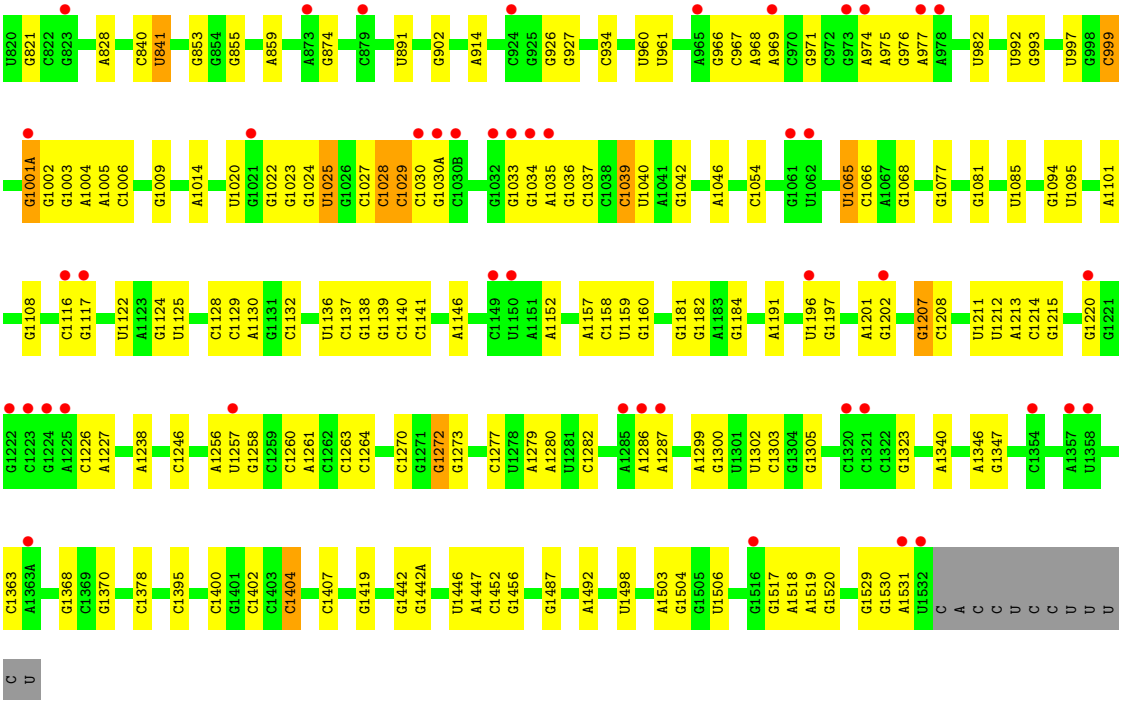
Chain 1a:



• Molecule 32: 16S Ribosomal RNA

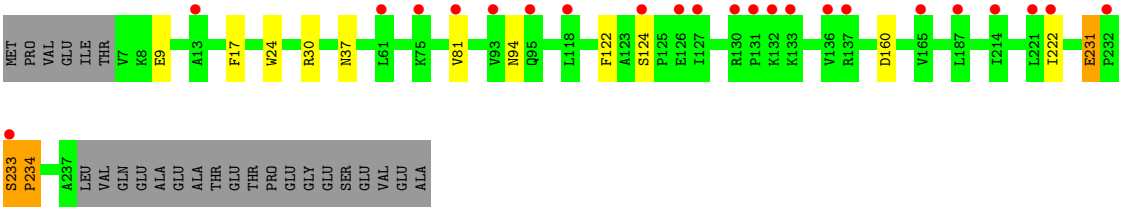
Chain 2a:





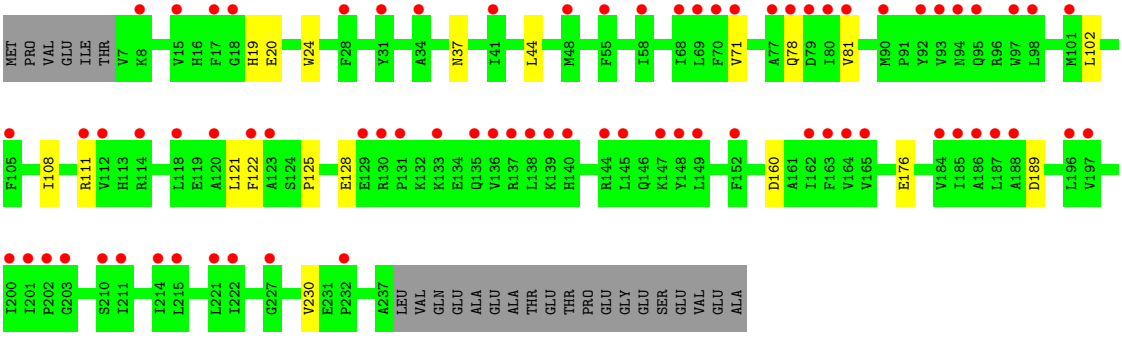
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



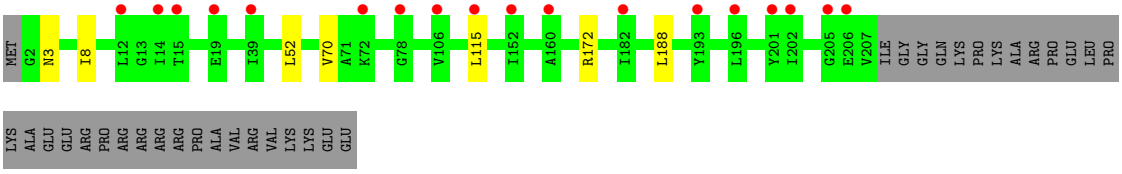
• Molecule 33: 30S ribosomal protein S2

Chain 2b:

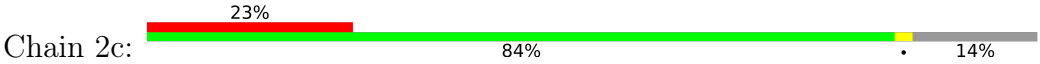


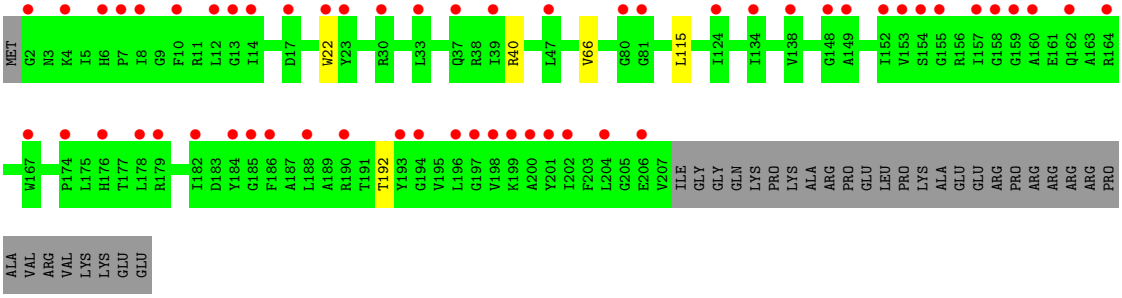
• Molecule 34: 30S ribosomal protein S3

Chain 1c:

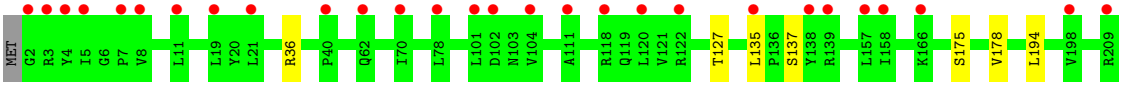


• Molecule 34: 30S ribosomal protein S3

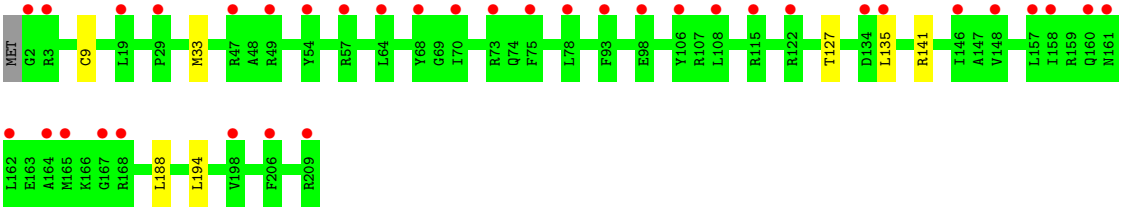




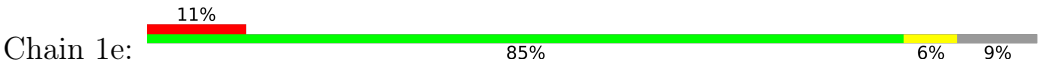
• Molecule 35: 30S ribosomal protein S4

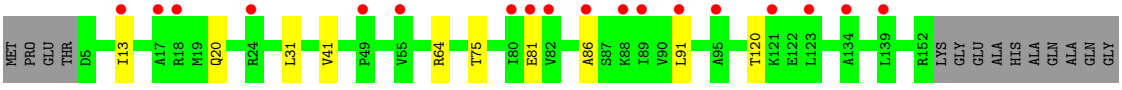


• Molecule 35: 30S ribosomal protein S4

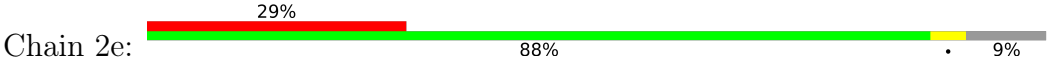


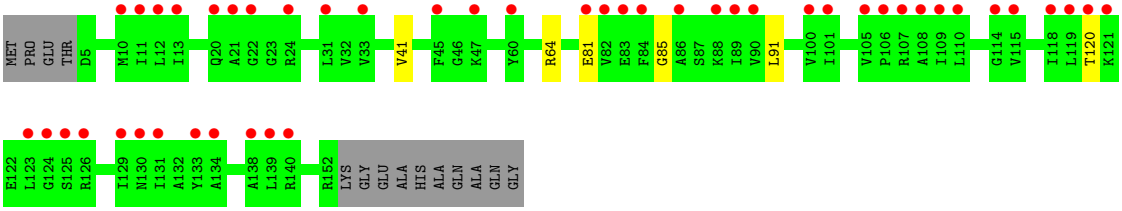
• Molecule 36: 30S ribosomal protein S5



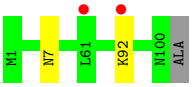


• Molecule 36: 30S ribosomal protein S5

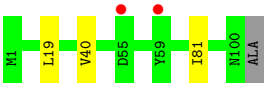




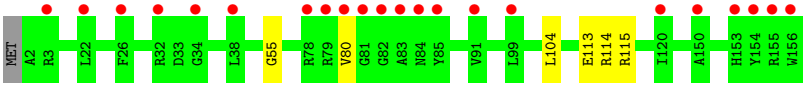
• Molecule 37: 30S ribosomal protein S6



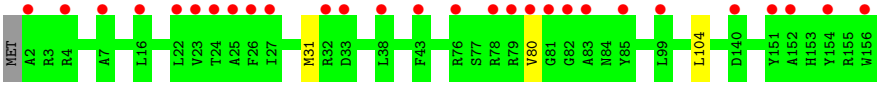
• Molecule 37: 30S ribosomal protein S6



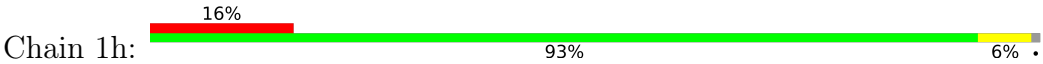
• Molecule 38: 30S ribosomal protein S7

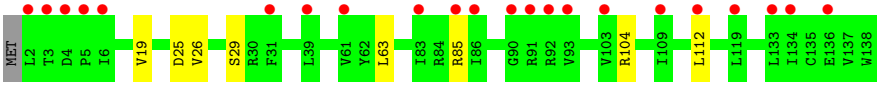


• Molecule 38: 30S ribosomal protein S7

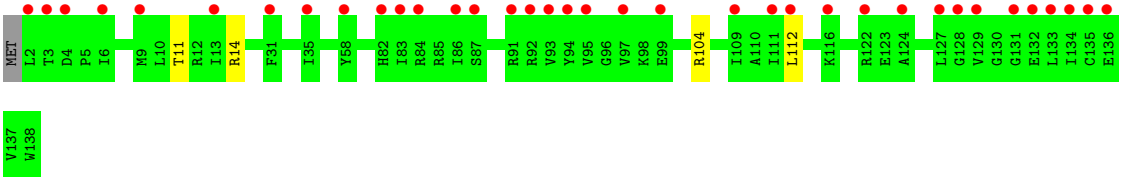


• Molecule 39: 30S ribosomal protein S8



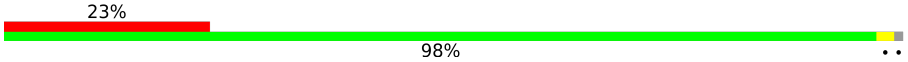


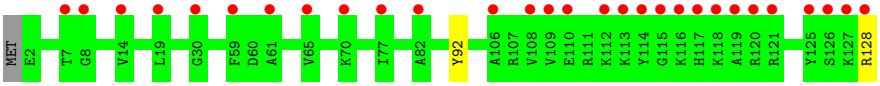
• Molecule 39: 30S ribosomal protein S8



• Molecule 40: 30S ribosomal protein S9

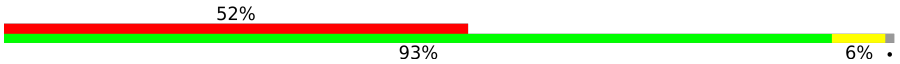
Chain 1i:

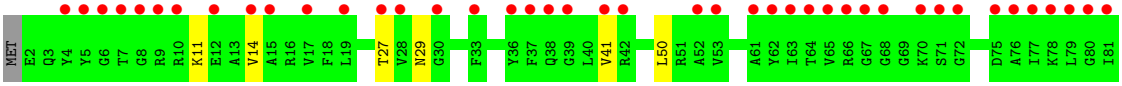


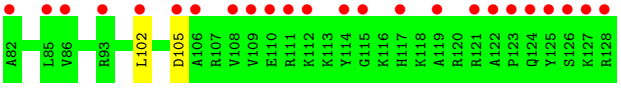


• Molecule 40: 30S ribosomal protein S9

Chain 2i:

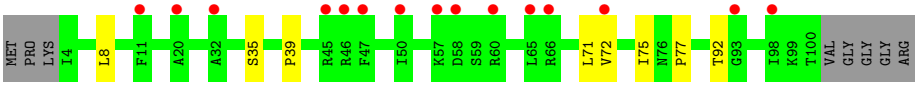






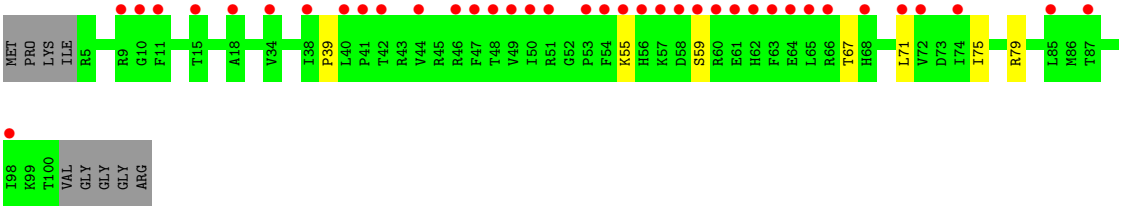
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



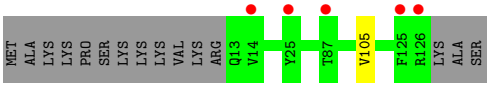
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



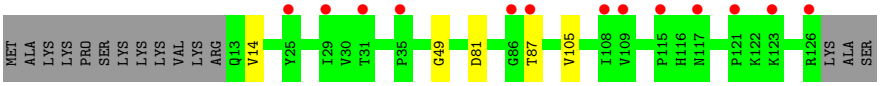
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



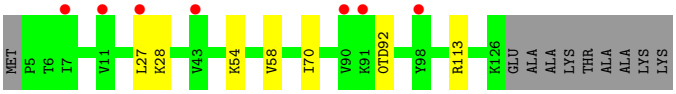
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



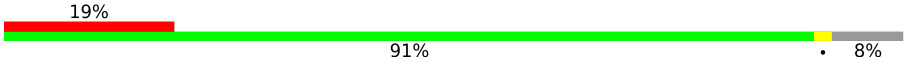
• Molecule 43: 30S ribosomal protein S12

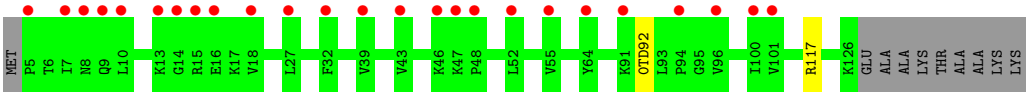
Chain 1l:



• Molecule 43: 30S ribosomal protein S12

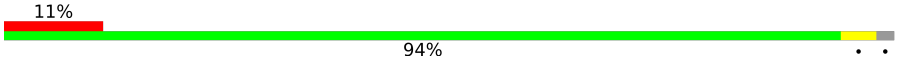
Chain 2l:

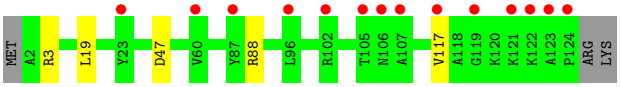




• Molecule 44: 30S ribosomal protein S13

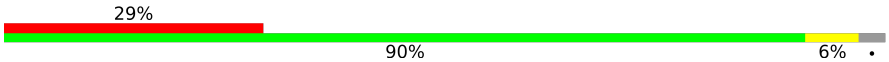
Chain 1m:

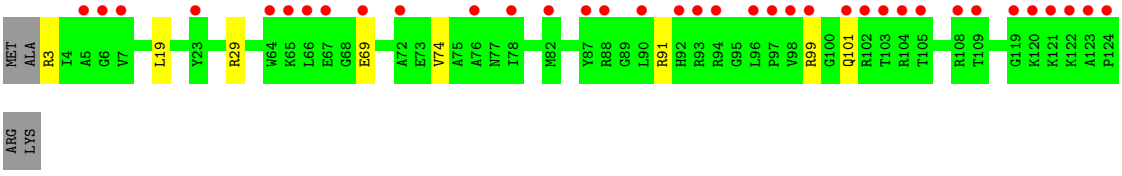




• Molecule 44: 30S ribosomal protein S13

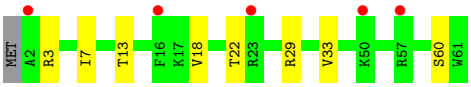
Chain 2m:





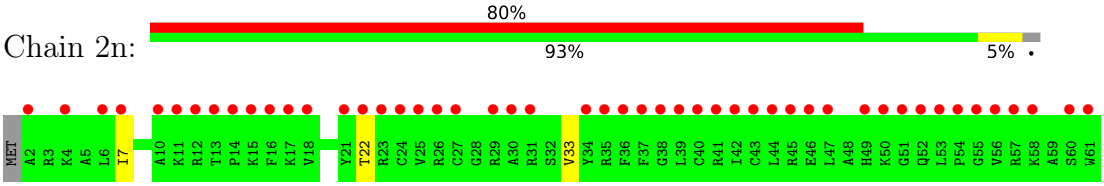
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



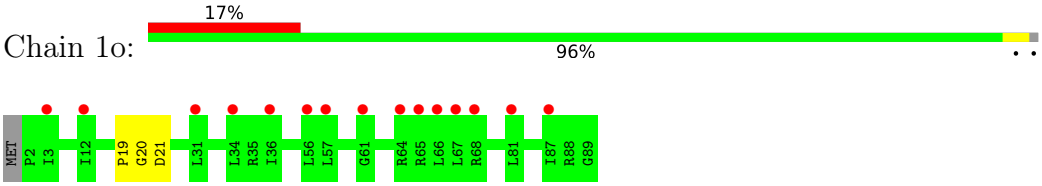
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



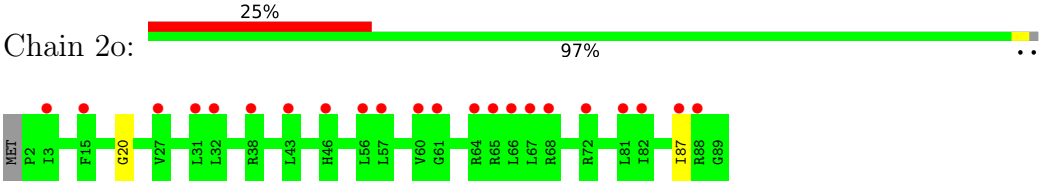
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



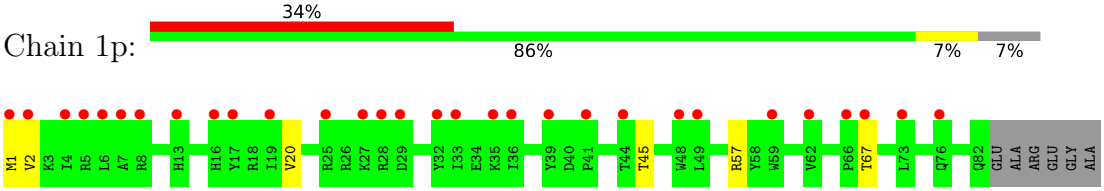
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



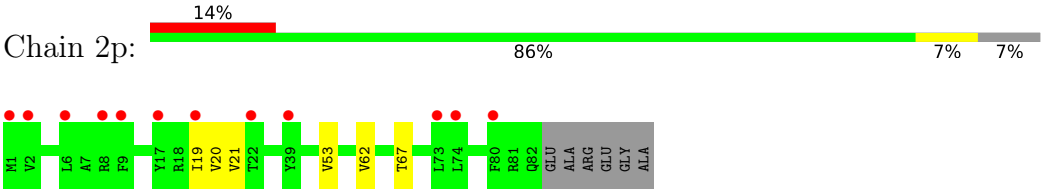
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



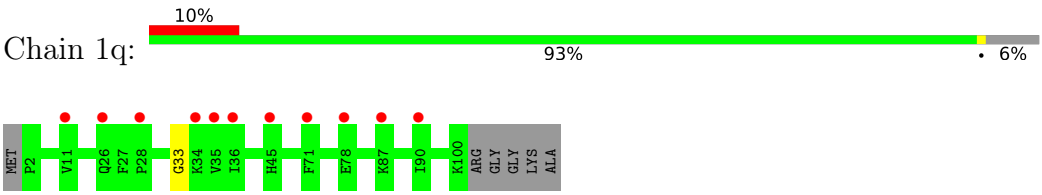
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



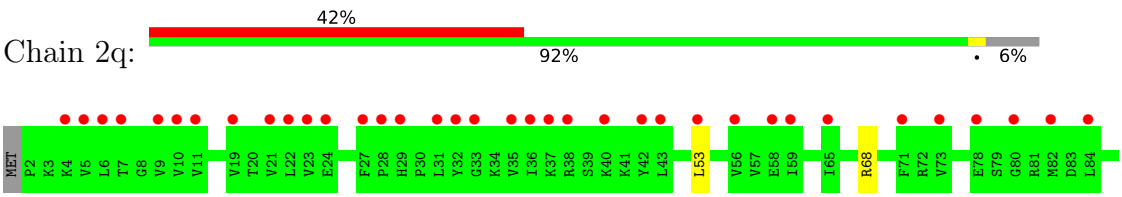
• Molecule 48: 30S ribosomal protein S17

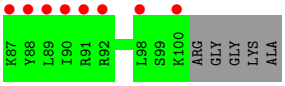
Chain 1q:



• Molecule 48: 30S ribosomal protein S17

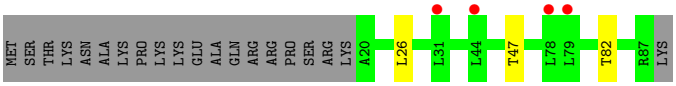
Chain 2q:





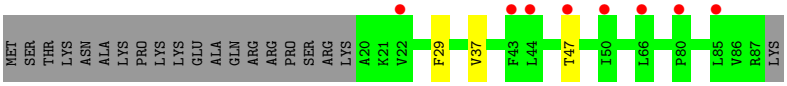
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



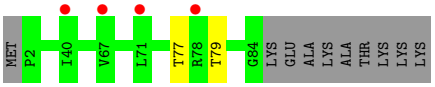
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



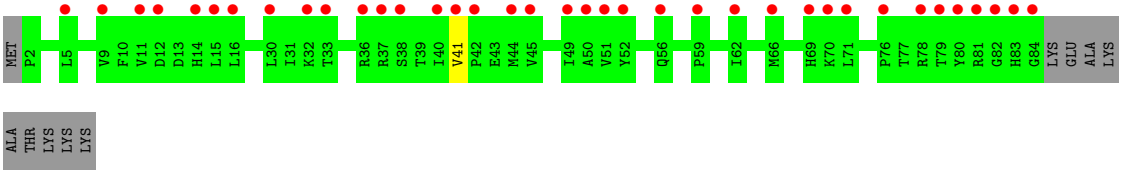
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



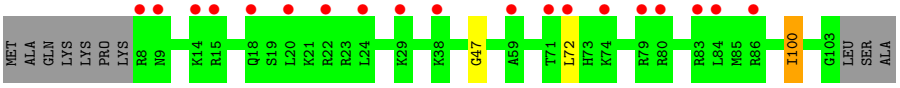
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



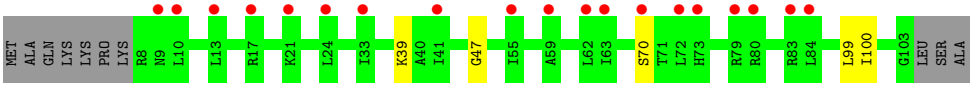
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



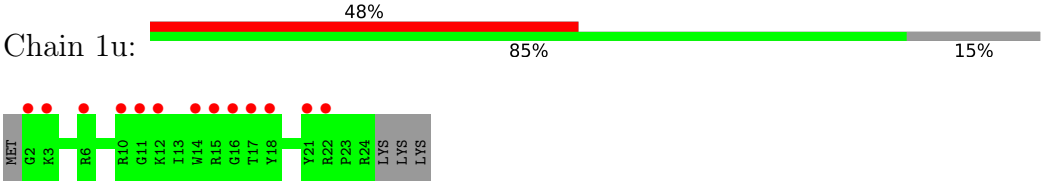
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



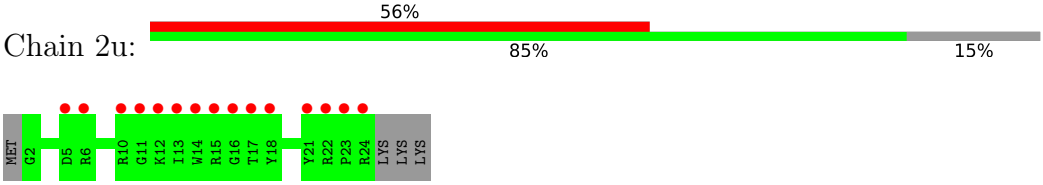
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



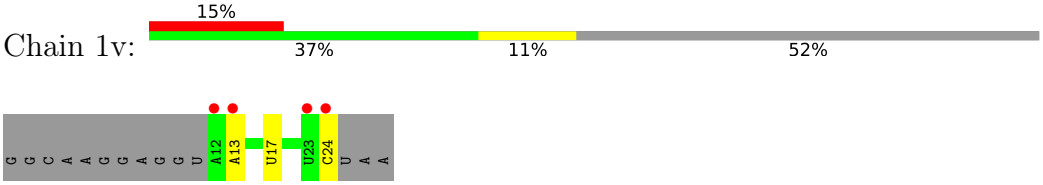
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



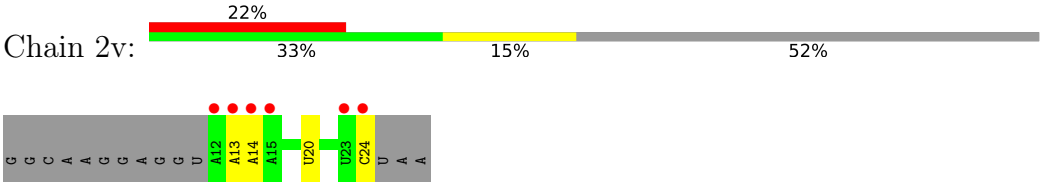
• Molecule 53: mRNA

Chain 1v:



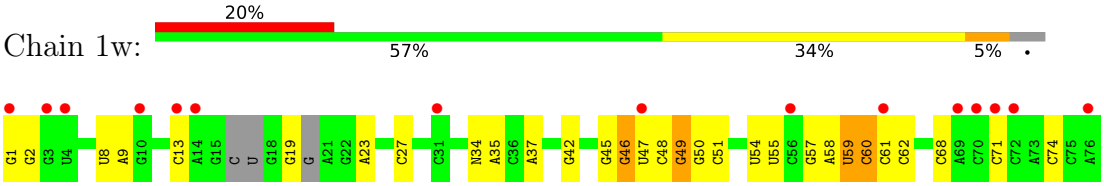
• Molecule 53: mRNA

Chain 2v:



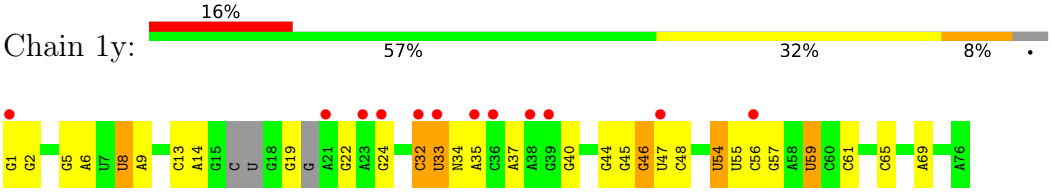
• Molecule 54: A-site and E-site tRNAs

Chain 1w:



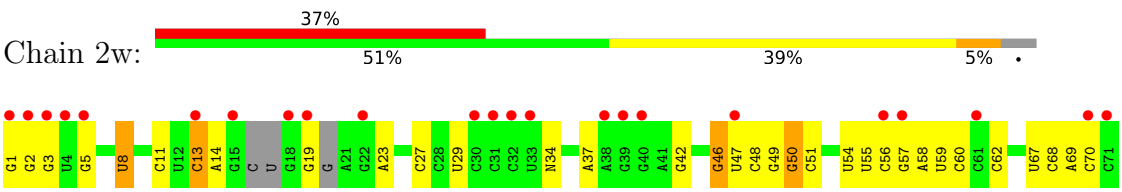
• Molecule 54: A-site and E-site tRNAs

Chain 1y:



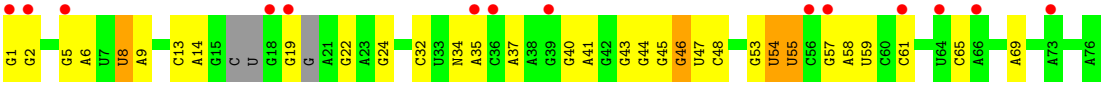
• Molecule 54: A-site and E-site tRNAs

Chain 2w:



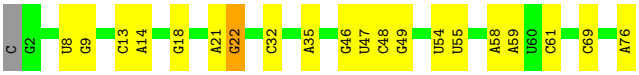
• Molecule 54: A-site and E-site tRNAs

Chain 2y:



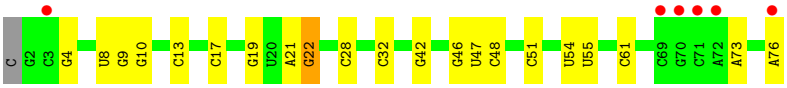
• Molecule 55: P-site tRNA

Chain 1x:



• Molecule 55: P-site tRNA

Chain 2x:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.02Å 447.76Å 618.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	254.43 – 2.75 309.19 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (254.43-2.75) 99.5 (309.19-2.75)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.235 , 0.284 0.236 , 0.284	Depositor DCC
R_{free} test set	74125 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	300702	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: MA6, 2MG, 4SU, 7MG, 2MA, OMU, K, UR3, MG, 5MU, PSU, LUJ, OMG, 5MC, M2G, CM0, SF4, OMC, 0TD, 6MZ, 4OC, ZN

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	0.34	0/69011	0.82	22/107720 (0.0%)
1	2A	0.26	0/67295	0.79	28/105042 (0.0%)
2	1B	0.34	1/2882 (0.0%)	0.76	0/4494
2	2B	0.30	1/2879 (0.0%)	0.77	1/4487 (0.0%)
3	1D	0.29	0/2186	0.52	0/2944
3	2D	0.27	0/2186	0.49	0/2944
4	1E	0.30	0/1592	0.48	0/2149
4	2E	0.26	0/1592	0.47	0/2149
5	1F	0.28	0/1619	0.47	0/2193
5	2F	0.26	0/1615	0.44	0/2188
6	1G	0.27	0/1448	0.45	0/1957
6	2G	0.26	0/1453	0.46	0/1963
7	1H	0.27	0/1356	0.45	0/1834
7	2H	0.25	0/1356	0.43	0/1834
8	1I	0.26	0/1112	0.45	0/1514
8	2I	0.25	0/1079	0.44	0/1475
9	1N	0.27	0/1144	0.46	0/1543
9	2N	0.25	0/1144	0.43	0/1543
10	1O	0.31	0/943	0.49	0/1269
10	2O	0.28	0/943	0.48	0/1269
11	1P	0.28	0/1152	0.48	0/1533
11	2P	0.26	0/1152	0.46	0/1533
12	1Q	0.32	0/1143	0.47	0/1527
12	2Q	0.26	0/1143	0.45	0/1527
13	1R	0.28	0/982	0.46	0/1312
13	2R	0.24	0/982	0.46	0/1312
14	1S	0.26	0/883	0.45	0/1176
14	2S	0.26	0/880	0.43	0/1172
15	1T	0.28	0/1105	0.47	0/1477
15	2T	0.26	0/1097	0.44	0/1468
16	1U	0.30	0/977	0.43	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.26	0/977	0.41	0/1301
17	1V	0.29	0/782	0.49	0/1049
17	2V	0.27	0/782	0.50	0/1049
18	1W	0.29	0/897	0.46	0/1205
18	2W	0.26	0/897	0.42	0/1205
19	1X	0.30	0/764	0.51	0/1025
19	2X	0.26	0/764	0.46	0/1025
20	1Y	0.28	0/819	0.50	0/1095
20	2Y	0.26	0/819	0.47	0/1095
21	1Z	0.27	0/1267	0.48	0/1717
21	2Z	0.26	0/1299	0.48	0/1763
22	10	0.29	0/662	0.48	0/881
22	20	0.27	0/662	0.46	0/881
23	11	0.28	0/762	0.46	0/1014
23	21	0.26	0/762	0.47	0/1014
24	12	0.27	0/590	0.41	0/781
24	22	0.25	0/590	0.38	0/781
25	13	0.28	0/474	0.46	0/635
25	23	0.24	0/469	0.43	0/630
26	14	0.30	0/565	0.55	0/761
26	24	0.26	0/545	0.50	0/737
27	15	0.29	0/469	0.51	0/635
27	25	0.29	0/469	0.47	0/635
28	16	0.28	0/460	0.48	0/613
28	26	0.26	0/456	0.46	0/608
29	17	0.26	0/426	0.47	0/561
29	27	0.25	0/426	0.45	0/561
30	18	0.28	0/525	0.48	0/691
30	28	0.25	0/525	0.45	0/691
31	19	0.29	0/310	0.47	0/407
31	29	0.24	0/310	0.47	0/407
32	1a	0.26	0/35795	0.80	19/55864 (0.0%)
32	2a	0.26	2/35886 (0.0%)	0.84	47/56005 (0.1%)
33	1b	0.32	0/1881	0.50	2/2542 (0.1%)
33	2b	0.26	0/1860	0.44	0/2518
34	1c	0.26	0/1572	0.45	0/2126
34	2c	0.25	0/1566	0.44	0/2119
35	1d	0.29	1/1685 (0.1%)	0.42	0/2262
35	2d	0.27	0/1704	0.42	0/2284
36	1e	0.26	0/1145	0.46	0/1543
36	2e	0.26	0/1149	0.47	0/1548
37	1f	0.25	0/823	0.43	0/1115
37	2f	0.26	0/829	0.44	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.26	0/1250	0.41	0/1679
38	2g	0.25	0/1254	0.39	0/1683
39	1h	0.26	0/1108	0.45	0/1494
39	2h	0.25	0/1108	0.44	0/1494
40	1i	0.26	0/1002	0.47	0/1346
40	2i	0.26	0/997	0.46	0/1343
41	1j	0.24	0/722	0.45	0/982
41	2j	0.26	0/727	0.46	0/988
42	1k	0.25	0/844	0.44	0/1145
42	2k	0.26	0/848	0.45	0/1149
43	1l	0.26	0/937	0.48	0/1260
43	2l	0.26	0/937	0.48	0/1260
44	1m	0.25	0/969	0.45	0/1302
44	2m	0.26	0/961	0.46	0/1291
45	1n	0.26	0/501	0.43	0/664
45	2n	0.27	0/501	0.42	0/664
46	1o	0.25	0/739	0.41	0/985
46	2o	0.23	0/739	0.43	0/985
47	1p	0.25	0/697	0.46	0/939
47	2p	0.25	0/693	0.46	0/935
48	1q	0.24	0/836	0.45	0/1117
48	2q	0.25	0/836	0.44	0/1117
49	1r	0.24	0/560	0.43	0/746
49	2r	0.24	0/560	0.42	0/746
50	1s	0.26	0/667	0.50	0/900
50	2s	0.27	0/661	0.51	0/893
51	1t	0.25	0/730	0.43	0/965
51	2t	0.25	0/729	0.42	0/965
52	1u	0.24	0/203	0.43	0/266
52	2u	0.23	0/203	0.45	0/266
53	1v	0.36	0/308	0.95	2/477 (0.4%)
53	2v	0.30	0/308	0.82	0/477
54	1w	0.67	5/1600 (0.3%)	1.24	11/2482 (0.4%)
54	1y	0.66	5/1600 (0.3%)	1.20	15/2482 (0.6%)
54	2w	0.45	1/1600 (0.1%)	1.06	4/2482 (0.2%)
54	2y	0.44	1/1600 (0.1%)	0.96	1/2482 (0.0%)
55	1x	0.40	0/1725	1.03	9/2689 (0.3%)
55	2x	0.36	0/1725	1.03	9/2689 (0.3%)
All	All	0.29	17/316735 (0.0%)	0.74	170/474180 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	14	0	1
33	1b	0	1
All	All	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	59	U	C4-O4	13.16	1.34	1.23
54	1y	59	U	C4-O4	13.03	1.34	1.23
54	1y	32	C	C4-N4	-11.30	1.23	1.33
54	1w	60	C	C4-N4	-11.27	1.23	1.33
54	1w	1	G	OP3-P	-10.52	1.48	1.61
54	2w	1	G	OP3-P	-10.52	1.48	1.61
2	2B	1	U	OP3-P	-10.49	1.48	1.61
54	1y	1	G	OP3-P	-10.43	1.48	1.61
54	2y	1	G	OP3-P	-10.43	1.48	1.61
2	1B	1	U	OP3-P	-10.17	1.49	1.61
32	2a	1272	G	C6-N1	-8.23	1.33	1.39
32	2a	1272	G	N1-C2	-7.84	1.31	1.37
54	1y	32	C	N3-C4	6.75	1.38	1.33
54	1w	60	C	N3-C4	6.28	1.38	1.33
54	1w	59	U	N3-C4	-5.45	1.33	1.38
35	1d	36	ARG	C-N	5.38	1.44	1.34
54	1y	59	U	N3-C4	-5.34	1.33	1.38

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	60	C	N3-C4-C5	-19.32	114.17	121.90
32	2a	1272	G	N3-C2-N2	18.90	133.13	119.90
54	1y	32	C	N3-C4-C5	-18.38	114.55	121.90
32	2a	1263	C	N1-C2-O2	17.46	129.37	118.90
32	2a	1272	G	C5-C6-O6	17.13	138.88	128.60
54	1w	60	C	C2-N3-C4	15.74	127.77	119.90
32	2a	1272	G	N1-C2-N2	-15.70	102.07	116.20
54	1y	32	C	C2-N3-C4	14.18	126.99	119.90
32	2a	1272	G	C6-N1-C2	12.54	132.62	125.10
54	1y	59	U	N3-C4-C5	11.66	121.60	114.60
54	1w	59	U	N3-C4-C5	11.55	121.53	114.60
54	1y	59	U	C2-N3-C4	-11.48	120.11	127.00
54	1w	59	U	C2-N3-C4	-11.33	120.20	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1263	C	C2-N3-C4	11.22	125.51	119.90
32	2a	1272	G	C5-C6-N1	-10.71	106.14	111.50
32	2a	1263	C	C5-C6-N1	10.21	126.11	121.00
54	1w	60	C	N1-C2-O2	10.05	124.93	118.90
1	2A	2136	C	N1-C2-O2	9.57	124.64	118.90
32	2a	1263	C	N3-C2-O2	-9.42	115.31	121.90
1	1A	1086	A	N1-C6-N6	-8.84	113.30	118.60
54	1y	59	U	C5-C4-O4	-8.60	120.74	125.90
54	1w	60	C	C5-C4-N4	8.58	126.20	120.20
32	2a	1158	C	C2-N1-C1'	8.57	128.23	118.80
32	2a	1272	G	N1-C6-O6	-8.23	114.96	119.90
32	2a	1158	C	N1-C2-O2	8.23	123.84	118.90
54	1w	59	U	C5-C4-O4	-8.21	120.97	125.90
32	1a	1030(B)	C	C2-N1-C1'	8.04	127.64	118.80
54	1w	59	U	N1-C2-N3	7.99	119.69	114.90
54	1y	32	C	C5-C4-N4	7.98	125.79	120.20
54	1y	59	U	N1-C2-N3	7.93	119.66	114.90
32	2a	1272	G	C2-N3-C4	-7.91	107.94	111.90
54	1y	22	G	N1-C6-O6	7.70	124.52	119.90
1	1A	1075	C	N1-C2-O2	7.67	123.50	118.90
1	1A	2167	U	C2-N1-C1'	7.61	126.83	117.70
32	2a	1272	G	C4-N9-C1'	7.55	136.32	126.50
1	1A	1075	C	C2-N3-C4	7.50	123.65	119.90
1	2A	2167	U	N1-C2-O2	7.40	127.98	122.80
32	2a	754	C	C2-N1-C1'	7.32	126.85	118.80
32	1a	1030(B)	C	N1-C2-O2	7.31	123.28	118.90
32	2a	1263	C	C6-N1-C2	-7.24	117.40	120.30
1	2A	1313	U	C2-N1-C1'	7.23	126.38	117.70
32	2a	754	C	N1-C2-O2	7.21	123.23	118.90
1	1A	2167	U	N1-C2-O2	7.20	127.84	122.80
32	2a	1272	G	C8-N9-C1'	-7.20	117.64	127.00
32	1a	1025	U	N1-C2-O2	7.15	127.80	122.80
55	2x	17	C	N1-C2-O2	7.11	123.17	118.90
55	1x	46	G	C6-N1-C2	-7.10	120.84	125.10
32	2a	1263	C	C2-N1-C1'	6.98	126.48	118.80
32	2a	999	C	N1-C2-O2	6.94	123.06	118.90
1	1A	2167	U	N3-C2-O2	-6.90	117.37	122.20
55	2x	17	C	C2-N1-C1'	6.89	126.38	118.80
1	2A	2167	U	C2-N1-C1'	6.89	125.96	117.70
32	2a	1001(A)	G	N3-C4-N9	6.85	130.11	126.00
32	2a	1039	C	C5-C4-N4	-6.85	115.41	120.20
1	2A	2167	U	N3-C2-O2	-6.78	117.46	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2897	U	C2-N1-C1'	6.74	125.78	117.70
2	2B	80	U	O4'-C1'-N1	6.68	113.54	108.20
1	1A	12	U	C2-N1-C1'	6.67	125.70	117.70
32	2a	1263	C	C4-C5-C6	-6.67	114.07	117.40
32	2a	1029	C	N1-C2-O2	6.63	122.88	118.90
1	2A	2136	C	N3-C2-O2	-6.61	117.27	121.90
53	1v	17	U	C2-N3-C4	6.55	130.93	127.00
1	1A	1063	G	C5-C6-O6	6.55	132.53	128.60
1	2A	2473	U	C2-N1-C1'	6.50	125.51	117.70
1	1A	512	G	O4'-C1'-N9	6.42	113.34	108.20
54	2w	50	G	C5-C6-O6	-6.36	124.78	128.60
55	2x	17	C	N3-C2-O2	-6.34	117.46	121.90
32	1a	1030(B)	C	C6-N1-C2	-6.29	117.78	120.30
54	1w	49	G	N3-C4-N9	6.28	129.76	126.00
32	1a	1027	C	C6-N1-C1'	6.25	128.30	120.80
32	1a	1030(B)	C	N3-C2-O2	-6.23	117.54	121.90
54	1y	32	C	N1-C2-O2	6.21	122.63	118.90
54	1y	22	G	C6-C5-N7	-6.21	126.68	130.40
32	1a	1025	U	C2-N1-C1'	6.19	125.13	117.70
32	2a	1054	C	C2-N1-C1'	6.19	125.61	118.80
53	1v	17	U	C5-C4-O4	6.17	129.60	125.90
55	1x	22	G	N1-C6-O6	-6.17	116.20	119.90
32	2a	1158	C	C6-N1-C1'	-6.16	113.40	120.80
54	1w	60	C	N1-C2-N3	-6.12	114.92	119.20
32	1a	1002	G	N3-C4-N9	6.11	129.66	126.00
55	2x	22	G	N1-C6-O6	-6.09	116.25	119.90
32	2a	1039	C	C2-N1-C1'	6.09	125.50	118.80
32	2a	841	U	C5-C6-N1	6.08	125.74	122.70
32	2a	1158	C	N3-C2-O2	-6.08	117.65	121.90
32	1a	1027	C	C2-N1-C1'	-6.06	112.14	118.80
54	1y	32	C	N1-C2-N3	-6.05	114.97	119.20
1	1A	2789	C	O4'-C1'-N1	5.95	112.96	108.20
55	1x	46	G	N3-C2-N2	-5.93	115.75	119.90
1	1A	1174	A	OP1-P-O3'	5.90	118.18	105.20
32	2a	1264	C	N1-C2-O2	5.87	122.42	118.90
32	2a	1028	C	C2-N3-C4	5.87	122.83	119.90
1	2A	528	A	OP1-P-O3'	5.86	118.09	105.20
32	2a	1039	C	N3-C4-N4	5.78	122.05	118.00
1	1A	1063	G	C6-N1-C2	5.78	128.57	125.10
32	1a	266	G	P-O3'-C3'	5.76	126.61	119.70
54	1y	22	G	C4-C5-C6	5.75	122.25	118.80
54	2w	29	U	C5-C4-O4	5.74	129.34	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	35	A	C6-N1-C2	5.73	122.04	118.60
1	2A	1142	U	C2-N1-C1'	5.71	124.55	117.70
1	2A	2897	U	N1-C2-O2	5.70	126.79	122.80
1	2A	2154	G	C5-C6-O6	-5.69	125.19	128.60
1	2A	2155	G	N3-C2-N2	5.67	123.87	119.90
1	1A	1176	G	OP1-P-O3'	5.67	117.68	105.20
32	2a	1054	C	N1-C2-O2	5.67	122.30	118.90
32	1a	1002	G	C4-N9-C1'	5.65	133.85	126.50
32	2a	1263	C	N1-C2-N3	-5.62	115.27	119.20
1	1A	847	U	C2-N1-C1'	5.60	124.42	117.70
32	1a	1002	G	N3-C4-C5	-5.60	125.80	128.60
55	1x	35	A	C5-C6-N6	5.60	128.18	123.70
32	2a	1025	U	N1-C2-O2	5.59	126.71	122.80
32	2a	1029	C	C2-N3-C4	5.58	122.69	119.90
33	1b	233	SER	C-N-CD	5.51	139.97	128.40
32	2a	1395	C	N1-C2-O2	5.51	122.20	118.90
1	1A	2789	C	C2-N1-C1'	-5.50	112.75	118.80
55	2x	22	G	C6-C5-N7	5.48	133.69	130.40
1	2A	214	G	O4'-C1'-N9	5.46	112.57	108.20
54	1w	60	C	C5-C6-N1	5.45	123.73	121.00
1	2A	1420	U	C2-N1-C1'	5.45	124.23	117.70
32	2a	1001(A)	G	C4-N9-C1'	5.44	133.57	126.50
32	2a	754	C	N3-C2-O2	-5.43	118.10	121.90
1	2A	528	A	P-O3'-C3'	5.43	126.22	119.70
54	2w	50	G	N1-C6-O6	5.43	123.16	119.90
1	2A	2140	C	N1-C2-O2	5.41	122.14	118.90
32	1a	1027	C	N3-C4-C5	-5.40	119.74	121.90
32	2a	754	C	C6-N1-C1'	-5.40	114.32	120.80
54	1y	56	C	N1-C2-O2	5.39	122.14	118.90
1	2A	1644	C	N1-C2-O2	5.39	122.13	118.90
55	1x	22	G	C4-C5-C6	-5.38	115.57	118.80
32	2a	1065	U	P-O3'-C3'	5.36	126.13	119.70
55	1x	14	A	C4-C5-C6	5.32	119.66	117.00
1	2A	2155	G	C6-N1-C2	5.30	128.28	125.10
1	1A	1313	U	C2-N1-C1'	5.29	124.05	117.70
32	2a	204	U	C2-N1-C1'	5.29	124.04	117.70
55	1x	22	G	C8-N9-C1'	5.25	133.82	127.00
1	2A	2473	U	N1-C2-O2	5.25	126.47	122.80
32	2a	1001(A)	G	C6-C5-N7	-5.25	127.25	130.40
32	1a	1067	A	P-O3'-C3'	5.24	125.99	119.70
32	2a	841	U	C2-N1-C1'	5.24	123.98	117.70
32	2a	266	G	P-O3'-C3'	5.22	125.97	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	46	G	C6-N1-C2	-5.22	121.97	125.10
1	1A	1174	A	P-O3'-C3'	5.22	125.96	119.70
1	1A	1086	A	C5-C6-N6	5.21	127.87	123.70
32	1a	1030(B)	C	C6-N1-C1'	-5.21	114.55	120.80
54	2y	22	G	N1-C6-O6	5.20	123.02	119.90
32	1a	1025	U	C6-N1-C1'	-5.19	113.94	121.20
1	1A	2167	U	C5-C6-N1	5.17	125.28	122.70
32	1a	841	U	C5-C6-N1	5.16	125.28	122.70
33	1b	231	GLU	C-N-CD	5.16	139.24	128.40
55	2x	22	G	N3-C4-N9	-5.16	122.90	126.00
54	1y	22	G	N3-C4-N9	5.16	129.09	126.00
1	2A	1210	A	P-O3'-C3'	5.16	125.89	119.70
1	1A	548	A	P-O3'-C3'	5.15	125.88	119.70
1	2A	1992	G	P-O3'-C3'	5.15	125.88	119.70
1	2A	1313	U	N1-C2-O2	5.14	126.40	122.80
1	2A	1644	C	C2-N1-C1'	5.13	124.45	118.80
1	2A	928	G	C6-C5-N7	-5.13	127.32	130.40
55	2x	17	C	C6-N1-C2	-5.12	118.25	120.30
1	2A	1380	G	O5'-P-OP2	-5.12	101.09	105.70
55	1x	14	A	C5-N7-C8	5.11	106.45	103.90
1	1A	1063	G	N3-C2-N2	5.10	123.47	119.90
54	2w	13	C	P-O3'-C3'	5.10	125.82	119.70
54	1y	33	U	C2-N1-C1'	5.10	123.82	117.70
1	1A	1992	G	P-O3'-C3'	5.09	125.81	119.70
55	2x	22	G	C8-N9-C1'	5.08	133.60	127.00
1	2A	2866	U	C2-N1-C1'	5.05	123.76	117.70
32	1a	560	U	C3'-C2'-C1'	5.05	105.54	101.50
32	2a	687	A	P-O3'-C3'	5.04	125.75	119.70
1	2A	2136	C	C2-N1-C1'	5.03	124.34	118.80
32	1a	1158	C	C2-N1-C1'	5.01	124.32	118.80
32	2a	1039	C	C6-N1-C1'	-5.00	114.79	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	63	TYR	Peptide
33	1b	124	SER	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	255 (93%)	17 (6%)	1 (0%)	34	53
3	2D	273/276 (99%)	261 (96%)	11 (4%)	1 (0%)	34	53
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	47
4	2E	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	29	47
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	29	47
5	2F	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	15	27
6	1G	179/182 (98%)	163 (91%)	15 (8%)	1 (1%)	25	42
6	2G	179/182 (98%)	162 (90%)	15 (8%)	2 (1%)	14	25
7	1H	172/180 (96%)	164 (95%)	7 (4%)	1 (1%)	25	42
7	2H	172/180 (96%)	157 (91%)	14 (8%)	1 (1%)	25	42
8	1I	144/148 (97%)	134 (93%)	9 (6%)	1 (1%)	22	39
8	2I	144/148 (97%)	133 (92%)	9 (6%)	2 (1%)	11	19
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
9	2N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	39
11	2P	147/150 (98%)	140 (95%)	7 (5%)	0	100	100
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
14	1S	108/112 (96%)	105 (97%)	3 (3%)	0	100 100
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100 100
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100 100
15	2T	129/146 (88%)	122 (95%)	5 (4%)	2 (2%)	9 16
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
17	1V	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	7 13
17	2V	99/101 (98%)	93 (94%)	6 (6%)	0	100 100
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
18	2W	110/113 (97%)	110 (100%)	0	0	100 100
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100 100
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
20	1Y	105/110 (96%)	100 (95%)	4 (4%)	1 (1%)	15 27
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100 100
21	1Z	148/206 (72%)	131 (88%)	14 (10%)	3 (2%)	7 13
21	2Z	156/206 (76%)	137 (88%)	15 (10%)	4 (3%)	5 8
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100 100
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100 100
24	12	68/72 (94%)	68 (100%)	0	0	100 100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
25	23	57/60 (95%)	56 (98%)	0	1 (2%)	8 15
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1 1
26	24	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1 1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
27	25	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
28	16	51/54 (94%)	47 (92%)	4 (8%)	0	100 100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
33	1b	229/256 (90%)	201 (88%)	23 (10%)	5 (2%)	6 11
33	2b	229/256 (90%)	203 (89%)	22 (10%)	4 (2%)	9 16
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100 100
34	2c	204/239 (85%)	187 (92%)	16 (8%)	1 (0%)	29 47
35	1d	206/209 (99%)	200 (97%)	6 (3%)	0	100 100
35	2d	206/209 (99%)	200 (97%)	6 (3%)	0	100 100
36	1e	146/162 (90%)	137 (94%)	8 (6%)	1 (1%)	22 39
36	2e	146/162 (90%)	137 (94%)	8 (6%)	1 (1%)	22 39
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100 100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
38	1g	153/156 (98%)	147 (96%)	3 (2%)	3 (2%)	7 13
38	2g	153/156 (98%)	142 (93%)	10 (6%)	1 (1%)	22 39
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100 100
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100 100
40	1i	125/128 (98%)	115 (92%)	10 (8%)	0	100 100
40	2i	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	19 34
41	1j	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	4 6
41	2j	94/105 (90%)	83 (88%)	7 (7%)	4 (4%)	2 3
42	1k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17 31
42	2k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8 15
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100 100
43	2l	119/132 (90%)	113 (95%)	6 (5%)	0	100 100
44	1m	121/126 (96%)	111 (92%)	10 (8%)	0	100 100
44	2m	120/126 (95%)	109 (91%)	9 (8%)	2 (2%)	9 16
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100 100
46	1o	86/89 (97%)	83 (96%)	1 (1%)	2 (2%)	6 10
46	2o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13 23
47	1p	80/88 (91%)	78 (98%)	2 (2%)	0	100 100
47	2p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12 21
48	1q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	15 27
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100 100
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100 100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100 100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100 100
50	2s	81/93 (87%)	69 (85%)	12 (15%)	0	100 100
51	1t	94/106 (89%)	88 (94%)	4 (4%)	2 (2%)	7 12
51	2t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	7 12
52	1u	21/27 (78%)	21 (100%)	0	0	100 100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
All	All	11370/12128 (94%)	10699 (94%)	596 (5%)	75 (1%)	22 39

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1H	126	PRO
8	1I	10	GLU
26	14	65	ASP
33	1b	17	PHE
51	1t	100	ILE
5	2F	130	ALA
7	2H	126	PRO
8	2I	10	GLU
26	24	55	ARG
26	24	56	VAL
33	2b	125	PRO
33	2b	128	GLU
5	1F	130	ALA
26	14	45	GLY
38	1g	114	ARG
41	1j	75	ILE
6	2G	47	LYS

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Mol	Chain	Res	Type
21	2Z	146	ILE
26	24	47	GLN
26	24	65	ASP
41	2j	75	ILE
42	2k	49	GLY
17	1V	53	GLU
21	1Z	2	GLU
33	1b	234	PRO
33	2b	20	GLU
41	2j	79	ARG
4	1E	52	LEU
6	1G	84	LYS
20	1Y	103	GLY
26	14	53	GLU
33	1b	9	GLU
46	1o	20	GLY
51	1t	47	GLY
5	2F	89	VAL
51	2t	47	GLY
51	2t	100	ILE
3	1D	3	VAL
17	1V	43	GLU
26	14	55	ARG
33	1b	233	SER
36	1e	86	ALA
3	2D	3	VAL
8	2I	145	VAL
15	2T	37	GLY
21	2Z	141	VAL
41	2j	55	LYS
44	2m	99	ARG
44	2m	101	GLN
46	2o	20	GLY
21	1Z	134	PRO
38	1g	80	VAL
4	2E	52	LEU
15	2T	127	ALA
33	2b	78	GLN
34	2c	66	VAL
36	2e	85	GLY
40	2i	11	LYS
21	1Z	165	VAL

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Mol	Chain	Res	Type
33	1b	231	GLU
11	1P	93	GLY
38	2g	80	VAL
38	1g	55	GLY
41	1j	39	PRO
21	2Z	165	VAL
25	23	50	VAL
41	2j	39	PRO
42	1k	105	VAL
46	1o	19	PRO
48	1q	33	GLY
6	2G	52	ILE
21	2Z	134	PRO
42	2k	105	VAL
41	1j	77	PRO
47	2p	53	VAL

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%)	203 (94%)	12 (6%)	21	36
3	2D	215/218 (99%)	207 (96%)	8 (4%)	34	54
4	1E	164/166 (99%)	156 (95%)	8 (5%)	25	43
4	2E	164/166 (99%)	157 (96%)	7 (4%)	29	48
5	1F	160/166 (96%)	150 (94%)	10 (6%)	18	31
5	2F	159/166 (96%)	145 (91%)	14 (9%)	10	17
6	1G	143/156 (92%)	133 (93%)	10 (7%)	15	26
6	2G	143/156 (92%)	136 (95%)	7 (5%)	25	43
7	1H	144/148 (97%)	139 (96%)	5 (4%)	36	56
7	2H	144/148 (97%)	140 (97%)	4 (3%)	43	63
8	1I	113/124 (91%)	101 (89%)	12 (11%)	6	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	2I	105/124 (85%)	98 (93%)	7 (7%)	16 28
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%)	99 (99%)	1 (1%)	76 85
10	2O	100/100 (100%)	99 (99%)	1 (1%)	76 85
11	1P	115/116 (99%)	111 (96%)	4 (4%)	36 56
11	2P	115/116 (99%)	114 (99%)	1 (1%)	78 87
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18 31
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	35 55
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6 10
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19 34
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11 21
14	2S	85/88 (97%)	83 (98%)	2 (2%)	49 68
15	1T	115/127 (91%)	112 (97%)	3 (3%)	46 66
15	2T	113/127 (89%)	109 (96%)	4 (4%)	36 56
16	1U	93/94 (99%)	89 (96%)	4 (4%)	29 48
16	2U	93/94 (99%)	90 (97%)	3 (3%)	39 59
17	1V	80/82 (98%)	75 (94%)	5 (6%)	18 31
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18 31
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38 58
18	2W	90/92 (98%)	85 (94%)	5 (6%)	21 36
19	1X	77/78 (99%)	76 (99%)	1 (1%)	69 81
19	2X	77/78 (99%)	72 (94%)	5 (6%)	17 30
20	1Y	85/91 (93%)	77 (91%)	8 (9%)	8 15
20	2Y	85/91 (93%)	77 (91%)	8 (9%)	8 15
21	1Z	135/179 (75%)	125 (93%)	10 (7%)	13 24
21	2Z	137/179 (76%)	130 (95%)	7 (5%)	24 41
22	10	65/67 (97%)	63 (97%)	2 (3%)	40 60
22	20	65/67 (97%)	65 (100%)	0	100 100
23	11	80/83 (96%)	78 (98%)	2 (2%)	47 67
23	21	80/83 (96%)	78 (98%)	2 (2%)	47 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	12	65/67 (97%)	64 (98%)	1 (2%)	65 78
24	22	65/67 (97%)	64 (98%)	1 (2%)	65 78
25	13	51/52 (98%)	44 (86%)	7 (14%)	3 5
25	23	50/52 (96%)	48 (96%)	2 (4%)	31 51
26	14	59/63 (94%)	49 (83%)	10 (17%)	2 3
26	24	53/63 (84%)	49 (92%)	4 (8%)	13 23
27	15	50/52 (96%)	45 (90%)	5 (10%)	7 13
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%)	47 (94%)	3 (6%)	19 33
29	17	41/42 (98%)	36 (88%)	5 (12%)	5 7
29	27	41/42 (98%)	37 (90%)	4 (10%)	8 13
30	18	54/55 (98%)	48 (89%)	6 (11%)	6 10
30	28	54/55 (98%)	52 (96%)	2 (4%)	34 54
31	19	34/34 (100%)	33 (97%)	1 (3%)	42 62
31	29	34/34 (100%)	33 (97%)	1 (3%)	42 62
33	1b	192/220 (87%)	183 (95%)	9 (5%)	26 45
33	2b	187/220 (85%)	172 (92%)	15 (8%)	12 21
34	1c	142/188 (76%)	135 (95%)	7 (5%)	25 43
34	2c	140/188 (74%)	136 (97%)	4 (3%)	42 62
35	1d	169/181 (93%)	163 (96%)	6 (4%)	35 55
35	2d	173/181 (96%)	166 (96%)	7 (4%)	31 51
36	1e	113/123 (92%)	104 (92%)	9 (8%)	12 21
36	2e	114/123 (93%)	109 (96%)	5 (4%)	28 47
37	1f	84/90 (93%)	82 (98%)	2 (2%)	49 68
37	2f	85/90 (94%)	82 (96%)	3 (4%)	36 56
38	1g	119/127 (94%)	116 (98%)	3 (2%)	47 67
38	2g	120/127 (94%)	118 (98%)	2 (2%)	60 76
39	1h	114/119 (96%)	106 (93%)	8 (7%)	15 26
39	2h	114/119 (96%)	110 (96%)	4 (4%)	36 56
40	1i	90/99 (91%)	88 (98%)	2 (2%)	52 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	2i	89/99 (90%)	82 (92%)	7 (8%)	12 22
41	1j	66/92 (72%)	61 (92%)	5 (8%)	13 23
41	2j	69/92 (75%)	66 (96%)	3 (4%)	29 48
42	1k	82/99 (83%)	82 (100%)	0	100 100
42	2k	83/99 (84%)	80 (96%)	3 (4%)	35 55
43	1l	96/108 (89%)	90 (94%)	6 (6%)	18 31
43	2l	96/108 (89%)	95 (99%)	1 (1%)	76 85
44	1m	93/101 (92%)	88 (95%)	5 (5%)	22 38
44	2m	92/101 (91%)	86 (94%)	6 (6%)	17 30
45	1n	49/50 (98%)	41 (84%)	8 (16%)	2 3
45	2n	49/50 (98%)	46 (94%)	3 (6%)	18 33
46	1o	78/80 (98%)	77 (99%)	1 (1%)	69 81
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69 81
47	1p	69/74 (93%)	63 (91%)	6 (9%)	10 18
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13 24
48	1q	94/97 (97%)	94 (100%)	0	100 100
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53 71
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24 41
49	2r	59/77 (77%)	56 (95%)	3 (5%)	24 41
50	1s	69/80 (86%)	67 (97%)	2 (3%)	42 62
50	2s	67/80 (84%)	66 (98%)	1 (2%)	65 78
51	1t	70/82 (85%)	68 (97%)	2 (3%)	42 62
51	2t	70/82 (85%)	67 (96%)	3 (4%)	29 48
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100
All	All	9303/10064 (92%)	8837 (95%)	466 (5%)	24 42

All (466) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	12	SER
3	1D	32	SER
3	1D	61	LEU

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Mol	Chain	Res	Type
3	1D	94	LEU
3	1D	99	ASP
3	1D	106	ILE
3	1D	134	ARG
3	1D	193	VAL
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	260	ARG
4	1E	21	VAL
4	1E	24	THR
4	1E	47	VAL
4	1E	113	PHE
4	1E	116	VAL
4	1E	170	LEU
4	1E	175	VAL
4	1E	181	LEU
5	1F	24	LEU
5	1F	52	LYS
5	1F	53	THR
5	1F	57	VAL
5	1F	88	VAL
5	1F	106	ARG
5	1F	170	LEU
5	1F	175	THR
5	1F	195	ASP
5	1F	201	VAL
6	1G	5	VAL
6	1G	43	LEU
6	1G	77	ILE
6	1G	79	ASN
6	1G	90	LEU
6	1G	126	ASP
6	1G	132	ASN
6	1G	139	LEU
6	1G	145	THR
6	1G	175	LEU
7	1H	15	VAL
7	1H	18	GLU
7	1H	45	VAL
7	1H	56	SER
7	1H	57	ASP

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Mol	Chain	Res	Type
8	1I	9	LEU
8	1I	20	ASP
8	1I	31	LEU
8	1I	38	LEU
8	1I	47	LEU
8	1I	74	ASN
8	1I	78	THR
8	1I	81	VAL
8	1I	92	VAL
8	1I	101	LEU
8	1I	127	VAL
8	1I	145	VAL
9	1N	17	ASP
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	46	VAL
9	1N	48	MET
9	1N	73	THR
9	1N	112	LEU
10	1O	28	SER
11	1P	42	SER
11	1P	59	LEU
11	1P	95	VAL
11	1P	101	VAL
12	1Q	8	LYS
12	1Q	35	VAL
12	1Q	98	LYS
12	1Q	101	ARG
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	138	ASP
13	1R	6	SER
13	1R	15	SER
13	1R	29	LEU
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	96	ARG
13	1R	100	LEU
13	1R	111	LEU

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Mol	Chain	Res	Type
13	1R	114	VAL
14	1S	3	ARG
14	1S	14	VAL
14	1S	20	ARG
14	1S	25	ARG
14	1S	69	VAL
14	1S	75	GLU
14	1S	110	LEU
15	1T	6	LEU
15	1T	28	VAL
15	1T	88	ILE
16	1U	8	VAL
16	1U	59	ARG
16	1U	74	LEU
16	1U	77	SER
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	72	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	17	VAL
18	1W	107	LEU
19	1X	70	LEU
20	1Y	14	LEU
20	1Y	43	ASN
20	1Y	49	VAL
20	1Y	70	SER
20	1Y	72	VAL
20	1Y	99	CYS
20	1Y	106	LEU
20	1Y	107	ASP
21	1Z	61	LEU
21	1Z	70	LEU
21	1Z	76	LEU
21	1Z	81	ARG
21	1Z	91	LEU
21	1Z	126	VAL
21	1Z	141	VAL
21	1Z	153	SER
21	1Z	165	VAL
21	1Z	171	ILE

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Mol	Chain	Res	Type
22	10	10	THR
22	10	14	ARG
23	11	30	VAL
23	11	35	THR
24	12	45	SER
25	13	3	ARG
25	13	17	LYS
25	13	23	LEU
25	13	30	ARG
25	13	34	GLU
25	13	54	VAL
25	13	56	VAL
26	14	27	THR
26	14	28	LYS
26	14	48	ARG
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	56	VAL
26	14	57	GLU
26	14	58	ARG
26	14	65	ASP
27	15	6	VAL
27	15	15	ARG
27	15	16	ARG
27	15	29	THR
27	15	58	LEU
28	16	9	LEU
28	16	19	ARG
28	16	48	VAL
28	16	50	ARG
28	16	51	GLU
29	17	1	MET
29	17	34	ARG
29	17	39	ARG
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
30	18	43	GLN

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Mol	Chain	Res	Type
30	18	58	ILE
31	19	7	VAL
33	1b	24	TRP
33	1b	30	ARG
33	1b	37	ASN
33	1b	81	VAL
33	1b	94	ASN
33	1b	122	PHE
33	1b	160	ASP
33	1b	222	ILE
33	1b	234	PRO
34	1c	3	ASN
34	1c	8	ILE
34	1c	52	LEU
34	1c	70	VAL
34	1c	115	LEU
34	1c	172	ARG
34	1c	188	LEU
35	1d	127	THR
35	1d	135	LEU
35	1d	137	SER
35	1d	175	SER
35	1d	178	VAL
35	1d	194	LEU
36	1e	13	ILE
36	1e	20	GLN
36	1e	31	LEU
36	1e	41	VAL
36	1e	64	ARG
36	1e	75	THR
36	1e	81	GLU
36	1e	91	LEU
36	1e	120	THR
37	1f	7	ASN
37	1f	92	LYS
38	1g	104	LEU
38	1g	113	GLU
38	1g	115	ARG
39	1h	19	VAL
39	1h	25	ASP
39	1h	26	VAL
39	1h	29	SER

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Mol	Chain	Res	Type
39	1h	63	LEU
39	1h	85	ARG
39	1h	104	ARG
39	1h	112	LEU
40	1i	92	TYR
40	1i	128	ARG
41	1j	8	LEU
41	1j	35	SER
41	1j	71	LEU
41	1j	72	VAL
41	1j	92	THR
43	1l	27	LEU
43	1l	28	LYS
43	1l	54	LYS
43	1l	58	VAL
43	1l	70	ILE
43	1l	113	ARG
44	1m	3	ARG
44	1m	19	LEU
44	1m	47	ASP
44	1m	88	ARG
44	1m	117	VAL
45	1n	3	ARG
45	1n	7	ILE
45	1n	13	THR
45	1n	18	VAL
45	1n	22	THR
45	1n	29	ARG
45	1n	33	VAL
45	1n	60	SER
46	1o	21	ASP
47	1p	1	MET
47	1p	2	VAL
47	1p	20	VAL
47	1p	45	THR
47	1p	57	ARG
47	1p	67	THR
49	1r	26	LEU
49	1r	47	THR
49	1r	82	THR
50	1s	77	THR
50	1s	79	THR

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Mol	Chain	Res	Type
51	1t	72	LEU
51	1t	100	ILE
3	2D	61	LEU
3	2D	94	LEU
3	2D	142	VAL
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	253	GLN
3	2D	261	LYS
4	2E	9	VAL
4	2E	21	VAL
4	2E	27	LEU
4	2E	33	VAL
4	2E	116	VAL
4	2E	119	ARG
4	2E	181	LEU
5	2F	20	LEU
5	2F	57	VAL
5	2F	70	THR
5	2F	88	VAL
5	2F	106	ARG
5	2F	107	LYS
5	2F	158	THR
5	2F	170	LEU
5	2F	175	THR
5	2F	183	VAL
5	2F	191	ARG
5	2F	192	LEU
5	2F	195	ASP
5	2F	201	VAL
6	2G	3	LEU
6	2G	18	GLU
6	2G	43	LEU
6	2G	47	LYS
6	2G	77	ILE
6	2G	79	ASN
6	2G	165	THR
7	2H	27	LYS
7	2H	45	VAL
7	2H	67	LEU
7	2H	71	LEU

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Mol	Chain	Res	Type
8	2I	38	LEU
8	2I	47	LEU
8	2I	76	THR
8	2I	101	LEU
8	2I	123	LEU
8	2I	127	VAL
8	2I	140	LEU
9	2N	32	THR
9	2N	34	LEU
9	2N	35	ARG
9	2N	38	HIS
9	2N	43	THR
9	2N	46	VAL
9	2N	60	ILE
9	2N	62	VAL
9	2N	63	THR
9	2N	83	LYS
9	2N	140	VAL
10	2O	22	ILE
11	2P	95	VAL
12	2Q	5	ARG
12	2Q	21	THR
12	2Q	109	VAL
12	2Q	110	THR
13	2R	6	SER
13	2R	29	LEU
13	2R	44	LEU
13	2R	65	LEU
13	2R	67	LEU
13	2R	111	LEU
14	2S	5	THR
14	2S	21	THR
15	2T	49	VAL
15	2T	57	PHE
15	2T	74	ARG
15	2T	96	ARG
16	2U	6	THR
16	2U	31	SER
16	2U	74	LEU
17	2V	7	THR
17	2V	51	VAL
17	2V	61	VAL

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Mol	Chain	Res	Type
17	2V	62	LEU
17	2V	72	VAL
18	2W	11	ARG
18	2W	15	ARG
18	2W	23	LEU
18	2W	67	ASP
18	2W	107	LEU
19	2X	23	GLU
19	2X	35	THR
19	2X	75	ASP
19	2X	82	GLN
19	2X	92	LEU
20	2Y	14	LEU
20	2Y	37	VAL
20	2Y	43	ASN
20	2Y	55	TYR
20	2Y	61	ILE
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	99	CYS
21	2Z	19	ARG
21	2Z	42	VAL
21	2Z	67	LEU
21	2Z	70	LEU
21	2Z	155	LEU
21	2Z	157	LEU
21	2Z	174	VAL
23	21	11	ARG
23	21	52	ARG
24	22	35	LEU
25	23	30	ARG
25	23	54	VAL
26	24	48	ARG
26	24	49	PHE
26	24	56	VAL
26	24	63	TYR
27	25	6	VAL
27	25	33	CYS
27	25	58	LEU
28	26	9	LEU
28	26	48	VAL
28	26	51	GLU

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Mol	Chain	Res	Type
29	27	1	MET
29	27	24	THR
29	27	39	ARG
29	27	43	THR
30	28	30	ARG
30	28	32	LEU
31	29	14	CYS
33	2b	19	HIS
33	2b	24	TRP
33	2b	37	ASN
33	2b	44	LEU
33	2b	71	VAL
33	2b	81	VAL
33	2b	102	LEU
33	2b	108	ILE
33	2b	111	ARG
33	2b	121	LEU
33	2b	122	PHE
33	2b	160	ASP
33	2b	176	GLU
33	2b	189	ASP
33	2b	230	VAL
34	2c	22	TRP
34	2c	40	ARG
34	2c	115	LEU
34	2c	192	THR
35	2d	9	CYS
35	2d	33	MET
35	2d	127	THR
35	2d	135	LEU
35	2d	141	ARG
35	2d	188	LEU
35	2d	194	LEU
36	2e	41	VAL
36	2e	64	ARG
36	2e	81	GLU
36	2e	91	LEU
36	2e	120	THR
37	2f	19	LEU
37	2f	40	VAL
37	2f	81	ILE
38	2g	31	MET

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Mol	Chain	Res	Type
38	2g	104	LEU
39	2h	11	THR
39	2h	14	ARG
39	2h	104	ARG
39	2h	112	LEU
40	2i	14	VAL
40	2i	27	THR
40	2i	29	ASN
40	2i	41	VAL
40	2i	50	LEU
40	2i	102	LEU
40	2i	105	ASP
41	2j	59	SER
41	2j	67	THR
41	2j	71	LEU
42	2k	14	VAL
42	2k	81	ASP
42	2k	87	THR
43	2l	117	ARG
44	2m	3	ARG
44	2m	19	LEU
44	2m	29	ARG
44	2m	69	GLU
44	2m	74	VAL
44	2m	91	ARG
45	2n	7	ILE
45	2n	22	THR
45	2n	33	VAL
46	2o	87	ILE
47	2p	19	ILE
47	2p	20	VAL
47	2p	21	VAL
47	2p	62	VAL
47	2p	67	THR
48	2q	53	LEU
48	2q	68	ARG
49	2r	29	PHE
49	2r	37	VAL
49	2r	47	THR
50	2s	41	VAL
51	2t	39	LYS
51	2t	70	SER

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Mol	Chain	Res	Type
51	2t	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	116	GLN
3	1D	126	GLN
5	1F	169	ASN
8	1I	11	ASN
8	1I	104	GLN
10	1O	3	GLN
14	1S	38	GLN
14	1S	61	ASN
16	1U	81	HIS
18	1W	60	ASN
19	1X	31	HIS
20	1Y	6	HIS
21	1Z	55	HIS
21	1Z	73	GLN
22	10	50	ASN
30	18	35	GLN
31	19	34	GLN
33	1b	16	HIS
33	1b	37	ASN
33	1b	78	GLN
33	1b	94	ASN
34	1c	110	ASN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	20	GLN
36	1e	78	HIS
38	1g	28	ASN
38	1g	51	GLN
38	1g	110	GLN
40	1i	3	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	73	GLN
41	1j	56	HIS
43	1l	99	HIS

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Mol	Chain	Res	Type
44	1m	92	HIS
46	1o	62	GLN
47	1p	14	ASN
48	1q	26	GLN
49	1r	63	GLN
50	1s	23	ASN
50	1s	83	HIS
51	1t	16	HIS
4	2E	48	GLN
5	2F	69	HIS
5	2F	203	GLN
6	2G	123	ASN
12	2Q	123	HIS
12	2Q	141	GLN
15	2T	79	HIS
16	2U	66	ASN
20	2Y	43	ASN
21	2Z	34	ASN
21	2Z	55	HIS
21	2Z	65	GLN
21	2Z	132	ASN
33	2b	37	ASN
33	2b	94	ASN
33	2b	212	GLN
35	2d	74	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	125	HIS
36	2e	73	ASN
36	2e	78	HIS
37	2f	100	ASN
38	2g	68	ASN
38	2g	86	GLN
39	2h	78	GLN
40	2i	3	GLN
40	2i	58	HIS
40	2i	73	GLN
41	2j	21	GLN
41	2j	56	HIS
43	2l	99	HIS
49	2r	63	GLN

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Mol	Chain	Res	Type
50	2s	23	ASN
50	2s	69	HIS
50	2s	83	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	448 (15%)	19 (0%)
1	2A	2790/2915 (95%)	514 (18%)	19 (0%)
2	1B	120/121 (99%)	11 (9%)	1 (0%)
2	2B	118/121 (97%)	28 (23%)	0
32	1a	1494/1521 (98%)	250 (16%)	0
32	2a	1498/1521 (98%)	281 (18%)	0
53	1v	12/27 (44%)	2 (16%)	0
53	2v	12/27 (44%)	4 (33%)	0
54	1w	68/76 (89%)	24 (35%)	0
54	1y	68/76 (89%)	24 (35%)	0
54	2w	68/76 (89%)	28 (41%)	0
54	2y	68/76 (89%)	28 (41%)	0
55	1x	75/77 (97%)	13 (17%)	0
55	2x	75/77 (97%)	15 (20%)	0
All	All	9329/9626 (96%)	1670 (17%)	39 (0%)

All (1670) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	196	A
1	1A	197	A

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Mol	Chain	Res	Type
1	1A	199	A
1	1A	201	C
1	1A	205	G
1	1A	214	G
1	1A	216	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	230	U
1	1A	233	A
1	1A	248	G
1	1A	266	G
1	1A	271(A)	A
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	345	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	418	G
1	1A	421	U
1	1A	428	A
1	1A	443	A
1	1A	444	C
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	467	G
1	1A	481	G

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Mol	Chain	Res	Type
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	512	G
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	551	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	634	C
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	764	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	790	C
1	1A	792	G

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Mol	Chain	Res	Type
1	1A	802	A
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	865	C
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	892	G
1	1A	894	C
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	899	A
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	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	1012	U
1	1A	1013	C
1	1A	1022	G

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Mol	Chain	Res	Type
1	1A	1025	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
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	1059	G
1	1A	1064	C
1	1A	1066	U
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1093	G
1	1A	1094	U
1	1A	1097	U
1	1A	1098	A
1	1A	1100	C
1	1A	1101	U
1	1A	1109	C
1	1A	1111	A
1	1A	1112	G
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1171	G
1	1A	1173	G

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Mol	Chain	Res	Type
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1211	U
1	1A	1212	G
1	1A	1220	A
1	1A	1227	G
1	1A	1229	G
1	1A	1237	A
1	1A	1244	G
1	1A	1248	G
1	1A	1253	A
1	1A	1256	G
1	1A	1267	U
1	1A	1271	G
1	1A	1272	A
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1320	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1379	A
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1437	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1478	G

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Mol	Chain	Res	Type
1	1A	1482	G
1	1A	1490	A
1	1A	1493	C
1	1A	1494	A
1	1A	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1542	A
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1612	C
1	1A	1646	C
1	1A	1647	G
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1667	G
1	1A	1671	U
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	1740	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A

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Mol	Chain	Res	Type
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1828	G
1	1A	1847	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
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	1940	U
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
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	2080	G

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Mol	Chain	Res	Type
1	1A	2101	G
1	1A	2107	C
1	1A	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2125	G
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	2138	C
1	1A	2140	C
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2147	G
1	1A	2149	G
1	1A	2150	U
1	1A	2151	G
1	1A	2152	G
1	1A	2155	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2162	G
1	1A	2163	C
1	1A	2164	C
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2169	A
1	1A	2171	A
1	1A	2172	U
1	1A	2174	C
1	1A	2178	C
1	1A	2184	G
1	1A	2198	A

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Mol	Chain	Res	Type
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2218	U
1	1A	2225	A
1	1A	2238	G
1	1A	2249	U
1	1A	2268	A
1	1A	2269	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2309	A
1	1A	2314	C
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	2389	G
1	1A	2396	G
1	1A	2406	U
1	1A	2410	G
1	1A	2424	C
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2445	G
1	1A	2448	A
1	1A	2474	C
1	1A	2476	A

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Mol	Chain	Res	Type
1	1A	2490	G
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2549	G
1	1A	2554	U
1	1A	2556	C
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2609	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2638	G
1	1A	2646	C
1	1A	2654	A
1	1A	2663	G
1	1A	2689	U
1	1A	2691	C
1	1A	2702	U
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2734	A
1	1A	2739	U
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
1	1A	2794	C
1	1A	2802	G

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Mol	Chain	Res	Type
1	1A	2803	C
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2873	A
1	1A	2879	C
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2897	U
2	1B	2	C
2	1B	15	A
2	1B	25	A
2	1B	35	U
2	1B	42	C
2	1B	50	G
2	1B	56	G
2	1B	73	A
2	1B	85	G
2	1B	110	G
2	1B	120	A
32	1a	9	G
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	54	C
32	1a	55	A
32	1a	61	G
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	92	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	111	G
32	1a	116	A

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Mol	Chain	Res	Type
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	159	G
32	1a	162	A
32	1a	164	U
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	231	G
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	316	G
32	1a	321	A
32	1a	328	C
32	1a	332	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	382	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G

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Mol	Chain	Res	Type
32	1a	412	A
32	1a	413	G
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	435	C
32	1a	439	A
32	1a	451	A
32	1a	452	A
32	1a	461	A
32	1a	484	G
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	531	U
32	1a	532	A
32	1a	534	U
32	1a	539	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
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	628	G
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	666	G
32	1a	687	A
32	1a	688	G
32	1a	695	A

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Mol	Chain	Res	Type
32	1a	702	A
32	1a	717	C
32	1a	723	U
32	1a	728	A
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	766	A
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	821	G
32	1a	828	A
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	864	A
32	1a	870	U
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	932	C
32	1a	934	C
32	1a	935	A
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

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Mol	Chain	Res	Type
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1007	C
32	1a	1008	C
32	1a	1011	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	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	1037	C
32	1a	1039	C
32	1a	1043	C
32	1a	1044	A
32	1a	1054	C
32	1a	1055	A
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1124	G
32	1a	1125	U
32	1a	1131	G

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Mol	Chain	Res	Type
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1157	A
32	1a	1159	U
32	1a	1160	G
32	1a	1182	G
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1312	G
32	1a	1320	C
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A

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Mol	Chain	Res	Type
32	1a	1364	U
32	1a	1370	G
32	1a	1397	C
32	1a	1400	5MC
32	1a	1416	G
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1447	A
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	24	C
54	1w	2	G
54	1w	9	A
54	1w	13	C
54	1w	19	G
54	1w	23	A
54	1w	27	C
54	1w	35	A
54	1w	42	G
54	1w	45	G
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	49	G
54	1w	50	G
54	1w	51	C
54	1w	57	G
54	1w	58	A
54	1w	59	U

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Mol	Chain	Res	Type
54	1w	60	C
54	1w	61	C
54	1w	62	C
54	1w	68	C
54	1w	71	C
54	1w	74	C
55	1x	9	G
55	1x	13	C
55	1x	18	G
55	1x	21	A
55	1x	22	G
55	1x	47	U
55	1x	48	C
55	1x	49	G
55	1x	58	A
55	1x	59	A
55	1x	61	C
55	1x	69	C
55	1x	76	A
54	1y	2	G
54	1y	5	G
54	1y	6	A
54	1y	8	4SU
54	1y	9	A
54	1y	13	C
54	1y	14	A
54	1y	19	G
54	1y	24	G
54	1y	32	C
54	1y	33	U
54	1y	35	A
54	1y	40	G
54	1y	44	G
54	1y	45	G
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	54	5MU
54	1y	57	G
54	1y	59	U
54	1y	61	C
54	1y	65	C

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Mol	Chain	Res	Type
54	1y	69	A
1	2A	8	A
1	2A	10	G
1	2A	11	G
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	139	G
1	2A	141	A
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	221	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	233	A
1	2A	245	G
1	2A	248	G
1	2A	249	C
1	2A	250	G

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Mol	Chain	Res	Type
1	2A	266	G
1	2A	267	C
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	280	C
1	2A	290	G
1	2A	294	A
1	2A	311	A
1	2A	312	G
1	2A	329	G
1	2A	330	A
1	2A	332	A
1	2A	342	G
1	2A	352	G
1	2A	363(B)	G
1	2A	386	G
1	2A	399	G
1	2A	402	A
1	2A	403	U
1	2A	411	G
1	2A	422	A
1	2A	435	C
1	2A	442	G
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	505	A
1	2A	508	G
1	2A	509	C

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Mol	Chain	Res	Type
1	2A	513	A
1	2A	514	A
1	2A	528	A
1	2A	529	A
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	586	A
1	2A	592	G
1	2A	593	G
1	2A	595	C
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	653	A
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	699	A
1	2A	717	G
1	2A	730	C
1	2A	734	A
1	2A	753	C
1	2A	764	A
1	2A	771	G
1	2A	775	G
1	2A	782	A

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Mol	Chain	Res	Type
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	804	A
1	2A	805	G
1	2A	811	U
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	832	G
1	2A	854	G
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	878	A
1	2A	879	G
1	2A	883	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	897	C
1	2A	898	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U

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Mol	Chain	Res	Type
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	990	A
1	2A	996	A
1	2A	997	G
1	2A	1003	G
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1043	C
1	2A	1117	G
1	2A	1122	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1143	A
1	2A	1144	G
1	2A	1155	A
1	2A	1171	G
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1225	G
1	2A	1242	A
1	2A	1248	G
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A

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Mol	Chain	Res	Type
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1320	C
1	2A	1342	A
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
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	1451	C
1	2A	1455	G
1	2A	1459	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	1494	A
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U

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Mol	Chain	Res	Type
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1514	U
1	2A	1531	C
1	2A	1532	C
1	2A	1541	G
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1553	A
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1582	C
1	2A	1584	C
1	2A	1586	A
1	2A	1588	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1695	G
1	2A	1696	G
1	2A	1700	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	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A

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Mol	Chain	Res	Type
1	2A	1778	U
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1847	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1990	C
1	2A	1992	G
1	2A	1993	U
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C

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Mol	Chain	Res	Type
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2093	G
1	2A	2102	U
1	2A	2106	G
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2141	G
1	2A	2146	C
1	2A	2151	G
1	2A	2153	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2162	G
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G

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Mol	Chain	Res	Type
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2178	C
1	2A	2182	G
1	2A	2189	U
1	2A	2194	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	2235	G
1	2A	2238	G
1	2A	2239	G
1	2A	2248	C
1	2A	2267	A
1	2A	2273	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2294	C
1	2A	2302	G
1	2A	2305	A
1	2A	2307	G
1	2A	2308	G
1	2A	2309	A
1	2A	2316	C
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2343	C
1	2A	2346	A

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Mol	Chain	Res	Type
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2355	C
1	2A	2366	A
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2391	G
1	2A	2395	C
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2419	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	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	2478	A
1	2A	2480	C
1	2A	2487	G
1	2A	2490	G
1	2A	2494	G
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2535	G
1	2A	2554	U
1	2A	2562	U
1	2A	2566	A

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Mol	Chain	Res	Type
1	2A	2567	G
1	2A	2572	A
1	2A	2573	C
1	2A	2582	G
1	2A	2585	U
1	2A	2586	C
1	2A	2588	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2661	G
1	2A	2662	A
1	2A	2689	U
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2732	G
1	2A	2733	A
1	2A	2748	A
1	2A	2751	G
1	2A	2757	A
1	2A	2759	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2780	G
1	2A	2793	G
1	2A	2807	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2836	U
1	2A	2839	G
1	2A	2858	C

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Mol	Chain	Res	Type
1	2A	2861	G
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2883	A
1	2A	2886	G
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2896	C
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	7	G
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	19	G
2	2B	20	C
2	2B	40	U
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	66	A
2	2B	67	G
2	2B	69	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	101	G
2	2B	108	U
2	2B	109	C
2	2B	110	G
2	2B	114	C
2	2B	119	G
2	2B	120	A
32	2a	7	G
32	2a	9	G
32	2a	32	A

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Mol	Chain	Res	Type
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	52	G
32	2a	54	C
32	2a	66	G
32	2a	73	G
32	2a	78	G
32	2a	80	G
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	117	G
32	2a	120	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	144	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	222	U
32	2a	247	G
32	2a	249	U
32	2a	250	A
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	301	G

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Mol	Chain	Res	Type
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	342	C
32	2a	345	C
32	2a	348	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	415	A
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	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	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	527	7MG
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	560	U
32	2a	561	U
32	2a	562	C
32	2a	564	C
32	2a	568	G
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	602	A
32	2a	607	A
32	2a	619	U
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	655	A
32	2a	665	A
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	693	G
32	2a	695	A
32	2a	702	A
32	2a	703	G
32	2a	723	U
32	2a	724	G
32	2a	729	A
32	2a	731	G
32	2a	735	C
32	2a	749	C
32	2a	754	C
32	2a	755	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	812	C
32	2a	815	A
32	2a	817	C

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Mol	Chain	Res	Type
32	2a	818	G
32	2a	819	A
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	855	G
32	2a	859	A
32	2a	874	G
32	2a	891	U
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1014	A
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1024	G

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Mol	Chain	Res	Type
32	2a	1025	U
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1033	G
32	2a	1034	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1042	G
32	2a	1046	A
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	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1116	C
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1128	C
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A

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Mol	Chain	Res	Type
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1181	G
32	2a	1182	G
32	2a	1184	G
32	2a	1191	A
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	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1215	G
32	2a	1220	G
32	2a	1226	C
32	2a	1227	A
32	2a	1238	A
32	2a	1246	C
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1261	A
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1279	A
32	2a	1280	A
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G

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Mol	Chain	Res	Type
32	2a	1323	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1378	C
32	2a	1404	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1487	G
32	2a	1492	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
53	2v	13	A
53	2v	14	A
53	2v	20	U
53	2v	24	C
54	2w	2	G
54	2w	3	G
54	2w	5	G
54	2w	8	4SU
54	2w	11	C
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	23	A
54	2w	27	C
54	2w	42	G
54	2w	46	7MG

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Mol	Chain	Res	Type
54	2w	47	U
54	2w	48	C
54	2w	49	G
54	2w	50	G
54	2w	51	C
54	2w	56	C
54	2w	57	G
54	2w	58	A
54	2w	59	U
54	2w	60	C
54	2w	62	C
54	2w	67	U
54	2w	68	C
54	2w	69	A
54	2w	70	C
54	2w	74	C
55	2x	4	G
55	2x	9	G
55	2x	10	G
55	2x	13	C
55	2x	19	G
55	2x	21	A
55	2x	22	G
55	2x	28	C
55	2x	42	G
55	2x	47	U
55	2x	48	C
55	2x	51	C
55	2x	61	C
55	2x	73	A
55	2x	76	A
54	2y	2	G
54	2y	5	G
54	2y	6	A
54	2y	8	4SU
54	2y	9	A
54	2y	13	C
54	2y	14	A
54	2y	19	G
54	2y	24	G
54	2y	32	C
54	2y	35	A

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Mol	Chain	Res	Type
54	2y	40	G
54	2y	41	A
54	2y	43	G
54	2y	44	G
54	2y	45	G
54	2y	46	7MG
54	2y	47	U
54	2y	48	C
54	2y	53	G
54	2y	54	5MU
54	2y	55	PSU
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	61	C
54	2y	65	C
54	2y	69	A

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	895	U
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1210	A
1	1A	1442	G
1	1A	1508	A
1	1A	1653	G
1	1A	1663	C
1	1A	1992	G
1	1A	2126	A
1	1A	2134	A
1	1A	2183	C
2	1B	1	U
1	2A	195	A

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Mol	Chain	Res	Type
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	827	U
1	2A	856	C
1	2A	893	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1608	A
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2756	U

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

80 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	$\#\|Z\| > 2$
1	OMG	1A	2251	55,56,1	18,26,27	0.97	1 (5%)	19,38,41	1.12	2 (10%)
32	5MC	1a	967	32	18,22,23	0.94	2 (11%)	26,32,35	1.18	3 (11%)
32	MA6	2a	1519	32	19,26,27	1.01	1 (5%)	18,38,41	1.61	3 (16%)
32	M2G	2a	966	32	20,27,28	1.49	3 (15%)	22,40,43	0.95	2 (9%)
54	CM0	2w	34	54	22,26,27	1.49	5 (22%)	28,37,40	1.70	4 (14%)
54	5MU	2y	54	54	19,22,23	1.45	5 (26%)	28,32,35	1.98	8 (28%)
54	PSU	1w	55	54	18,21,22	1.37	1 (5%)	22,30,33	1.89	4 (18%)
32	PSU	1a	516	32,56	18,21,22	1.37	2 (11%)	22,30,33	1.86	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	0TD	1l	92	43	7,9,10	4.93	1 (14%)	6,11,13	7.18	3 (50%)
1	5MU	2A	1915	1	19,22,23	1.47	5 (26%)	28,32,35	2.07	6 (21%)
32	5MC	1a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.12	2 (7%)
54	7MG	1y	46	54	22,26,27	1.47	4 (18%)	29,39,42	2.66	5 (17%)
32	MA6	1a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.66	4 (22%)
32	2MG	2a	1207	32	18,26,27	0.91	1 (5%)	16,38,41	1.08	1 (6%)
55	5MU	1x	54	55	19,22,23	1.41	5 (26%)	28,32,35	1.79	5 (17%)
1	5MC	2A	1962	56,1	18,22,23	0.98	2 (11%)	26,32,35	1.11	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.35	3 (16%)	22,30,33	1.86	3 (13%)
54	CM0	1y	34	54	22,26,27	1.55	4 (18%)	28,37,40	1.84	4 (14%)
54	PSU	2w	55	54	18,21,22	1.33	2 (11%)	22,30,33	1.82	4 (18%)
32	MA6	2a	1518	32	19,26,27	1.04	1 (5%)	18,38,41	1.68	4 (22%)
1	OMC	1A	1920	1	19,22,23	0.81	0	26,31,34	0.93	2 (7%)
32	MA6	1a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.68	6 (33%)
1	5MU	2A	1939	1	19,22,23	1.40	6 (31%)	28,32,35	2.13	6 (21%)
1	5MU	1A	1915	1	19,22,23	1.45	5 (26%)	28,32,35	2.05	6 (21%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.09	2 (12%)
1	OMU	1A	2552	56,1	19,22,23	1.27	3 (15%)	26,31,34	1.84	6 (23%)
1	PSU	2A	1911	1	18,21,22	1.34	2 (11%)	22,30,33	1.80	3 (13%)
43	0TD	2l	92	43	7,9,10	4.82	1 (14%)	6,11,13	4.80	3 (50%)
54	6MZ	1w	37	54	18,25,26	0.92	1 (5%)	16,36,39	2.05	4 (25%)
54	4SU	1y	8	54	18,21,22	1.79	5 (27%)	26,30,33	2.02	5 (19%)
32	5MC	2a	1400	32	18,22,23	0.95	2 (11%)	26,32,35	1.19	3 (11%)
54	5MU	2w	54	54	19,22,23	1.40	5 (26%)	28,32,35	1.88	6 (21%)
54	6MZ	2w	37	54	18,25,26	0.93	1 (5%)	16,36,39	1.87	3 (18%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
32	5MC	1a	1404	32	18,22,23	1.00	2 (11%)	26,32,35	1.15	3 (11%)
32	5MC	2a	967	32	18,22,23	0.98	2 (11%)	26,32,35	1.10	2 (7%)
55	5MC	2x	32	55	18,22,23	1.00	2 (11%)	26,32,35	1.26	3 (11%)
54	PSU	1y	55	54	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
54	CM0	2y	34	54	22,26,27	1.51	3 (13%)	28,37,40	1.82	5 (17%)
54	5MU	1w	54	54	19,22,23	1.40	5 (26%)	28,32,35	2.14	8 (28%)
32	5MC	2a	1404	32	18,22,23	0.97	2 (11%)	26,32,35	1.19	3 (11%)
32	4OC	2a	1402	32	20,23,24	0.77	0	26,32,35	1.02	2 (7%)
32	7MG	2a	527	32,56	22,26,27	1.33	3 (13%)	29,39,42	2.48	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	4SU	2w	8	54	18,21,22	1.70	4 (22%)	26,30,33	2.02	5 (19%)
32	5MC	1a	1407	32	18,22,23	0.96	2 (11%)	26,32,35	1.18	2 (7%)
1	5MC	2A	1942	1	18,22,23	0.93	2 (11%)	26,32,35	1.12	2 (7%)
32	PSU	2a	516	32	18,21,22	1.32	2 (11%)	22,30,33	1.81	3 (13%)
54	5MU	1y	54	54	19,22,23	1.45	5 (26%)	28,32,35	2.05	5 (17%)
1	PSU	1A	1917	1	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
32	5MC	2a	1407	32	18,22,23	0.97	2 (11%)	26,32,35	1.12	2 (7%)
1	5MC	1A	1942	1	18,22,23	0.97	2 (11%)	26,32,35	1.18	3 (11%)
1	OMG	2A	2251	55,56,1	18,26,27	0.95	1 (5%)	19,38,41	1.03	2 (10%)
55	4SU	2x	8	55,56	18,21,22	1.90	5 (27%)	26,30,33	1.71	7 (26%)
32	7MG	1a	527	32,56	22,26,27	1.37	3 (13%)	29,39,42	2.49	5 (17%)
1	OMC	2A	1920	1	19,22,23	0.82	0	26,31,34	0.96	1 (3%)
54	7MG	2y	46	54	22,26,27	1.41	4 (18%)	29,39,42	2.60	6 (20%)
54	6MZ	1y	37	54	18,25,26	0.97	1 (5%)	16,36,39	2.16	4 (25%)
55	4SU	1x	8	55	18,21,22	1.98	4 (22%)	26,30,33	1.68	7 (26%)
55	PSU	1x	55	55,56	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)
32	UR3	2a	1498	32	19,22,23	1.03	2 (10%)	26,32,35	1.49	1 (3%)
54	6MZ	2y	37	54	18,25,26	0.96	1 (5%)	16,36,39	2.09	4 (25%)
54	4SU	1w	8	54	18,21,22	1.75	5 (27%)	26,30,33	1.98	5 (19%)
32	4OC	1a	1402	32	20,23,24	0.76	0	26,32,35	0.90	1 (3%)
55	5MC	1x	32	55	18,22,23	1.02	2 (11%)	26,32,35	1.20	3 (11%)
1	PSU	1A	2605	56,1	18,21,22	1.37	3 (16%)	22,30,33	1.80	3 (13%)
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	28,32,35	2.00	6 (21%)
1	5MC	1A	1962	1	18,22,23	0.96	2 (11%)	26,32,35	1.17	3 (11%)
32	M2G	1a	966	32	20,27,28	1.43	3 (15%)	22,40,43	0.90	2 (9%)
1	PSU	1A	1911	1	18,21,22	1.37	3 (16%)	22,30,33	1.91	3 (13%)
54	4SU	2y	8	54	18,21,22	1.74	4 (22%)	26,30,33	1.84	5 (19%)
1	2MA	2A	2503	1	17,25,26	0.98	1 (5%)	17,37,40	1.00	2 (11%)
54	7MG	1w	46	54	22,26,27	1.41	2 (9%)	29,39,42	2.39	7 (24%)
1	OMU	2A	2552	56,1	19,22,23	1.27	3 (15%)	26,31,34	1.81	6 (23%)
32	UR3	1a	1498	32	19,22,23	0.99	2 (10%)	26,32,35	1.46	2 (7%)
54	CM0	1w	34	54	22,26,27	1.53	4 (18%)	28,37,40	1.73	5 (17%)
1	5MU	1A	1939	56,1	19,22,23	1.42	6 (31%)	28,32,35	2.21	6 (21%)
54	PSU	2y	55	54	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	2MA	1A	2503	56,1	17,25,26	0.98	1 (5%)	17,37,40	1.05	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	7MG	2w	46	54	22,26,27	1.27	2 (9%)	29,39,42	2.54	6 (20%)
55	PSU	2x	55	55	18,21,22	1.32	2 (11%)	22,30,33	1.91	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1A	2251	55,56,1	-	0/5/27/28	0/3/3/3
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	6/7/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	CM0	2w	34	54	-	7/12/30/31	0/2/2/2
54	5MU	2y	54	54	-	3/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	1/7/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
32	2MG	2a	1207	32	-	2/5/27/28	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	56,1	-	2/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	CM0	1y	34	54	-	4/12/30/31	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	MA6	1a	1518	32	-	1/7/29/30	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	OMU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
54	6MZ	1w	37	54	-	0/5/27/28	0/3/3/3
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	6MZ	2w	37	54	-	2/5/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	CM0	2y	34	54	-	6/12/30/31	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	4/9/29/30	0/2/2/2
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3
54	4SU	2w	8	54	-	2/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,56,1	-	0/5/27/28	0/3/3/3
55	4SU	2x	8	55,56	-	1/7/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
54	7MG	2y	46	54	-	5/7/37/38	0/3/3/3
54	6MZ	1y	37	54	-	1/5/27/28	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	6MZ	2y	37	54	-	1/5/27/28	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	2A	2503	1	-	1/3/25/26	0/3/3/3
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
1	OMU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	CM0	1w	34	54	-	1/12/30/31	0/2/2/2
1	5MU	1A	1939	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
1	2MA	1A	2503	56,1	-	2/3/25/26	0/3/3/3
54	7MG	2w	46	54	-	0/7/37/38	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2

All (203) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.69	1.69	1.82
43	2l	92	0TD	CB-SB	-12.47	1.69	1.82
32	2a	966	M2G	C2-N3	4.92	1.36	1.30
54	1y	34	CM0	C6-C5	4.84	1.39	1.34
54	1w	34	CM0	C6-C5	4.78	1.39	1.34
54	2y	34	CM0	C6-C5	4.64	1.39	1.34
54	1w	8	4SU	C4-S4	-4.49	1.59	1.68
55	2x	8	4SU	C4-S4	-4.45	1.60	1.68
54	2w	34	CM0	C6-C5	4.40	1.39	1.34
54	1y	8	4SU	C4-S4	-4.39	1.60	1.68
55	1x	8	4SU	C4-S4	-4.38	1.60	1.68
32	1a	966	M2G	C2-N3	4.34	1.36	1.30
54	2y	8	4SU	C4-S4	-4.30	1.60	1.68
54	2w	8	4SU	C4-S4	-4.19	1.60	1.68
55	1x	8	4SU	C4-N3	-4.17	1.33	1.37
54	1w	46	7MG	C4-N9	-4.14	1.32	1.37
54	1w	55	PSU	C6-C5	3.98	1.40	1.35
55	2x	8	4SU	C4-N3	-3.94	1.33	1.37
54	2w	55	PSU	C6-C5	3.72	1.39	1.35
54	1y	55	PSU	C6-C5	3.69	1.39	1.35
54	2y	55	PSU	C6-C5	3.54	1.39	1.35
55	1x	55	PSU	C6-C5	3.54	1.39	1.35
54	1y	8	4SU	C4-N3	-3.52	1.33	1.37
55	1x	8	4SU	C2-N3	-3.42	1.31	1.38
32	2a	516	PSU	C6-C5	3.39	1.39	1.35
32	1a	516	PSU	C6-C5	3.39	1.39	1.35
54	1y	46	7MG	C5-C4	3.29	1.48	1.38
1	2A	1917	PSU	C6-C5	3.28	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	527	7MG	C4-N9	-3.24	1.34	1.37
1	2A	2605	PSU	C6-C5	3.24	1.39	1.35
54	2y	46	7MG	C5-C4	3.20	1.48	1.38
1	1A	1917	PSU	C6-C5	3.20	1.39	1.35
54	2y	8	4SU	C4-N3	-3.15	1.34	1.37
55	2x	55	PSU	C6-C5	3.14	1.39	1.35
1	1A	1911	PSU	C6-C5	3.13	1.39	1.35
55	1x	32	5MC	C6-C5	3.13	1.39	1.34
1	2A	1911	PSU	C6-C5	3.10	1.38	1.35
32	1a	527	7MG	C4-N9	-3.10	1.34	1.37
55	1x	8	4SU	C5-C4	-3.08	1.38	1.42
1	1A	2605	PSU	C6-C5	3.03	1.38	1.35
32	1a	527	7MG	C5-C4	3.03	1.48	1.38
54	1w	8	4SU	C4-N3	-3.02	1.34	1.37
54	2w	46	7MG	C5-C4	3.00	1.47	1.38
54	1y	54	5MU	C6-C5	2.99	1.39	1.34
1	2A	1915	5MU	C6-C5	2.98	1.39	1.34
32	2a	527	7MG	C5-C4	2.95	1.47	1.38
54	2w	54	5MU	C6-C5	2.94	1.39	1.34
1	2A	1962	5MC	C6-C5	2.89	1.39	1.34
55	2x	8	4SU	C5-C4	-2.88	1.38	1.42
54	1y	46	7MG	C6-N1	-2.87	1.33	1.38
55	2x	32	5MC	C6-C5	2.86	1.39	1.34
54	1w	46	7MG	C5-C4	2.85	1.47	1.38
54	1w	8	4SU	C5-C4	-2.85	1.38	1.42
32	1a	966	M2G	C2-N2	2.85	1.40	1.35
32	2a	966	M2G	C2-N2	2.85	1.40	1.35
32	1a	1404	5MC	C6-C5	2.85	1.39	1.34
32	2a	1407	5MC	C6-C5	2.85	1.39	1.34
32	2a	1404	5MC	C6-C5	2.82	1.39	1.34
1	1A	1915	5MU	C6-C5	2.82	1.39	1.34
54	2y	54	5MU	C6-C5	2.82	1.39	1.34
55	2x	54	5MU	C6-C5	2.82	1.39	1.34
1	1A	2552	OMU	C4-N3	-2.81	1.33	1.38
1	2A	1939	5MU	C6-C5	2.81	1.39	1.34
32	2a	967	5MC	C6-C5	2.79	1.39	1.34
54	2w	8	4SU	C4-N3	-2.79	1.34	1.37
32	1a	1400	5MC	C6-C5	2.78	1.39	1.34
55	1x	54	5MU	C4-N3	-2.78	1.33	1.38
1	1A	2605	PSU	C4-N3	-2.77	1.33	1.38
54	1w	34	CM0	C4-N3	-2.76	1.33	1.38
54	2y	54	5MU	C2-N1	2.75	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C6-C5	2.75	1.39	1.34
32	1a	1407	5MC	C6-C5	2.75	1.39	1.34
1	2A	2251	OMG	C6-N1	-2.72	1.33	1.37
1	1A	1911	PSU	C4-N3	-2.72	1.33	1.38
54	2w	34	CM0	C4-N3	-2.72	1.33	1.38
54	2w	8	4SU	C2-N1	2.71	1.42	1.38
1	1A	1939	5MU	C4-N3	-2.71	1.33	1.38
54	2y	46	7MG	C6-N1	-2.71	1.33	1.38
1	1A	1942	5MC	C6-C5	2.70	1.39	1.34
32	2a	1400	5MC	C6-C5	2.70	1.39	1.34
55	1x	54	5MU	C6-C5	2.70	1.39	1.34
54	1y	34	CM0	C4-N3	-2.69	1.33	1.38
32	1a	1207	2MG	C6-N1	-2.68	1.33	1.37
54	1y	46	7MG	C8-N9	2.68	1.47	1.46
32	2a	1518	MA6	C5-C4	2.68	1.48	1.40
54	2w	46	7MG	C4-N9	-2.67	1.34	1.37
1	2A	1911	PSU	C4-N3	-2.67	1.33	1.38
32	1a	967	5MC	C6-C5	2.67	1.39	1.34
1	1A	1962	5MC	C6-C5	2.66	1.39	1.34
1	1A	1915	5MU	C4-N3	-2.66	1.33	1.38
54	1w	54	5MU	C6-C5	2.66	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.66	1.33	1.38
54	2y	54	5MU	C4-N3	-2.65	1.33	1.38
1	1A	1917	PSU	C4-N3	-2.64	1.33	1.38
54	2y	8	4SU	C5-C4	-2.63	1.39	1.42
1	1A	1915	5MU	C2-N1	2.62	1.42	1.38
32	2a	1519	MA6	C5-C4	2.62	1.47	1.40
54	2w	54	5MU	C4-N3	-2.61	1.34	1.38
54	2y	34	CM0	C4-N3	-2.61	1.34	1.38
54	2y	55	PSU	C4-N3	-2.60	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.60	1.33	1.38
54	1y	8	4SU	C5-C4	-2.59	1.39	1.42
1	2A	1915	5MU	C4-C5	2.59	1.49	1.44
1	2A	1915	5MU	C4-N3	-2.59	1.34	1.38
1	1A	2251	OMG	C6-N1	-2.59	1.34	1.37
54	2y	37	6MZ	C5-C4	2.58	1.47	1.40
1	2A	1939	5MU	C4-N3	-2.58	1.34	1.38
1	2A	1942	5MC	C6-C5	2.56	1.38	1.34
54	1y	37	6MZ	C5-C4	2.55	1.47	1.40
55	2x	8	4SU	C2-N3	-2.55	1.33	1.38
1	2A	1917	PSU	C4-N3	-2.55	1.34	1.38
32	1a	516	PSU	C4-N3	-2.54	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	8	4SU	C5-C4	-2.54	1.39	1.42
54	1y	54	5MU	C2-N1	2.54	1.42	1.38
54	2w	37	6MZ	C5-C4	2.54	1.47	1.40
55	2x	54	5MU	C4-N3	-2.54	1.34	1.38
55	1x	55	PSU	C4-N3	-2.54	1.34	1.38
54	1w	37	6MZ	C5-C4	2.53	1.47	1.40
54	1y	54	5MU	C4-C5	2.52	1.49	1.44
55	2x	55	PSU	C4-N3	-2.52	1.34	1.38
54	1w	54	5MU	C4-C5	2.52	1.49	1.44
32	1a	1518	MA6	C5-C4	2.49	1.47	1.40
55	2x	54	5MU	C4-C5	2.47	1.48	1.44
32	1a	966	M2G	C6-N1	-2.47	1.34	1.37
32	1a	1519	MA6	C5-C4	2.46	1.47	1.40
54	1y	54	5MU	C4-N3	-2.46	1.34	1.38
54	1y	8	4SU	C2-N1	2.44	1.42	1.38
32	1a	527	7MG	C6-N1	-2.44	1.34	1.38
1	2A	2552	OMU	C5-C4	2.41	1.49	1.43
32	2a	516	PSU	C4-N3	-2.41	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.40	1.33	1.38
54	2y	46	7MG	C8-N9	2.40	1.47	1.46
1	1A	2552	OMU	C5-C4	2.39	1.48	1.43
54	1y	55	PSU	C4-N3	-2.38	1.34	1.38
54	2y	34	CM0	C2-N1	2.37	1.42	1.38
54	1w	54	5MU	C4-N3	-2.37	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.37	1.34	1.38
1	2A	1915	5MU	C2-N1	2.36	1.42	1.38
54	1y	34	CM0	C2-N1	2.35	1.42	1.38
1	2A	1939	5MU	C6-N1	-2.35	1.34	1.38
54	2y	54	5MU	C4-C5	2.34	1.48	1.44
1	1A	2552	OMU	C2-N3	-2.33	1.33	1.38
54	2w	55	PSU	C4-N3	-2.33	1.34	1.38
55	2x	8	4SU	C2-N1	2.32	1.42	1.38
1	1A	1962	5MC	C6-N1	-2.32	1.34	1.38
32	2a	527	7MG	C6-N1	-2.31	1.34	1.38
32	1a	967	5MC	C6-N1	-2.31	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.31	1.34	1.38
54	1w	54	5MU	C2-N1	2.30	1.42	1.38
32	2a	966	M2G	C6-N1	-2.29	1.34	1.37
32	2a	1498	UR3	C2-N1	2.28	1.41	1.38
32	2a	1404	5MC	C6-N1	-2.27	1.34	1.38
1	1A	1915	5MU	C4-C5	2.25	1.48	1.44
55	1x	54	5MU	C4-C5	2.25	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1207	2MG	C6-N1	-2.25	1.34	1.37
54	2y	8	4SU	C2-N1	2.24	1.42	1.38
1	1A	1939	5MU	C4-C5	2.24	1.48	1.44
32	2a	1400	5MC	C6-N1	-2.23	1.34	1.38
55	2x	54	5MU	C2-N1	2.22	1.42	1.38
32	1a	1400	5MC	C6-N1	-2.22	1.34	1.38
54	2w	54	5MU	C2-N1	2.22	1.42	1.38
32	1a	1404	5MC	C6-N1	-2.21	1.34	1.38
54	2w	34	CM0	C2-N1	2.21	1.42	1.38
54	1w	54	5MU	C6-N1	-2.20	1.34	1.38
55	1x	54	5MU	C2-N3	-2.19	1.34	1.38
54	1w	8	4SU	C2-N1	2.19	1.42	1.38
1	1A	1939	5MU	C2-N3	-2.18	1.34	1.38
1	2A	1939	5MU	C4-C5	2.18	1.48	1.44
55	1x	32	5MC	C6-N1	-2.16	1.34	1.38
54	1w	34	CM0	C2-N1	2.16	1.41	1.38
55	1x	54	5MU	C2-N1	2.15	1.41	1.38
32	2a	967	5MC	C6-N1	-2.15	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.14	1.34	1.38
55	2x	32	5MC	C6-N1	-2.12	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.11	1.34	1.38
54	1w	34	CM0	C2-N3	-2.10	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.10	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.09	1.34	1.38
54	1y	54	5MU	C6-N1	-2.09	1.34	1.38
54	2w	34	CM0	C2-N3	-2.08	1.34	1.38
32	1a	1498	UR3	C2-N1	2.07	1.41	1.38
54	2w	54	5MU	C4-C5	2.07	1.48	1.44
1	1A	2503	2MA	C2-N3	2.07	1.35	1.31
55	2x	54	5MU	C6-N1	-2.07	1.34	1.38
32	1a	1498	UR3	C6-C5	2.06	1.39	1.35
32	2a	1407	5MC	C6-N1	-2.06	1.34	1.38
54	1y	8	4SU	C2-N3	-2.05	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.05	1.34	1.37
1	2A	2605	PSU	C2-N3	-2.04	1.34	1.37
54	1w	8	4SU	C2-N3	-2.04	1.34	1.38
54	2w	54	5MU	C6-N1	-2.04	1.34	1.38
1	1A	1911	PSU	C2-N3	-2.04	1.34	1.37
1	2A	2503	2MA	C2-N3	2.04	1.35	1.31
32	2a	1498	UR3	C6-C5	2.04	1.39	1.35
54	2w	34	CM0	C6-N1	-2.03	1.34	1.38
1	1A	1915	5MU	C2-N3	-2.02	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	46	7MG	C4-N9	-2.02	1.35	1.37
54	1y	34	CM0	C2-N3	-2.02	1.34	1.38
1	2A	2552	OMU	C2-N3	-2.02	1.34	1.38
54	1y	46	7MG	C2-N3	2.01	1.38	1.33
1	1A	1939	5MU	C2-N1	2.01	1.41	1.38
54	2y	54	5MU	C6-N1	-2.01	1.34	1.38
1	2A	1939	5MU	C2-N1	2.00	1.41	1.38

All (305) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-17.07	71.55	102.44
43	2l	92	0TD	CSB-SB-CB	-10.93	82.66	102.44
54	1y	46	7MG	N9-C4-N3	9.93	140.32	125.47
54	2y	46	7MG	N9-C4-N3	9.63	139.87	125.47
32	1a	527	7MG	N9-C4-N3	8.77	138.59	125.47
54	2w	46	7MG	N9-C4-N3	8.71	138.49	125.47
32	2a	527	7MG	N9-C4-N3	8.57	138.28	125.47
54	1w	46	7MG	N9-C4-N3	7.55	136.76	125.47
54	1y	37	6MZ	C2-N1-C6	6.10	121.82	116.59
32	1a	1498	UR3	C4-N3-C2	-6.10	118.82	124.56
1	2A	1917	PSU	N1-C2-N3	6.08	122.02	115.13
32	2a	1498	UR3	C4-N3-C2	-6.03	118.89	124.56
54	1w	37	6MZ	C2-N1-C6	6.01	121.75	116.59
54	1y	55	PSU	N1-C2-N3	6.00	121.93	115.13
54	2w	37	6MZ	C2-N1-C6	6.00	121.73	116.59
54	2y	37	6MZ	C2-N1-C6	5.96	121.70	116.59
1	1A	1911	PSU	N1-C2-N3	5.96	121.88	115.13
55	2x	55	PSU	N1-C2-N3	5.92	121.84	115.13
32	1a	516	PSU	N1-C2-N3	5.90	121.82	115.13
55	1x	55	PSU	N1-C2-N3	5.86	121.77	115.13
54	2y	55	PSU	N1-C2-N3	5.84	121.75	115.13
1	1A	1917	PSU	N1-C2-N3	5.81	121.72	115.13
54	1y	8	4SU	C4-N3-C2	-5.77	121.74	127.34
1	2A	2605	PSU	N1-C2-N3	5.76	121.65	115.13
54	1w	8	4SU	C5-C4-N3	5.68	119.96	114.69
1	2A	1911	PSU	N1-C2-N3	5.62	121.50	115.13
54	1w	46	7MG	N9-C8-N7	-5.60	95.37	103.38
1	1A	1939	5MU	C4-N3-C2	-5.60	120.10	127.35
1	1A	2605	PSU	N1-C2-N3	5.57	121.44	115.13
32	2a	527	7MG	N9-C8-N7	-5.53	95.48	103.38
32	2a	516	PSU	N1-C2-N3	5.52	121.39	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	527	7MG	C5-C4-N3	-5.51	117.63	128.13
54	1y	46	7MG	C5-C4-N3	-5.49	117.66	128.13
54	2w	8	4SU	C4-N3-C2	-5.46	122.04	127.34
54	2w	46	7MG	C5-C4-N3	-5.46	117.73	128.13
54	2w	34	CM0	C4-N3-C2	-5.46	120.29	127.35
54	1w	55	PSU	N1-C2-N3	5.44	121.30	115.13
54	1w	8	4SU	C4-N3-C2	-5.42	122.08	127.34
54	2w	8	4SU	C5-C4-N3	5.41	119.71	114.69
54	2y	8	4SU	C5-C4-N3	5.40	119.69	114.69
54	1w	54	5MU	C4-N3-C2	-5.39	120.38	127.35
54	2w	55	PSU	N1-C2-N3	5.36	121.21	115.13
54	1y	8	4SU	C5-C4-N3	5.34	119.64	114.69
1	2A	1939	5MU	C4-N3-C2	-5.34	120.44	127.35
54	1y	34	CM0	C4-N3-C2	-5.33	120.45	127.35
54	2y	46	7MG	C5-C4-N3	-5.32	117.99	128.13
1	2A	1915	5MU	C4-N3-C2	-5.28	120.52	127.35
1	1A	2552	OMU	N3-C2-N1	5.26	121.87	114.89
54	2y	34	CM0	C4-N3-C2	-5.25	120.55	127.35
32	2a	527	7MG	C5-C4-N3	-5.20	118.22	128.13
54	1y	34	CM0	N3-C2-N1	5.20	121.79	114.89
54	2w	46	7MG	N9-C8-N7	-5.17	95.99	103.38
54	1y	54	5MU	N3-C2-N1	5.16	121.73	114.89
54	1w	34	CM0	C4-N3-C2	-5.13	120.71	127.35
1	2A	1915	5MU	N3-C2-N1	5.13	121.70	114.89
54	1y	54	5MU	C4-N3-C2	-5.12	120.72	127.35
54	1w	54	5MU	N3-C2-N1	5.09	121.65	114.89
54	1w	34	CM0	N3-C2-N1	5.09	121.64	114.89
32	1a	527	7MG	N9-C8-N7	-5.08	96.11	103.38
54	2w	34	CM0	N3-C2-N1	5.04	121.58	114.89
54	2y	8	4SU	C4-N3-C2	-4.99	122.49	127.34
1	2A	2552	OMU	N3-C2-N1	4.99	121.52	114.89
55	2x	54	5MU	N3-C2-N1	4.99	121.51	114.89
54	2y	34	CM0	N3-C2-N1	4.98	121.50	114.89
1	1A	1939	5MU	C5-C4-N3	4.98	119.56	115.31
1	2A	1939	5MU	N3-C2-N1	4.97	121.48	114.89
1	1A	1939	5MU	N3-C2-N1	4.95	121.46	114.89
54	2y	46	7MG	N9-C8-N7	-4.93	96.32	103.38
55	2x	54	5MU	C4-N3-C2	-4.91	120.99	127.35
1	1A	1915	5MU	C4-N3-C2	-4.91	121.00	127.35
1	1A	1915	5MU	N3-C2-N1	4.77	121.22	114.89
1	1A	1915	5MU	C5-C4-N3	4.74	119.36	115.31
54	1y	46	7MG	N9-C8-N7	-4.74	96.60	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	54	5MU	N3-C2-N1	4.69	121.11	114.89
55	2x	8	4SU	C5-C4-N3	4.68	119.03	114.69
54	2y	54	5MU	C4-N3-C2	-4.61	121.39	127.35
1	1A	1939	5MU	C5-C6-N1	-4.54	118.66	123.34
55	1x	8	4SU	C5-C4-N3	4.54	118.90	114.69
54	2w	54	5MU	C4-N3-C2	-4.53	121.49	127.35
54	1w	46	7MG	C5-C4-N3	-4.52	119.51	128.13
54	2w	54	5MU	N3-C2-N1	4.50	120.87	114.89
54	2w	46	7MG	C2-N3-C4	4.48	120.29	112.30
1	1A	2552	OMU	C4-N3-C2	-4.47	120.68	126.58
1	2A	1939	5MU	C5-C4-N3	4.45	119.11	115.31
1	2A	1939	5MU	O4-C4-C5	-4.40	119.80	124.90
54	2y	34	CM0	C7-O5-C5	4.36	123.29	117.58
54	1y	54	5MU	C5-C4-N3	4.33	119.01	115.31
54	1y	46	7MG	C2-N3-C4	4.33	120.01	112.30
1	2A	1915	5MU	C5-C4-N3	4.31	118.99	115.31
55	1x	54	5MU	N3-C2-N1	4.31	120.61	114.89
32	1a	527	7MG	C2-N3-C4	4.29	119.94	112.30
54	1w	54	5MU	C5-C4-N3	4.28	118.97	115.31
1	1A	1939	5MU	O4-C4-C5	-4.27	119.96	124.90
1	2A	1939	5MU	C5-C6-N1	-4.25	118.97	123.34
1	2A	2552	OMU	C4-N3-C2	-4.22	121.02	126.58
32	2a	527	7MG	C2-N3-C4	4.19	119.76	112.30
55	1x	54	5MU	C4-N3-C2	-4.17	121.95	127.35
54	2y	54	5MU	C5-C4-N3	4.16	118.86	115.31
54	2y	46	7MG	C2-N3-C4	4.12	119.64	112.30
54	1w	54	5MU	O4-C4-C5	-4.10	120.15	124.90
55	2x	8	4SU	C1'-N1-C2	4.09	124.98	117.57
1	2A	1915	5MU	C5-C6-N1	-4.08	119.14	123.34
54	1w	46	7MG	C2-N3-C4	4.07	119.56	112.30
54	1y	34	CM0	C7-O5-C5	4.05	122.88	117.58
55	2x	54	5MU	C5-C4-N3	4.05	118.77	115.31
55	2x	55	PSU	C4-N3-C2	-4.03	120.53	126.34
54	1w	55	PSU	O2-C2-N1	-4.03	118.35	122.79
1	1A	1911	PSU	C4-N3-C2	-4.01	120.56	126.34
1	1A	1915	5MU	O4-C4-C5	-3.98	120.29	124.90
1	2A	2605	PSU	C4-N3-C2	-3.96	120.63	126.34
54	2w	54	5MU	C5-C4-N3	3.92	118.65	115.31
54	2w	54	5MU	O4-C4-C5	-3.91	120.37	124.90
1	1A	1962	5MC	C5-C6-N1	-3.90	119.33	123.34
1	2A	1917	PSU	C4-N3-C2	-3.88	120.75	126.34
32	2a	1404	5MC	C5-C6-N1	-3.87	119.36	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	54	5MU	C5-C4-N3	3.85	118.60	115.31
1	1A	2605	PSU	C4-N3-C2	-3.84	120.80	126.34
1	1A	1917	PSU	C4-N3-C2	-3.82	120.83	126.34
54	1w	54	5MU	C5-C6-N1	-3.80	119.42	123.34
32	2a	516	PSU	C4-N3-C2	-3.80	120.86	126.34
54	2y	55	PSU	C4-N3-C2	-3.79	120.87	126.34
54	1y	55	PSU	O2-C2-N1	-3.78	118.62	122.79
55	1x	55	PSU	C4-N3-C2	-3.76	120.92	126.34
54	1y	8	4SU	N3-C2-N1	3.75	119.86	114.89
1	2A	1911	PSU	C4-N3-C2	-3.73	120.97	126.34
32	1a	516	PSU	C4-N3-C2	-3.72	120.97	126.34
32	2a	1400	5MC	C5-C6-N1	-3.70	119.53	123.34
55	1x	32	5MC	C5-C6-N1	-3.69	119.54	123.34
54	1y	54	5MU	O4-C4-C5	-3.69	120.62	124.90
55	2x	54	5MU	O4-C4-C5	-3.68	120.64	124.90
32	2a	1519	MA6	C4-C5-N7	-3.66	105.59	109.40
54	1w	8	4SU	C5-C4-S4	-3.63	119.79	124.47
54	2w	55	PSU	C4-N3-C2	-3.63	121.11	126.34
32	2a	1518	MA6	C4-C5-N7	-3.62	105.62	109.40
54	2w	8	4SU	C5-C4-S4	-3.62	119.80	124.47
1	2A	1917	PSU	O2-C2-N1	-3.62	118.81	122.79
54	1y	55	PSU	C4-N3-C2	-3.60	121.15	126.34
54	1y	37	6MZ	C9-N6-C6	-3.58	119.79	122.87
1	1A	1942	5MC	C5-C6-N1	-3.56	119.68	123.34
54	2y	54	5MU	O4-C4-C5	-3.54	120.80	124.90
32	1a	1519	MA6	C4-C5-N7	-3.51	105.74	109.40
32	1a	1400	5MC	C5-C6-N1	-3.51	119.73	123.34
54	1w	55	PSU	C4-N3-C2	-3.50	121.30	126.34
55	1x	8	4SU	C1'-N1-C2	3.48	123.86	117.57
32	1a	967	5MC	C5-C6-N1	-3.43	119.81	123.34
1	2A	1962	5MC	C5-C6-N1	-3.43	119.81	123.34
32	1a	1407	5MC	C5-C6-N1	-3.43	119.81	123.34
1	2A	1915	5MU	O4-C4-C5	-3.42	120.94	124.90
54	2w	8	4SU	C1'-N1-C2	3.42	123.75	117.57
54	2w	54	5MU	C5-C6-N1	-3.41	119.83	123.34
32	2a	967	5MC	C5-C6-N1	-3.40	119.84	123.34
55	2x	54	5MU	C5-C6-N1	-3.39	119.85	123.34
1	1A	1911	PSU	O2-C2-N1	-3.37	119.08	122.79
55	2x	32	5MC	C5-C6-N1	-3.36	119.89	123.34
1	2A	2552	OMU	C2'-C1'-N1	-3.36	107.71	114.22
32	1a	1518	MA6	N3-C2-N1	-3.35	123.44	128.68
54	2y	37	6MZ	C9-N6-C6	-3.35	119.99	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	46	7MG	C5-C4-N9	-3.34	102.01	106.35
32	1a	1518	MA6	C4-C5-N7	-3.33	105.92	109.40
32	2a	1518	MA6	N3-C2-N1	-3.33	123.47	128.68
1	2A	1911	PSU	O2-C2-N1	-3.33	119.12	122.79
32	2a	1519	MA6	C9-N6-C6	-3.32	109.46	119.51
55	2x	55	PSU	O2-C2-N1	-3.32	119.14	122.79
54	1y	37	6MZ	N3-C2-N1	-3.30	123.52	128.68
54	2y	55	PSU	O2-C2-N1	-3.30	119.16	122.79
55	1x	54	5MU	C5-C6-N1	-3.29	119.95	123.34
54	1w	37	6MZ	C9-N6-C6	-3.28	120.05	122.87
43	1l	92	0TD	OD2-CG-CB	3.28	120.24	113.15
32	1a	1519	MA6	N3-C2-N1	-3.28	123.56	128.68
54	2w	8	4SU	N3-C2-N1	3.27	119.23	114.89
55	1x	54	5MU	O4-C4-C5	-3.27	121.11	124.90
32	2a	1518	MA6	C9-N6-C6	-3.27	109.61	119.51
43	2l	92	0TD	OD2-CG-CB	3.27	120.21	113.15
1	2A	1942	5MC	C5-C6-N1	-3.27	119.98	123.34
54	2w	55	PSU	O2-C2-N1	-3.26	119.20	122.79
32	2a	516	PSU	O2-C2-N1	-3.25	119.21	122.79
54	2y	46	7MG	C5-C4-N9	-3.24	102.14	106.35
54	1y	54	5MU	C5-C6-N1	-3.22	120.02	123.34
54	2y	8	4SU	C5-C4-S4	-3.21	120.33	124.47
54	1y	8	4SU	C1'-N1-C2	3.20	123.37	117.57
54	2y	37	6MZ	N3-C2-N1	-3.19	123.69	128.68
54	1w	8	4SU	N3-C2-N1	3.16	119.08	114.89
55	1x	55	PSU	O2-C2-N1	-3.15	119.32	122.79
1	1A	1917	PSU	O2-C2-N1	-3.13	119.34	122.79
54	2w	37	6MZ	N3-C2-N1	-3.12	123.80	128.68
32	2a	1519	MA6	N3-C2-N1	-3.11	123.82	128.68
32	1a	516	PSU	O2-C2-N1	-3.11	119.37	122.79
32	2a	1407	5MC	C5-C6-N1	-3.10	120.14	123.34
1	1A	1915	5MU	C5-C6-N1	-3.09	120.16	123.34
32	1a	1519	MA6	C9-N6-C6	-3.08	110.19	119.51
32	1a	1518	MA6	C9-N6-C6	-3.07	110.21	119.51
32	1a	1404	5MC	C5-C6-N1	-3.06	120.19	123.34
1	1A	2552	OMU	O2-C2-N1	-3.02	118.77	122.79
54	1w	37	6MZ	N3-C2-N1	-3.01	123.97	128.68
1	2A	2552	OMU	O2-C2-N1	-3.00	118.79	122.79
1	1A	2552	OMU	C2'-C1'-N1	-2.99	108.43	114.22
54	2y	37	6MZ	C4-C5-N7	-2.97	106.30	109.40
54	2w	46	7MG	C5-C6-N1	2.97	116.22	110.99
32	1a	1404	5MC	C5-C4-N3	-2.96	118.48	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	32	5MC	O2-C2-N3	-2.96	117.52	122.33
54	2y	54	5MU	C5-C6-N1	-2.94	120.32	123.34
32	1a	1407	5MC	C5-C4-N3	-2.92	118.52	121.67
54	1w	37	6MZ	C4-C5-N7	-2.91	106.37	109.40
1	1A	2552	OMU	C5-C4-N3	2.89	119.16	114.84
54	1y	37	6MZ	C4-C5-N7	-2.87	106.41	109.40
55	1x	32	5MC	C5-C4-N3	-2.85	118.59	121.67
54	1y	8	4SU	C5-C4-S4	-2.85	120.80	124.47
1	2A	2605	PSU	O2-C2-N1	-2.85	119.66	122.79
54	2y	54	5MU	C1'-N1-C2	2.80	122.65	117.57
1	2A	1939	5MU	O2-C2-N1	-2.78	119.09	122.79
54	2y	8	4SU	N3-C2-N1	2.76	118.56	114.89
55	2x	8	4SU	C4-N3-C2	-2.76	124.66	127.34
32	2a	1407	5MC	C5-C4-N3	-2.76	118.70	121.67
55	2x	32	5MC	C5-C4-N3	-2.72	118.74	121.67
54	2w	37	6MZ	C4-C5-N7	-2.71	106.58	109.40
55	1x	8	4SU	C6-C5-C4	-2.68	117.63	119.95
1	1A	1939	5MU	O2-C2-N1	-2.67	119.23	122.79
1	1A	1942	5MC	C5-C4-N3	-2.67	118.79	121.67
54	1w	34	CM0	O2-C2-N1	-2.67	119.24	122.79
32	2a	527	7MG	C5-C6-N1	2.66	115.68	110.99
1	2A	2552	OMU	C5-C4-N3	2.64	118.79	114.84
32	1a	527	7MG	C5-C6-N1	2.62	115.60	110.99
54	1w	54	5MU	O2-C2-N1	-2.62	119.31	122.79
54	2y	8	4SU	C1'-N1-C2	2.60	122.28	117.57
54	2w	54	5MU	O2-C2-N1	-2.60	119.34	122.79
54	2w	34	CM0	O2-C2-N1	-2.59	119.34	122.79
55	1x	8	4SU	O2-C2-N3	-2.59	116.68	121.50
54	1y	34	CM0	O2-C2-N1	-2.58	119.36	122.79
1	1A	2605	PSU	O2-C2-N1	-2.56	119.97	122.79
32	1a	1400	5MC	C5-C4-N3	-2.56	118.92	121.67
32	1a	967	5MC	C5-C4-N3	-2.54	118.93	121.67
54	1w	46	7MG	C5-C6-N1	2.53	115.46	110.99
54	1w	8	4SU	C1'-N1-C2	2.53	122.15	117.57
1	2A	1962	5MC	C5-C4-N3	-2.51	118.96	121.67
32	2a	1207	2MG	C8-N7-C5	2.51	107.77	102.99
32	2a	1400	5MC	C5-C4-N3	-2.50	118.97	121.67
55	1x	8	4SU	O2-C2-N1	2.47	126.07	122.79
32	1a	1207	2MG	C8-N7-C5	2.47	107.69	102.99
1	1A	2503	2MA	C8-N7-C5	2.46	107.68	102.99
1	2A	1920	OMC	O2-C2-N3	-2.45	118.34	122.33
54	1w	55	PSU	C6-C5-C4	-2.45	116.48	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1404	5MC	C5-C4-N3	-2.44	119.04	121.67
1	2A	1942	5MC	C5-C4-N3	-2.43	119.05	121.67
54	2w	34	CM0	C7-O5-C5	2.43	120.75	117.58
32	2a	967	5MC	C5-C4-N3	-2.42	119.07	121.67
54	2y	34	CM0	O2-C2-N1	-2.41	119.59	122.79
55	2x	54	5MU	O2-C2-N1	-2.41	119.59	122.79
1	2A	2503	2MA	C8-N7-C5	2.40	107.57	102.99
1	1A	1915	5MU	C1'-N1-C2	2.40	121.91	117.57
32	1a	966	M2G	C5-C6-N1	2.39	118.18	113.95
1	2A	1915	5MU	O2-C2-N1	-2.39	119.61	122.79
1	1A	2503	2MA	C5-C6-N1	2.38	118.12	114.02
32	1a	1402	4OC	C6-C5-C4	2.38	119.87	116.96
32	2a	1518	MA6	C10-N6-C9	-2.35	108.56	116.12
43	2l	92	0TD	OD1-CG-CB	-2.34	117.55	122.44
1	2A	2251	OMG	C8-N7-C5	2.32	107.40	102.99
54	1w	34	CM0	C7-O5-C5	2.31	120.59	117.58
1	1A	2251	OMG	C5-C6-N1	2.30	118.01	113.95
54	2w	46	7MG	O6-C6-C5	-2.30	121.91	127.54
1	2A	2503	2MA	C5-C6-N1	2.30	117.98	114.02
1	1A	1962	5MC	C5-C4-N3	-2.29	119.20	121.67
32	1a	1207	2MG	CM2-N2-C2	-2.26	118.87	123.86
55	2x	8	4SU	C5-C4-S4	-2.25	121.57	124.47
55	2x	8	4SU	C1'-N1-C6	-2.25	115.94	120.84
55	1x	32	5MC	O2-C2-N3	-2.24	118.68	122.33
32	1a	1518	MA6	C10-N6-C6	-2.24	112.73	119.51
54	2y	54	5MU	C1'-N1-C6	-2.24	117.40	121.12
55	1x	8	4SU	C5-C4-S4	-2.23	121.59	124.47
55	2x	55	PSU	C5-C6-N1	-2.23	118.76	122.11
1	1A	2251	OMG	C8-N7-C5	2.23	107.24	102.99
55	2x	8	4SU	C6-C5-C4	-2.22	118.03	119.95
54	1w	46	7MG	O6-C6-C5	-2.21	122.12	127.54
32	1a	516	PSU	O4'-C1'-C2'	2.21	108.26	105.14
32	2a	527	7MG	C5-C4-N9	-2.20	103.49	106.35
54	1w	34	CM0	O3'-C3'-C2'	2.20	118.94	111.82
32	1a	1518	MA6	C10-N6-C9	-2.20	109.04	116.12
32	2a	1402	4OC	C6-C5-C4	2.20	119.65	116.96
32	2a	966	M2G	C5-C6-N1	2.19	117.82	113.95
1	2A	2552	OMU	O4-C4-C5	-2.19	121.31	125.16
32	2a	1402	4OC	O2-C2-N3	-2.18	118.78	122.33
32	1a	1404	5MC	O2-C2-N3	-2.17	118.80	122.33
54	2y	54	5MU	O2-C2-N3	-2.15	117.49	121.50
32	2a	966	M2G	C8-N7-C5	2.15	107.08	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	55	PSU	C6-C5-C4	-2.13	116.71	118.20
32	2a	1400	5MC	O2-C2-N3	-2.12	118.88	122.33
32	1a	1519	MA6	N1-C6-N6	2.12	119.29	117.06
1	2A	2251	OMG	C5-C6-N1	2.12	117.69	113.95
54	1w	54	5MU	C5M-C5-C6	-2.10	120.04	122.85
32	2a	1404	5MC	O2-C2-N3	-2.09	118.93	122.33
55	1x	8	4SU	C4-N3-C2	-2.09	125.31	127.34
43	1l	92	0TD	OD1-CG-CB	-2.08	118.08	122.44
54	1w	54	5MU	C5M-C5-C4	2.08	121.05	118.77
1	1A	1920	OMC	O2-C2-N3	-2.06	118.98	122.33
32	1a	966	M2G	C8-N7-C5	2.05	106.90	102.99
1	1A	1962	5MC	CM5-C5-C6	-2.05	120.12	122.85
32	1a	967	5MC	O2-C2-N3	-2.04	119.02	122.33
32	1a	1518	MA6	N1-C6-N6	2.04	119.20	117.06
1	1A	1920	OMC	C1'-N1-C2	2.03	122.96	118.42
54	2y	46	7MG	C5-C6-N1	2.03	114.57	110.99
54	2y	34	CM0	O5-C7-C8	-2.02	106.49	110.88
54	1w	46	7MG	C5-C4-N9	-2.02	103.73	106.35
1	1A	2552	OMU	O4-C4-C5	-2.01	121.62	125.16
55	2x	8	4SU	O2-C2-N3	-2.01	117.75	121.50
32	1a	1498	UR3	C3U-N3-C2	2.01	120.84	117.31
1	1A	1942	5MC	CM5-C5-C6	-2.01	120.17	122.85

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	C3'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
43	1l	92	0TD	O-C-CA-CB
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1207	2MG	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
54	1y	37	6MZ	N1-C6-N6-C9
54	2w	37	6MZ	C5-C6-N6-C9
54	2w	37	6MZ	N1-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
54	2y	37	6MZ	N1-C6-N6-C9
54	1w	46	7MG	O4'-C4'-C5'-O5'
54	1w	46	7MG	C3'-C4'-C5'-O5'
54	1y	46	7MG	C4'-C5'-O5'-P
54	1y	46	7MG	C3'-C4'-C5'-O5'
54	2y	46	7MG	C4'-C5'-O5'-P
54	2y	46	7MG	C3'-C4'-C5'-O5'
54	1y	54	5MU	C3'-C4'-C5'-O5'
54	1y	54	5MU	O4'-C4'-C5'-O5'
54	2y	54	5MU	C3'-C4'-C5'-O5'
54	2y	54	5MU	O4'-C4'-C5'-O5'
1	1A	1915	5MU	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	2y	8	4SU	O4'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C4'-C5'-O5'
54	2y	34	CM0	O5-C7-C8-O8
54	2y	34	CM0	O5-C7-C8-O9
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
54	2y	8	4SU	C3'-C4'-C5'-O5'
54	2y	55	PSU	C3'-C4'-C5'-O5'
54	1y	34	CM0	O5-C7-C8-O8
54	2y	34	CM0	C6-C5-O5-C7
54	1y	34	CM0	O4'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C4'-C5'-O5'
54	2y	46	7MG	O4'-C4'-C5'-O5'
54	2w	34	CM0	O5-C7-C8-O9
32	1a	1518	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	C5-C6-N6-C9
54	2w	34	CM0	O4'-C4'-C5'-O5'
54	2y	34	CM0	C4-C5-O5-C7
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
54	1y	34	CM0	O5-C7-C8-O9
54	2w	34	CM0	O5-C7-C8-O8
54	2w	34	CM0	C6-C5-O5-C7

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Mol	Chain	Res	Type	Atoms
54	1y	46	7MG	C2'-C1'-N9-C8
32	2a	1404	5MC	O4'-C4'-C5'-O5'
54	1y	34	CM0	C3'-C4'-C5'-O5'
54	2w	34	CM0	C3'-C4'-C5'-O5'
54	2w	34	CM0	C4-C5-O5-C7
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	1404	5MC	C3'-C4'-C5'-O5'
54	2w	34	CM0	C8-C7-O5-C5
54	2y	34	CM0	C8-C7-O5-C5
54	2y	46	7MG	C2'-C1'-N9-C8
43	1l	92	0TD	CA-CB-CG-OD2
1	1A	2503	2MA	C4'-C5'-O5'-P
32	2a	527	7MG	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P
54	1y	8	4SU	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C4'-C5'-O5'
54	2w	8	4SU	C2'-C1'-N1-C6
54	1w	34	CM0	C8-C7-O5-C5
54	1w	55	PSU	O4'-C1'-C5-C4
54	2y	55	PSU	O4'-C1'-C5-C4
32	2a	1519	MA6	N1-C6-N6-C9
32	2a	1402	4OC	C3'-C2'-O2'-CM2
54	2y	46	7MG	O4'-C1'-N9-C8
32	1a	527	7MG	C4'-C5'-O5'-P
54	1y	8	4SU	O4'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C1'-C2'-O2'-CM2
1	1A	1920	OMC	C2'-C1'-N1-C2
54	2y	54	5MU	C2'-C1'-N1-C2
55	2x	8	4SU	C2'-C1'-N1-C2
43	1l	92	0TD	CG-CB-SB-CSB
54	1y	8	4SU	C2'-C1'-N1-C2
54	2w	8	4SU	C2'-C1'-N1-C2
54	1y	46	7MG	O4'-C1'-N9-C8
1	2A	1962	5MC	C3'-C4'-C5'-O5'
43	2l	92	0TD	SB-CB-CG-OD1
32	2a	1518	MA6	N1-C6-N6-C9
1	1A	2503	2MA	O4'-C4'-C5'-O5'
54	2y	34	CM0	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2778 ligands modelled in this entry, 2770 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
57	LUJ	1A	4100	-	45,45,47	0.75	1 (2%)	61,67,69	1.11	3 (4%)
57	LUJ	1a	1832	56	47,47,47	0.76	1 (2%)	61,69,69	1.18	3 (4%)
60	SF4	2d	303	35	0,12,12	-	-	-		
57	LUJ	2A	3851	-	45,45,47	0.83	2 (4%)	61,67,69	1.54	8 (13%)
57	LUJ	2A	3852	-	45,45,47	0.75	1 (2%)	61,67,69	1.18	4 (6%)
57	LUJ	2a	3232	-	47,47,47	0.83	3 (6%)	61,69,69	1.32	5 (8%)
57	LUJ	1A	4099	-	45,45,47	0.79	1 (2%)	61,67,69	1.48	8 (13%)
60	SF4	1d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	LUJ	1A	4100	-	-	5/18/94/97	0/4/4/4
57	LUJ	1a	1832	56	-	5/21/97/97	0/4/4/4
60	SF4	2d	303	35	-	-	0/6/5/5
57	LUJ	2A	3851	-	-	4/18/94/97	0/4/4/4
57	LUJ	2A	3852	-	-	4/18/94/97	0/4/4/4
57	LUJ	2a	3232	-	-	6/21/97/97	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	LUJ	1A	4099	-	-	7/18/94/97	0/4/4/4
60	SF4	1d	501	35	-	-	0/6/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3851	LUJ	O4'-C1'	2.73	1.46	1.41
57	1A	4100	LUJ	O4'-C1'	2.68	1.46	1.41
57	2A	3851	LUJ	CBE-CBD	-2.34	1.50	1.53
57	1a	1832	LUJ	CBG-CBE	-2.27	1.50	1.53
57	1A	4099	LUJ	OAB-CBC	2.12	1.47	1.41
57	2a	3232	LUJ	O4'-C1'	2.09	1.45	1.41
57	2a	3232	LUJ	C1'-C2'	-2.07	1.50	1.52
57	2A	3852	LUJ	C1'-C2'	-2.05	1.50	1.52
57	2a	3232	LUJ	CBE-CBD	-2.02	1.51	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	2a	3232	LUJ	CBF-O3'-C3'	-6.22	102.56	117.96
57	1A	4099	LUJ	O1'-C1'-O4'	-5.36	105.63	111.43
57	1a	1832	LUJ	CBF-O3'-C3'	-5.23	105.01	117.96
57	2A	3851	LUJ	O1'-C1'-O4'	-5.10	105.91	111.43
57	2A	3852	LUJ	CBF-O3'-C3'	-4.69	106.35	117.96
57	1A	4099	LUJ	C1'-C2'-C3'	-4.21	97.04	102.10
57	2a	3232	LUJ	C1'-C2'-C3'	-4.14	97.13	102.10
57	2A	3851	LUJ	C1'-O1'-CAS	-4.12	107.78	117.96
57	1A	4100	LUJ	C2'-C3'-C4'	-4.09	95.98	103.22
57	2A	3851	LUJ	C2'-C3'-C4'	-4.01	96.12	103.22
57	1A	4100	LUJ	CBF-O3'-C3'	-3.91	108.30	117.96
57	1a	1832	LUJ	C2'-C3'-C4'	-3.76	96.55	103.22
57	1A	4099	LUJ	C1'-O1'-CAS	-3.73	108.73	117.96
57	2A	3852	LUJ	C1'-C2'-C3'	-3.64	97.73	102.10
57	2A	3851	LUJ	CBP-CBG-CBE	-3.58	107.35	112.15
57	2A	3852	LUJ	O4'-C1'-C2'	-3.39	100.61	104.98
57	1A	4100	LUJ	O1'-C1'-O4'	3.33	115.04	111.43
57	2a	3232	LUJ	C2'-C3'-C4'	-3.13	97.68	103.22
57	1A	4099	LUJ	C2'-C3'-C4'	-2.81	98.24	103.22
57	2A	3851	LUJ	OAB-CBC-OAF	2.80	118.50	110.67
57	1A	4099	LUJ	OAB-CBC-OAF	2.74	118.32	110.67
57	1A	4099	LUJ	CBP-CBG-CBE	-2.73	108.49	112.15
57	1a	1832	LUJ	C1'-C2'-C3'	-2.73	98.82	102.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	2A	3851	LUJ	C1'-C2'-C3'	-2.64	98.93	102.10
57	2A	3852	LUJ	C2'-C3'-C4'	-2.51	98.77	103.22
57	2A	3851	LUJ	CBC-OAB-CAT	2.34	123.77	117.96
57	1A	4099	LUJ	OAB-CAT-CAS	2.29	113.30	107.48
57	1A	4099	LUJ	OAG-CBM-CBO	2.20	110.10	106.01
57	2a	3232	LUJ	O4'-C1'-C2'	-2.15	102.21	104.98
57	2A	3851	LUJ	CBF-O3'-C3'	-2.02	112.97	117.96
57	2a	3232	LUJ	O3'-CBF-CBH	2.00	111.66	108.22

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	1a	1832	LUJ	CBE-CBG-CBP-CBQ
57	2a	3232	LUJ	CBI-CBG-CBP-CBQ
57	2a	3232	LUJ	CBE-CBG-CBP-CBQ
57	2a	3232	LUJ	O4'-C4'-C5'-O5'
57	2A	3852	LUJ	O4'-C4'-C5'-O5'
57	2A	3852	LUJ	C3'-C4'-C5'-O5'
57	2a	3232	LUJ	C3'-C4'-C5'-O5'
57	1A	4099	LUJ	OAF-CBC-OAB-CAT
57	2A	3851	LUJ	OAF-CBC-OAB-CAT
57	1A	4100	LUJ	O4'-C4'-C5'-O5'
57	1a	1832	LUJ	OAF-CBI-CBN-OAM
57	1A	4100	LUJ	C3'-C4'-C5'-O5'
57	1a	1832	LUJ	CBG-CBI-CBN-OAM
57	2a	3232	LUJ	CBG-CBP-CBQ-CBR
57	1A	4100	LUJ	OAF-CBI-CBN-OAM
57	2A	3851	LUJ	OAG-CBF-O3'-C3'
57	1a	1832	LUJ	CBI-CBG-CBP-CBQ
57	1A	4099	LUJ	C2'-C3'-O3'-CBF
57	1A	4100	LUJ	CBG-CBI-CBN-OAM
57	2A	3852	LUJ	CAS-CAT-OAB-CBC
57	1A	4100	LUJ	OAF-CBC-OAB-CAT
57	2a	3232	LUJ	CAS-CAT-OAB-CBC
57	1a	1832	LUJ	CAS-CAT-OAB-CBC
57	1A	4099	LUJ	OAG-CBM-CBO-NAR
57	2A	3851	LUJ	OAG-CBM-CBO-NAR
57	1A	4099	LUJ	CAS-CAT-OAB-CBC
57	1A	4099	LUJ	OAG-CBF-O3'-C3'
57	2A	3852	LUJ	OAF-CBC-OAB-CAT
57	2A	3851	LUJ	CAS-CAT-OAB-CBC

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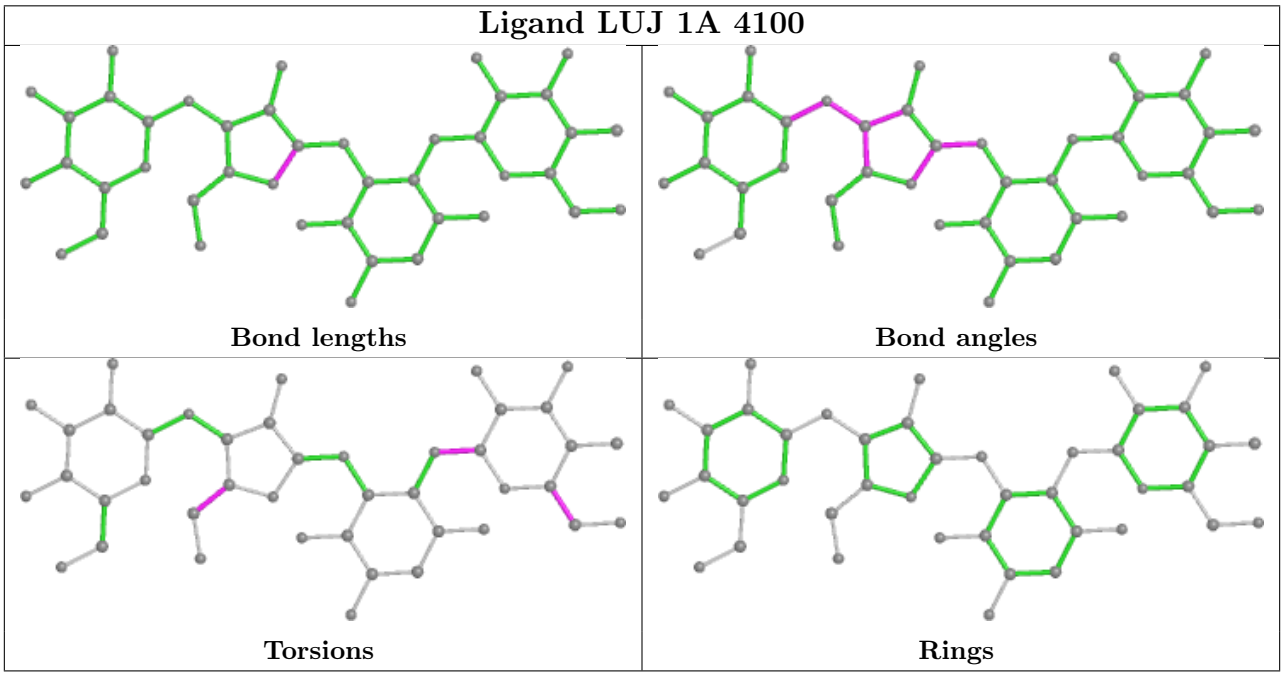
Mol	Chain	Res	Type	Atoms
57	1A	4099	LUJ	C2'-C1'-O1'-CAS
57	1A	4099	LUJ	CBL-CBM-CBO-NAR

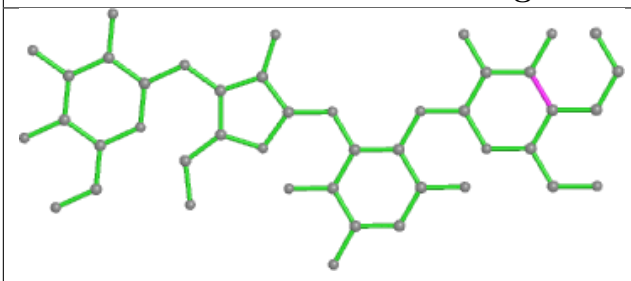
There are no ring outliers.

No monomer is involved in short contacts.

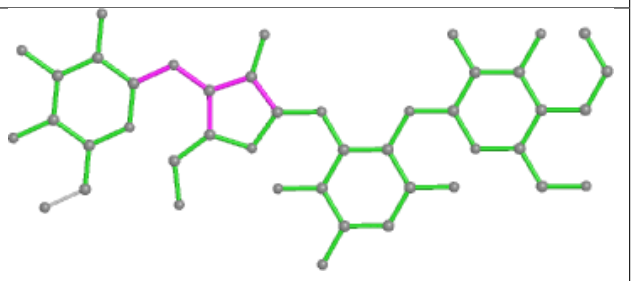
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



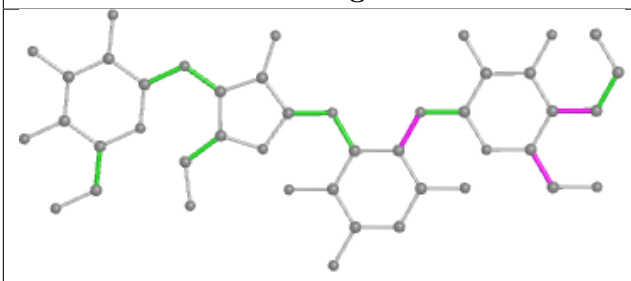
Ligand LUJ 1a 1832



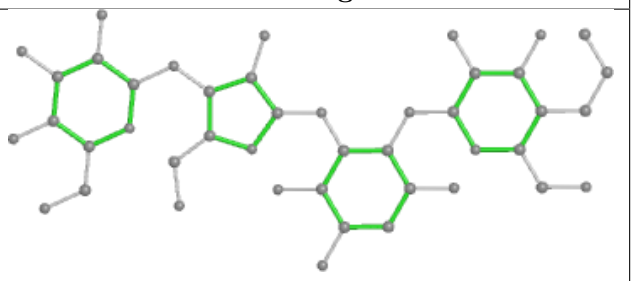
Bond lengths



Bond angles

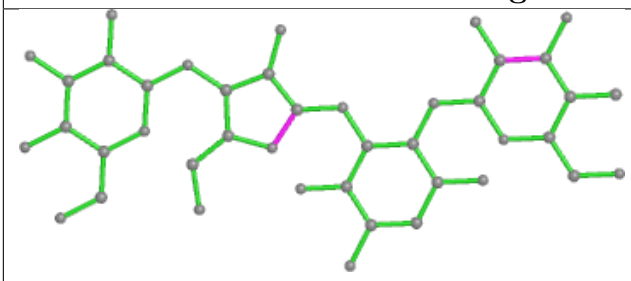


Torsions

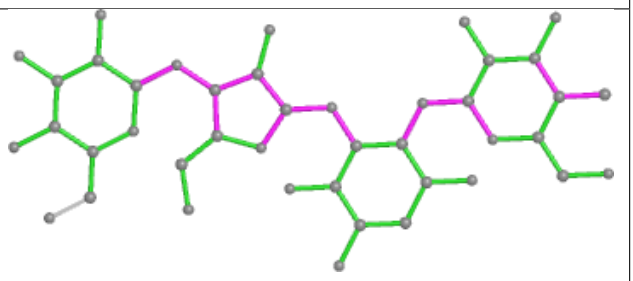


Rings

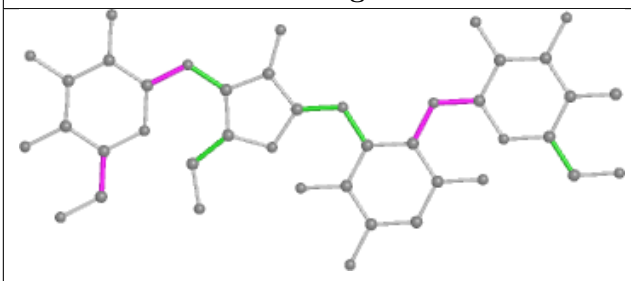
Ligand LUJ 2A 3851



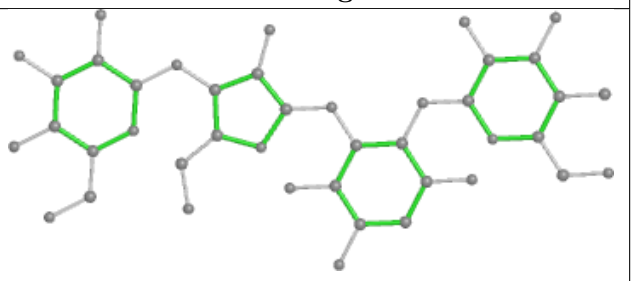
Bond lengths



Bond angles

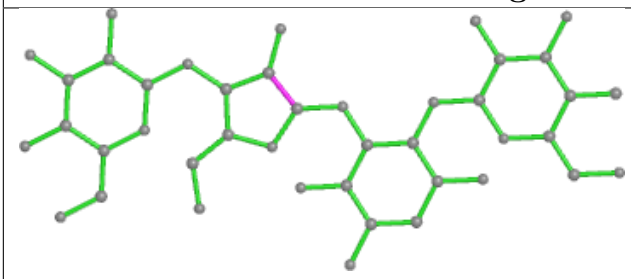


Torsions

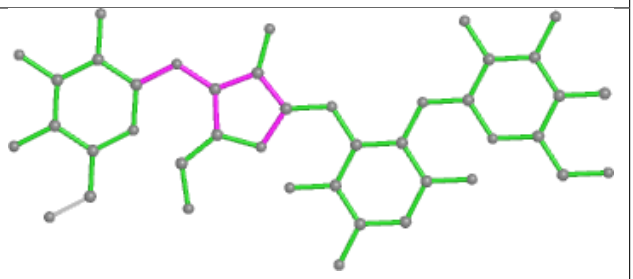


Rings

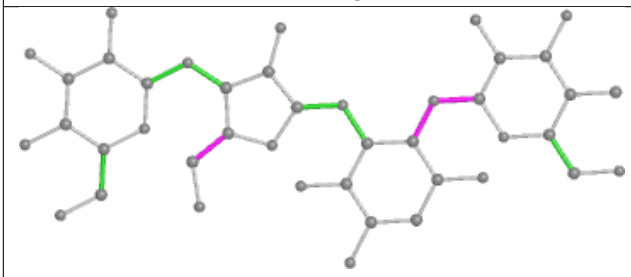
Ligand LUJ 2A 3852



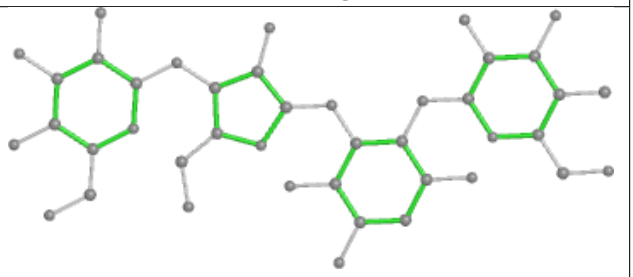
Bond lengths



Bond angles

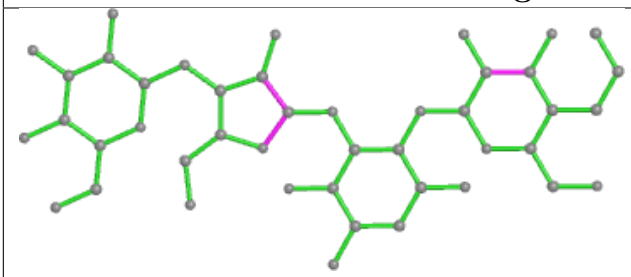


Torsions

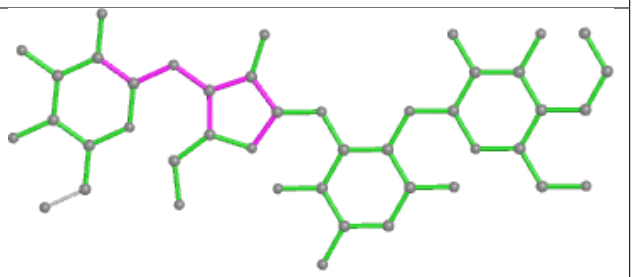


Rings

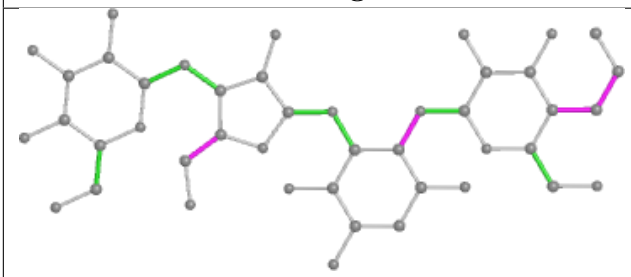
Ligand LUJ 2a 3232



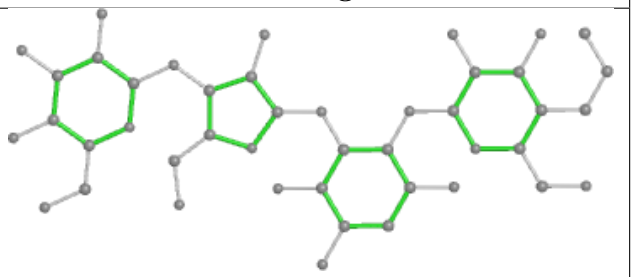
Bond lengths



Bond angles

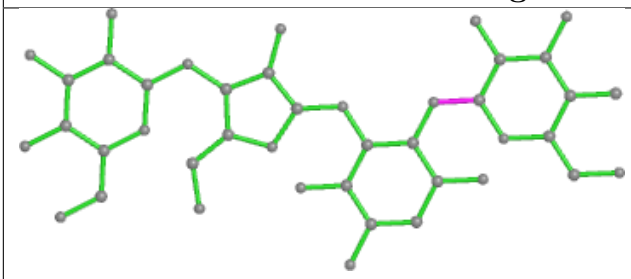


Torsions

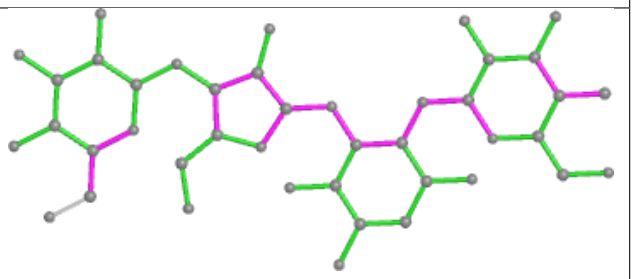


Rings

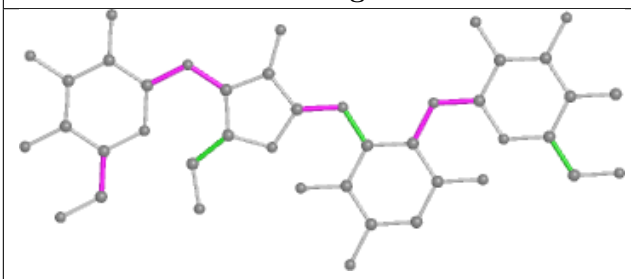
Ligand LUJ 1A 4099



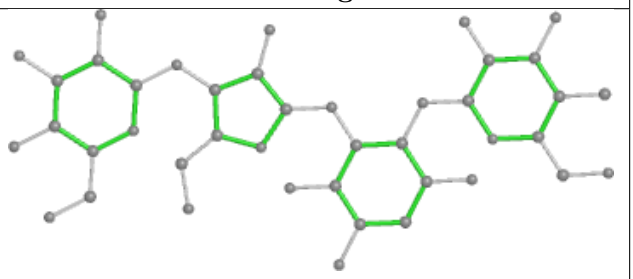
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.32	22 (0%) 86 90	11, 28, 86, 98	0
1	2A	2789/2915 (95%)	0.23	57 (2%) 65 73	26, 53, 86, 100	0
2	1B	120/121 (99%)	-0.03	0 100 100	21, 40, 53, 74	0
2	2B	120/121 (99%)	-0.06	1 (0%) 86 90	55, 70, 79, 87	0
3	1D	275/276 (99%)	0.79	14 (5%) 28 34	13, 31, 45, 74	0
3	2D	275/276 (99%)	0.82	19 (6%) 16 20	24, 44, 58, 69	0
4	1E	204/206 (99%)	0.59	4 (1%) 65 73	12, 33, 52, 69	0
4	2E	204/206 (99%)	0.73	15 (7%) 14 17	29, 55, 68, 76	0
5	1F	203/210 (96%)	0.45	3 (1%) 73 81	13, 35, 60, 77	0
5	2F	203/210 (96%)	0.69	13 (6%) 19 23	31, 61, 75, 79	0
6	1G	181/182 (99%)	0.60	8 (4%) 34 41	34, 52, 66, 76	0
6	2G	181/182 (99%)	0.92	25 (13%) 2 3	57, 70, 78, 92	0
7	1H	174/180 (96%)	0.25	1 (0%) 89 92	31, 45, 57, 63	0
7	2H	174/180 (96%)	1.40	48 (27%) 0 0	63, 76, 84, 89	0
8	1I	146/148 (98%)	0.43	8 (5%) 25 30	38, 64, 75, 80	0
8	2I	146/148 (98%)	0.51	9 (6%) 20 25	53, 65, 74, 78	0
9	1N	140/140 (100%)	0.52	2 (1%) 75 82	18, 31, 51, 68	0
9	2N	140/140 (100%)	1.07	27 (19%) 1 1	43, 59, 70, 82	0
10	1O	122/122 (100%)	0.68	2 (1%) 72 79	20, 34, 51, 57	0
10	2O	122/122 (100%)	0.87	14 (11%) 4 5	43, 55, 65, 67	0
11	1P	149/150 (99%)	0.55	0 100 100	13, 39, 62, 68	0
11	2P	149/150 (99%)	0.99	26 (17%) 1 1	34, 61, 73, 80	0
12	1Q	141/141 (100%)	0.49	1 (0%) 87 91	20, 33, 49, 65	0
12	2Q	141/141 (100%)	1.49	39 (27%) 0 0	43, 61, 71, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.52	0 100 100	16, 27, 43, 55	0
13	2R	118/118 (100%)	0.58	3 (2%) 57 66	36, 49, 58, 62	0
14	1S	110/112 (98%)	0.28	1 (0%) 84 89	29, 40, 52, 58	0
14	2S	110/112 (98%)	0.96	20 (18%) 1 1	52, 63, 75, 79	0
15	1T	131/146 (89%)	0.49	4 (3%) 49 58	26, 38, 61, 66	0
15	2T	131/146 (89%)	0.68	7 (5%) 26 31	45, 57, 72, 74	0
16	1U	116/118 (98%)	0.74	4 (3%) 45 53	14, 23, 36, 60	0
16	2U	116/118 (98%)	1.04	19 (16%) 1 1	38, 57, 70, 78	0
17	1V	101/101 (100%)	0.36	1 (0%) 82 87	13, 31, 48, 62	0
17	2V	101/101 (100%)	0.89	17 (16%) 1 1	43, 64, 72, 77	0
18	1W	112/113 (99%)	0.51	1 (0%) 84 89	16, 24, 43, 70	0
18	2W	112/113 (99%)	0.94	13 (11%) 4 5	37, 46, 60, 75	0
19	1X	95/96 (98%)	0.50	1 (1%) 80 86	17, 29, 48, 68	0
19	2X	95/96 (98%)	0.58	5 (5%) 26 31	41, 53, 65, 70	0
20	1Y	107/110 (97%)	0.54	2 (1%) 66 75	28, 43, 65, 70	0
20	2Y	107/110 (97%)	1.35	23 (21%) 0 0	56, 65, 77, 79	0
21	1Z	154/206 (74%)	0.47	5 (3%) 47 56	29, 56, 81, 89	0
21	2Z	160/206 (77%)	1.18	36 (22%) 0 0	55, 73, 87, 91	0
22	10	83/85 (97%)	1.04	7 (8%) 11 13	20, 28, 53, 69	0
22	20	83/85 (97%)	1.52	24 (28%) 0 0	39, 57, 71, 80	0
23	11	97/98 (98%)	0.83	5 (5%) 27 33	18, 36, 62, 69	0
23	21	97/98 (98%)	1.03	10 (10%) 6 7	30, 52, 69, 74	0
24	12	70/72 (97%)	0.54	1 (1%) 75 82	26, 40, 54, 68	0
24	22	70/72 (97%)	0.62	5 (7%) 16 19	50, 62, 71, 79	0
25	13	59/60 (98%)	0.30	0 100 100	17, 28, 48, 62	0
25	23	59/60 (98%)	1.61	17 (28%) 0 0	50, 61, 75, 82	0
26	14	69/71 (97%)	0.61	8 (11%) 4 5	41, 68, 81, 85	0
26	24	69/71 (97%)	0.81	12 (17%) 1 1	71, 77, 85, 87	0
27	15	59/60 (98%)	0.55	2 (3%) 45 53	12, 24, 44, 55	0
27	25	59/60 (98%)	0.63	5 (8%) 10 13	34, 47, 62, 67	0
28	16	53/54 (98%)	0.45	0 100 100	26, 34, 45, 51	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	1.20	10 (18%) 1 1	42, 53, 63, 70	0
29	17	48/49 (97%)	0.84	5 (10%) 6 7	14, 19, 50, 59	0
29	27	48/49 (97%)	1.46	8 (16%) 1 1	29, 38, 57, 71	0
30	18	64/65 (98%)	0.69	3 (4%) 31 37	18, 26, 35, 52	0
30	28	64/65 (98%)	1.80	26 (40%) 0 0	39, 49, 56, 66	0
31	19	37/37 (100%)	0.86	0 100 100	22, 32, 46, 47	0
31	29	37/37 (100%)	1.39	11 (29%) 0 0	54, 66, 75, 77	0
32	1a	1488/1521 (97%)	0.10	9 (0%) 89 92	29, 57, 83, 98	0
32	2a	1491/1521 (98%)	0.24	52 (3%) 44 52	43, 69, 87, 100	0
33	1b	231/256 (90%)	0.62	23 (9%) 7 7	54, 70, 78, 84	0
33	2b	231/256 (90%)	1.61	75 (32%) 0 0	65, 78, 85, 92	0
34	1c	206/239 (86%)	0.74	18 (8%) 10 12	47, 63, 73, 78	0
34	2c	206/239 (86%)	1.29	56 (27%) 0 0	64, 75, 81, 88	0
35	1d	208/209 (99%)	0.90	28 (13%) 3 3	50, 60, 70, 76	0
35	2d	208/209 (99%)	1.03	36 (17%) 1 1	50, 64, 73, 82	0
36	1e	148/162 (91%)	0.72	18 (12%) 4 4	45, 56, 65, 71	0
36	2e	148/162 (91%)	1.48	47 (31%) 0 0	56, 70, 76, 82	0
37	1f	100/101 (99%)	0.43	2 (2%) 65 73	41, 55, 64, 73	0
37	2f	100/101 (99%)	0.27	2 (2%) 65 73	50, 61, 69, 76	0
38	1g	155/156 (99%)	0.74	22 (14%) 2 3	52, 63, 75, 83	0
38	2g	155/156 (99%)	0.79	28 (18%) 1 1	61, 70, 79, 82	0
39	1h	137/138 (99%)	0.94	22 (16%) 1 1	48, 58, 64, 74	0
39	2h	137/138 (99%)	1.44	36 (26%) 0 0	61, 69, 75, 79	0
40	1i	127/128 (99%)	1.07	29 (22%) 0 0	44, 66, 75, 80	0
40	2i	127/128 (99%)	2.23	66 (51%) 0 0	66, 75, 82, 85	0
41	1j	97/105 (92%)	0.73	15 (15%) 2 2	49, 70, 80, 90	0
41	2j	96/105 (91%)	2.02	38 (39%) 0 0	64, 76, 83, 88	0
42	1k	114/129 (88%)	0.61	5 (4%) 34 41	37, 57, 66, 75	0
42	2k	114/129 (88%)	0.85	13 (11%) 5 5	51, 65, 74, 76	0
43	1l	121/132 (91%)	0.55	7 (5%) 23 28	36, 45, 56, 62	0
43	2l	121/132 (91%)	1.20	25 (20%) 1 1	49, 61, 69, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.94	14 (11%) 5 5	47, 62, 72, 85	0
44	2m	122/126 (96%)	1.84	36 (29%) 0 0	64, 73, 81, 90	0
45	1n	60/61 (98%)	0.93	5 (8%) 11 13	48, 57, 65, 69	0
45	2n	60/61 (98%)	3.70	49 (81%) 0 0	66, 76, 80, 81	0
46	1o	88/89 (98%)	0.95	15 (17%) 1 1	41, 54, 66, 70	0
46	2o	88/89 (98%)	1.32	22 (25%) 0 0	56, 66, 73, 78	0
47	1p	82/88 (93%)	1.61	30 (36%) 0 0	48, 59, 70, 79	0
47	2p	82/88 (93%)	1.11	12 (14%) 2 2	53, 62, 69, 75	0
48	1q	99/105 (94%)	0.93	11 (11%) 5 6	42, 57, 65, 71	0
48	2q	99/105 (94%)	1.71	44 (44%) 0 0	55, 66, 74, 76	0
49	1r	68/88 (77%)	0.67	4 (5%) 22 27	48, 57, 67, 72	0
49	2r	68/88 (77%)	0.70	8 (11%) 4 5	55, 65, 75, 83	0
50	1s	83/93 (89%)	0.45	4 (4%) 30 36	50, 61, 72, 78	0
50	2s	83/93 (89%)	1.85	37 (44%) 0 0	67, 77, 82, 86	0
51	1t	96/106 (90%)	1.07	19 (19%) 1 1	46, 60, 72, 74	0
51	2t	96/106 (90%)	1.19	19 (19%) 1 1	53, 64, 75, 77	0
52	1u	23/27 (85%)	2.22	13 (56%) 0 0	55, 59, 64, 65	0
52	2u	23/27 (85%)	3.35	15 (65%) 0 0	67, 74, 78, 80	0
53	1v	13/27 (48%)	1.87	4 (30%) 0 0	40, 50, 82, 92	0
53	2v	13/27 (48%)	2.52	6 (46%) 0 0	56, 72, 92, 94	0
54	1w	67/76 (88%)	0.90	15 (22%) 0 0	44, 81, 92, 95	0
54	1y	67/76 (88%)	1.09	12 (17%) 1 1	31, 89, 96, 96	0
54	2w	67/76 (88%)	2.00	28 (41%) 0 0	65, 89, 95, 101	0
54	2y	67/76 (88%)	1.28	14 (20%) 1 0	49, 92, 97, 99	0
55	1x	72/77 (93%)	0.15	0 100 100	30, 60, 74, 80	0
55	2x	72/77 (93%)	0.32	6 (8%) 11 13	50, 74, 82, 88	0
All	All	20878/21754 (95%)	0.62	1793 (8%) 10 13	11, 57, 82, 101	0

All (1793) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	21.0
44	2m	124	PRO	20.8

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Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	19.8
44	2m	122	LYS	15.9
44	1m	123	ALA	15.0
33	2b	165	VAL	13.1
45	2n	39	LEU	10.9
22	20	2	ALA	10.5
45	2n	25	VAL	9.9
45	2n	34	TYR	9.6
41	2j	47	PHE	9.5
23	21	2	SER	9.0
52	2u	14	TRP	9.0
22	20	7	LEU	8.7
21	2Z	149	SER	8.5
44	2m	102	ARG	8.1
34	2c	198	VAL	8.1
54	2w	56	C	8.0
44	2m	121	LYS	7.8
40	2i	115	GLY	7.7
33	2b	187	LEU	7.7
41	2j	65	LEU	7.5
54	2w	71	C	7.4
38	1g	79	ARG	7.2
38	1g	80	VAL	7.1
40	2i	66	ARG	7.0
40	2i	125	TYR	7.0
44	2m	6	GLY	7.0
46	2o	87	ILE	7.0
21	2Z	170	THR	6.8
45	2n	42	ILE	6.8
54	2y	36	C	6.7
22	10	7	LEU	6.6
22	20	4	LYS	6.5
33	2b	133	LYS	6.5
7	2H	113	VAL	6.5
29	17	48	LYS	6.5
29	27	47	ARG	6.4
3	1D	276	LYS	6.4
50	2s	84	GLY	6.4
52	2u	17	THR	6.4
53	2v	24	C	6.3
50	2s	83	HIS	6.3
39	2h	83	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
44	2m	120	LYS	6.2
54	2w	1	G	6.2
53	2v	12	A	6.2
33	1b	133	LYS	6.2
40	2i	9	ARG	6.2
34	2c	4	LYS	6.1
39	2h	2	LEU	6.1
35	1d	5	ILE	6.1
41	2j	50	ILE	6.1
54	2w	70	C	6.0
7	2H	105	LEU	6.0
17	2V	73	SER	6.0
3	2D	2	ALA	6.0
52	2u	11	GLY	6.0
40	2i	7	THR	6.0
54	1w	70	C	5.9
52	2u	13	ILE	5.9
41	2j	59	SER	5.9
52	2u	22	ARG	5.9
29	27	1	MET	5.8
34	2c	159	GLY	5.8
54	2w	31	C	5.8
45	2n	24	CYS	5.8
1	1A	2141	G	5.8
22	10	5	LYS	5.8
40	2i	36	TYR	5.8
34	2c	157	ILE	5.7
45	2n	36	PHE	5.7
55	2x	70	G	5.7
53	1v	13	A	5.7
38	1g	156	TRP	5.7
45	2n	35	ARG	5.7
36	2e	12	LEU	5.6
39	2h	99	GLU	5.6
12	2Q	104	PHE	5.6
54	2w	76	A	5.6
38	1g	84	ASN	5.6
36	2e	13	ILE	5.6
41	2j	40	LEU	5.5
45	2n	23	ARG	5.5
45	2n	11	LYS	5.5
11	2P	45	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	2A	2802	G	5.5
39	2h	112	LEU	5.5
52	1u	2	GLY	5.4
23	11	98	LEU	5.4
44	2m	90	LEU	5.4
41	2j	55	LYS	5.4
44	1m	122	LYS	5.4
54	1y	36	C	5.3
50	2s	71	LEU	5.3
44	2m	119	GLY	5.3
46	2o	60	VAL	5.3
34	2c	200	ALA	5.3
39	2h	111	ILE	5.3
7	2H	103	LEU	5.3
40	1i	106	ALA	5.2
41	2j	85	LEU	5.2
45	2n	2	ALA	5.2
44	2m	101	GLN	5.2
12	2Q	37	LEU	5.2
34	2c	193	TYR	5.2
22	10	6	GLY	5.1
41	2j	48	THR	5.1
41	2j	56	HIS	5.1
33	2b	70	PHE	5.1
50	2s	80	TYR	5.1
54	2w	73	A	5.1
38	2g	82	GLY	5.1
34	2c	124	ILE	5.0
54	2w	3	G	5.0
1	2A	2146	C	5.0
33	2b	197	VAL	5.0
43	2l	8	ASN	5.0
1	2A	2112	G	5.0
34	2c	197	GLY	5.0
20	2Y	106	LEU	5.0
45	2n	53	LEU	5.0
45	2n	29	ARG	5.0
33	2b	185	ILE	4.9
26	24	49	PHE	4.9
21	2Z	144	LEU	4.9
26	14	54	GLY	4.9
33	2b	139	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
42	2k	126	ARG	4.9
22	10	3	HIS	4.9
33	2b	188	ALA	4.9
27	15	60	VAL	4.9
29	27	48	LYS	4.9
44	2m	87	TYR	4.8
17	2V	72	VAL	4.8
38	2g	16	LEU	4.8
34	2c	149	ALA	4.8
24	22	1	MET	4.8
45	2n	37	PHE	4.8
52	2u	18	TYR	4.8
26	24	56	VAL	4.8
51	2t	24	LEU	4.8
22	20	3	HIS	4.8
40	2i	77	ILE	4.8
52	2u	15	ARG	4.7
36	2e	110	LEU	4.7
40	2i	14	VAL	4.7
46	1o	57	LEU	4.7
36	2e	133	TYR	4.7
39	1h	92	ARG	4.7
43	2l	15	ARG	4.7
33	2b	48	MET	4.7
1	2A	2111	C	4.7
33	2b	129	GLU	4.7
41	2j	51	ARG	4.7
35	2d	164	ALA	4.7
17	2V	71	LEU	4.7
1	2A	888	C	4.7
40	2i	114	TYR	4.7
42	2k	25	TYR	4.7
7	2H	107	VAL	4.7
21	2Z	140	ASP	4.7
34	2c	188	LEU	4.6
40	2i	65	VAL	4.6
53	2v	14	A	4.6
26	24	50	VAL	4.6
33	2b	93	VAL	4.6
48	2q	37	LYS	4.6
21	2Z	150	LEU	4.6
32	2a	1257	U	4.6

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Mol	Chain	Res	Type	RSRZ
36	2e	90	VAL	4.6
21	1Z	168	GLU	4.6
32	2a	1532	U	4.6
35	1d	8	VAL	4.6
38	2g	80	VAL	4.6
33	2b	97	TRP	4.6
1	2A	1026	U	4.6
7	2H	55	PRO	4.5
3	1D	2	ALA	4.5
36	2e	86	ALA	4.5
45	2n	41	ARG	4.5
45	2n	6	LEU	4.5
54	2y	1	G	4.5
1	2A	2896	C	4.5
54	1w	71	C	4.5
33	2b	120	ALA	4.5
41	2j	58	ASP	4.5
36	2e	31	LEU	4.5
50	2s	69	HIS	4.4
22	20	8	GLY	4.4
6	2G	146	TYR	4.4
30	28	29	LYS	4.4
32	2a	1030(A)	G	4.4
43	2l	32	PHE	4.4
33	2b	95	GLN	4.4
36	2e	82	VAL	4.4
39	2h	129	VAL	4.4
34	2c	6	HIS	4.4
12	2Q	66	ILE	4.4
7	2H	169	VAL	4.3
17	2V	75	PHE	4.3
36	2e	89	ILE	4.3
52	1u	14	TRP	4.3
29	17	46	VAL	4.3
45	2n	55	GLY	4.3
8	2I	1	MET	4.3
36	2e	123	LEU	4.3
6	2G	49	ASP	4.3
45	2n	44	LEU	4.3
54	2w	13	C	4.3
45	2n	38	GLY	4.3
1	2A	2117	A	4.2

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Mol	Chain	Res	Type	RSRZ
32	2a	80	G	4.2
29	27	46	VAL	4.2
52	2u	16	GLY	4.2
16	2U	17	ILE	4.2
12	2Q	103	MET	4.2
33	2b	81	VAL	4.2
45	2n	26	ARG	4.2
19	2X	69	TYR	4.2
53	2v	13	A	4.2
39	2h	128	GLY	4.2
50	2s	59	PRO	4.2
32	2a	1202	G	4.2
33	2b	164	VAL	4.2
7	2H	56	SER	4.2
54	2w	4	U	4.2
33	2b	114	ARG	4.2
41	2j	46	ARG	4.2
46	2o	64	ARG	4.2
41	2j	63	PHE	4.2
39	1h	3	THR	4.2
35	1d	70	ILE	4.2
47	2p	19	ILE	4.2
47	1p	19	ILE	4.1
54	2w	72	C	4.1
21	2Z	148	ASP	4.1
50	2s	40	ILE	4.1
8	2I	12	LEU	4.1
25	23	26	LEU	4.1
6	1G	139	LEU	4.1
45	2n	7	ILE	4.1
32	1a	1531	A	4.1
45	2n	50	LYS	4.1
21	2Z	139	VAL	4.1
41	2j	66	ARG	4.1
41	2j	11	PHE	4.1
33	2b	118	LEU	4.1
44	1m	96	LEU	4.1
10	2O	1	MET	4.1
36	2e	84	PHE	4.1
7	2H	148	ILE	4.1
51	2t	80	ARG	4.1
43	2l	18	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
45	2n	56	VAL	4.1
16	1U	117	GLN	4.1
30	28	41	ILE	4.0
48	1q	35	VAL	4.0
7	2H	159	GLU	4.0
34	2c	152	ILE	4.0
38	1g	154	TYR	4.0
33	2b	135	GLN	4.0
33	2b	215	LEU	4.0
28	26	54	ILE	4.0
54	2y	2	G	4.0
6	2G	34	LEU	4.0
33	2b	221	LEU	4.0
48	2q	9	VAL	4.0
20	2Y	105	ALA	4.0
25	23	60	GLU	4.0
35	1d	157	LEU	4.0
36	2e	120	THR	4.0
23	11	2	SER	4.0
48	2q	90	ILE	4.0
38	1g	83	ALA	4.0
34	2c	2	GLY	4.0
52	2u	6	ARG	4.0
35	1d	104	VAL	4.0
40	2i	128	ARG	3.9
1	2A	2113	U	3.9
43	1l	7	ILE	3.9
1	2A	2155	G	3.9
40	1i	113	LYS	3.9
40	2i	33	PHE	3.9
38	2g	4	ARG	3.9
45	2n	31	ARG	3.9
20	2Y	5	MET	3.9
39	2h	3	THR	3.9
46	2o	31	LEU	3.9
47	1p	6	LEU	3.9
6	2G	133	LEU	3.9
40	2i	4	TYR	3.9
40	2i	71	SER	3.9
9	2N	8	GLN	3.9
21	2Z	137	ILE	3.9
36	2e	131	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
48	1q	36	ILE	3.9
54	1y	33	U	3.9
7	2H	96	ALA	3.9
43	2l	55	VAL	3.9
45	2n	22	THR	3.9
39	1h	133	LEU	3.9
31	29	37	GLY	3.9
1	1A	2132	U	3.9
32	2a	1030(B)	C	3.9
1	2A	2154	G	3.9
6	2G	136	ARG	3.9
51	2t	62	LEU	3.9
40	2i	64	THR	3.9
26	24	67	TYR	3.9
54	2w	75	C	3.9
34	2c	160	ALA	3.8
44	2m	104	ARG	3.8
46	2o	68	ARG	3.8
39	2h	9	MET	3.8
40	2i	72	GLY	3.8
38	1g	85	TYR	3.8
3	2D	276	LYS	3.8
30	28	16	ILE	3.8
34	1c	14	ILE	3.8
41	1j	98	ILE	3.8
44	2m	5	ALA	3.8
44	2m	7	VAL	3.8
20	1Y	1	MET	3.8
33	2b	163	PHE	3.8
43	2l	7	ILE	3.8
33	2b	149	LEU	3.8
40	2i	17	VAL	3.8
40	2i	79	LEU	3.8
1	2A	2147	G	3.8
10	2O	65	THR	3.8
50	2s	79	THR	3.8
20	2Y	1	MET	3.8
54	2w	74	C	3.8
1	1A	1026	U	3.8
34	2c	186	PHE	3.8
40	1i	77	ILE	3.8
40	2i	28	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2118	U	3.8
33	2b	201	ILE	3.8
34	2c	154	SER	3.8
1	1A	2142	C	3.8
20	2Y	24	VAL	3.8
38	1g	78	ARG	3.8
22	10	4	LYS	3.8
29	17	47	ARG	3.7
38	1g	34	GLY	3.8
22	10	2	ALA	3.7
7	2H	35	VAL	3.7
52	2u	5	ASP	3.7
47	2p	1	MET	3.7
45	2n	51	GLY	3.7
35	1d	4	TYR	3.7
44	2m	23	TYR	3.7
41	2j	87	THR	3.7
45	2n	27	CYS	3.7
12	2Q	1	MET	3.7
25	23	17	LYS	3.7
35	1d	3	ARG	3.7
45	2n	45	ARG	3.7
46	2o	61	GLY	3.7
50	2s	30	LEU	3.7
34	2c	184	TYR	3.7
55	2x	72	A	3.7
41	2j	49	VAL	3.7
16	2U	43	GLY	3.7
54	2w	2	G	3.7
39	2h	13	ILE	3.7
44	2m	65	LYS	3.7
14	2S	3	ARG	3.7
45	2n	12	ARG	3.7
50	2s	78	ARG	3.7
40	2i	10	ARG	3.7
52	1u	21	TYR	3.7
34	2c	199	LYS	3.7
36	2e	20	GLN	3.7
48	2q	100	LYS	3.7
40	1i	19	LEU	3.7
34	2c	201	TYR	3.7
43	2l	39	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
40	1i	70	LYS	3.7
36	2e	125	SER	3.7
11	2P	51	PHE	3.6
41	2j	54	PHE	3.6
41	2j	62	HIS	3.6
40	2i	52	ALA	3.6
32	1a	1257	U	3.6
39	2h	93	VAL	3.6
7	2H	6	ARG	3.6
6	2G	139	LEU	3.6
5	2F	49	ALA	3.6
54	2w	32	C	3.6
7	2H	165	ALA	3.6
44	2m	76	ALA	3.6
50	2s	82	GLY	3.6
34	2c	182	ILE	3.6
45	2n	58	LYS	3.6
46	2o	32	LEU	3.6
22	20	6	GLY	3.6
34	2c	155	GLY	3.6
38	1g	81	GLY	3.6
35	1d	122	ARG	3.6
35	2d	49	ARG	3.6
12	2Q	38	GLU	3.6
34	2c	10	PHE	3.6
26	14	45	GLY	3.6
12	2Q	6	ARG	3.6
41	2j	44	VAL	3.6
48	2q	36	ILE	3.6
46	2o	72	ARG	3.6
21	2Z	171	ILE	3.6
33	2b	210	SER	3.6
1	2A	2174	C	3.6
48	2q	88	TYR	3.6
35	1d	21	LEU	3.6
40	2i	127	LYS	3.6
38	2g	27	ILE	3.6
50	2s	70	LYS	3.6
1	2A	2145	C	3.6
53	1v	24	C	3.6
1	2A	2132	U	3.5
33	2b	34	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
7	2H	114	VAL	3.5
36	1e	82	VAL	3.5
11	2P	30	THR	3.5
32	2a	965	A	3.5
54	2w	57	G	3.5
26	14	59	PHE	3.5
9	2N	44	PRO	3.5
23	21	26	ARG	3.5
33	2b	222	ILE	3.5
45	2n	13	THR	3.5
52	2u	10	ARG	3.5
9	2N	116	LEU	3.5
22	20	5	LYS	3.5
14	2S	20	ARG	3.5
33	2b	137	ARG	3.5
50	2s	38	SER	3.5
54	2y	73	A	3.5
23	11	70	VAL	3.5
35	1d	2	GLY	3.5
51	2t	41	ILE	3.5
1	2A	2897	U	3.5
16	2U	20	LEU	3.5
40	2i	62	TYR	3.5
39	2h	35	ILE	3.5
50	1s	71	LEU	3.5
33	2b	152	PHE	3.5
33	2b	92	TYR	3.5
21	2Z	169	GLU	3.5
41	2j	98	ILE	3.5
52	1u	17	THR	3.5
23	11	97	LEU	3.5
12	2Q	65	PHE	3.5
21	2Z	121	HIS	3.5
32	2a	974	A	3.5
33	1b	130	ARG	3.5
40	1i	121	ARG	3.5
42	1k	126	ARG	3.5
54	1w	56	C	3.5
10	2O	7	TYR	3.5
25	23	51	ALA	3.5
40	1i	8	GLY	3.5
40	1i	30	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
45	2n	30	ALA	3.5
6	2G	29	TRP	3.4
47	1p	28	ARG	3.5
33	2b	140	HIS	3.4
8	1I	1	MET	3.4
32	2a	1116	C	3.4
32	2a	1286	A	3.4
52	2u	21	TYR	3.4
55	2x	71	C	3.4
30	28	35	GLN	3.4
13	2R	68	ARG	3.4
28	26	10	LEU	3.4
28	26	11	LEU	3.4
35	2d	78	LEU	3.4
41	2j	41	PRO	3.4
6	2G	159	VAL	3.4
33	1b	214	ILE	3.4
39	1h	134	ILE	3.4
7	2H	2	SER	3.4
45	2n	17	LYS	3.4
51	2t	59	ALA	3.4
35	2d	160	GLN	3.4
33	1b	131	PRO	3.4
44	2m	97	PRO	3.4
33	2b	71	VAL	3.4
44	2m	103	THR	3.4
46	1o	66	LEU	3.4
36	1e	89	ILE	3.4
34	2c	13	GLY	3.4
38	2g	81	GLY	3.4
45	2n	15	LYS	3.4
21	2Z	96	VAL	3.4
21	2Z	151	HIS	3.4
45	2n	49	HIS	3.4
32	2a	873	A	3.4
8	2I	19	VAL	3.4
21	2Z	126	VAL	3.4
41	1j	72	VAL	3.4
34	2c	202	ILE	3.4
5	2F	62	ARG	3.4
36	2e	81	GLU	3.4
51	2t	73	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
45	2n	61	TRP	3.4
1	2A	2119	A	3.4
51	1t	38	LYS	3.4
41	2j	53	PRO	3.4
21	2Z	145	GLU	3.4
35	2d	70	ILE	3.4
41	2j	38	ILE	3.4
51	1t	80	ARG	3.4
16	2U	39	LEU	3.4
35	1d	120	LEU	3.4
7	2H	49	VAL	3.4
7	2H	97	ARG	3.4
33	2b	101	MET	3.3
11	2P	23	PRO	3.3
18	2W	92	ARG	3.3
47	2p	39	TYR	3.3
8	1I	3	VAL	3.3
50	2s	41	VAL	3.3
51	2t	63	ILE	3.3
33	2b	94	ASN	3.3
51	1t	9	ASN	3.3
54	2w	19	G	3.3
7	2H	41	MET	3.3
50	2s	81	ARG	3.3
33	2b	200	ILE	3.3
39	2h	6	ILE	3.3
32	2a	1285	A	3.3
40	2i	82	ALA	3.3
4	2E	115	GLY	3.3
9	2N	83	LYS	3.3
43	2l	13	LYS	3.3
9	2N	9	VAL	3.3
36	2e	100	VAL	3.3
7	2H	123	PHE	3.3
51	1t	74	LYS	3.3
21	2Z	160	GLY	3.3
32	2a	1224	G	3.3
40	2i	76	ALA	3.3
44	2m	66	LEU	3.3
33	2b	147	LYS	3.3
51	1t	83	ARG	3.3
12	2Q	47	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
33	2b	214	ILE	3.3
54	2w	39	G	3.3
40	1i	65	VAL	3.3
40	2i	63	ILE	3.3
18	2W	86	LEU	3.3
32	2a	1033	G	3.3
47	1p	1	MET	3.3
40	1i	128	ARG	3.3
25	23	25	ALA	3.2
33	1b	187	LEU	3.2
33	2b	232	PRO	3.2
54	1y	21	A	3.2
45	2n	47	LEU	3.2
12	2Q	33	GLY	3.2
14	2S	33	LYS	3.2
31	29	15	LYS	3.2
35	2d	93	PHE	3.2
6	1G	73	ALA	3.2
41	2j	18	ALA	3.2
8	1I	35	LEU	3.2
12	2Q	39	PRO	3.2
14	2S	32	LEU	3.2
40	2i	123	PRO	3.2
49	1r	31	LEU	3.2
40	1i	14	VAL	3.2
44	2m	98	VAL	3.2
16	2U	47	TYR	3.2
45	2n	21	TYR	3.2
54	1y	24	G	3.2
33	2b	77	ALA	3.2
48	2q	53	LEU	3.2
51	2t	72	LEU	3.2
25	23	54	VAL	3.2
50	2s	52	TYR	3.2
33	2b	123	ALA	3.2
1	2A	2140	C	3.2
38	1g	99	LEU	3.2
39	1h	2	LEU	3.2
44	2m	92	HIS	3.2
39	2h	97	VAL	3.2
41	2j	60	ARG	3.2
15	2T	110	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
34	1c	193	TYR	3.2
45	1n	2	ALA	3.2
15	2T	99	LEU	3.2
6	2G	28	VAL	3.2
9	2N	122	VAL	3.2
33	2b	28	PHE	3.2
9	2N	75	TYR	3.2
31	29	19	ARG	3.2
17	2V	79	VAL	3.2
25	23	47	VAL	3.2
47	1p	2	VAL	3.2
48	2q	23	VAL	3.2
32	2a	1032	G	3.2
38	2g	154	TYR	3.2
40	2i	106	ALA	3.2
39	2h	131	GLY	3.2
40	2i	30	GLY	3.2
44	1m	106	ASN	3.2
40	1i	120	ARG	3.2
41	2j	9	ARG	3.2
7	2H	133	VAL	3.1
48	2q	21	VAL	3.1
32	2a	1223	C	3.1
48	2q	32	TYR	3.1
50	2s	56	GLN	3.1
36	2e	10	MET	3.1
3	2D	205	VAL	3.1
12	2Q	22	LYS	3.1
40	1i	112	LYS	3.1
53	1v	12	A	3.1
5	2F	181	LEU	3.1
32	1a	1027	C	3.1
36	2e	107	ARG	3.1
36	2e	126	ARG	3.1
40	2i	67	GLY	3.1
33	2b	31	TYR	3.1
41	1j	65	LEU	3.1
45	2n	46	GLU	3.1
14	2S	5	THR	3.1
48	2q	5	VAL	3.1
29	27	31	LEU	3.1
34	2c	196	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
39	2h	132	GLU	3.1
45	2n	10	ALA	3.1
43	2l	5	PRO	3.1
54	1y	38	A	3.1
44	2m	109	THR	3.1
1	1A	1176	G	3.1
9	2N	84	LYS	3.1
34	1c	182	ILE	3.1
35	2d	162	LEU	3.1
38	2g	7	ALA	3.1
17	2V	81	TYR	3.1
35	2d	122	ARG	3.1
44	1m	102	ARG	3.1
12	2Q	35	VAL	3.1
48	2q	11	VAL	3.1
9	2N	91	LEU	3.1
30	28	61	LEU	3.1
34	2c	148	GLY	3.1
8	2I	92	VAL	3.1
33	1b	81	VAL	3.1
33	1b	136	VAL	3.1
4	2E	157	ALA	3.1
16	2U	35	ALA	3.1
33	2b	138	LEU	3.1
25	23	29	ARG	3.1
1	2A	2125	G	3.1
30	28	21	LYS	3.1
16	2U	40	PHE	3.1
1	2A	884	C	3.1
46	1o	67	LEU	3.1
3	2D	271	ILE	3.1
12	2Q	99	PRO	3.1
33	2b	131	PRO	3.1
47	1p	17	TYR	3.0
26	24	54	GLY	3.0
6	2G	109	VAL	3.0
7	2H	141	VAL	3.0
54	2w	18	G	3.0
21	2Z	51	ALA	3.0
39	2h	84	ARG	3.0
40	2i	12	GLU	3.0
40	2i	15	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
51	1t	86	ARG	3.0
26	14	55	ARG	3.0
12	2Q	20	ALA	3.0
17	1V	77	ALA	3.0
1	1A	2151	G	3.0
54	1w	61	C	3.0
5	2F	90	PHE	3.0
54	1w	76	A	3.0
47	1p	48	TRP	3.0
47	1p	7	ALA	3.0
34	2c	185	GLY	3.0
35	2d	98	GLU	3.0
36	1e	81	GLU	3.0
47	1p	32	TYR	3.0
42	2k	87	THR	3.0
1	2A	1847	A	3.0
32	2a	1196	U	3.0
49	1r	78	LEU	3.0
20	2Y	77	PRO	3.0
3	1D	275	LYS	3.0
4	2E	77	ILE	3.0
39	1h	86	ILE	3.0
41	2j	74	ILE	3.0
48	2q	59	ILE	3.0
9	2N	45	ASN	3.0
39	2h	31	PHE	3.0
41	1j	47	PHE	3.0
52	1u	18	TYR	3.0
1	2A	2115	G	3.0
5	2F	89	VAL	3.0
7	2H	144	VAL	3.0
40	2i	109	VAL	3.0
54	2w	40	G	3.0
14	2S	58	LEU	3.0
30	28	34	TRP	3.0
34	2c	33	LEU	3.0
34	2c	178	LEU	3.0
40	2i	80	GLY	3.0
54	1y	47	U	3.0
39	1h	6	ILE	3.0
26	24	63	TYR	3.0
48	2q	27	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
39	1h	103	VAL	3.0
43	1l	11	VAL	3.0
49	1r	79	LEU	3.0
50	2s	37	ARG	3.0
11	2P	39	LYS	3.0
14	2S	11	LYS	3.0
48	2q	71	PHE	3.0
40	2i	110	GLU	3.0
54	2w	61	C	2.9
23	21	60	PHE	2.9
9	2N	72	TYR	2.9
14	2S	17	ARG	2.9
48	2q	35	VAL	2.9
17	2V	74	LYS	2.9
28	26	20	ASN	2.9
50	1s	40	ILE	2.9
20	2Y	90	LEU	2.9
38	2g	79	ARG	2.9
51	2t	13	LEU	2.9
52	1u	6	ARG	2.9
7	2H	125	VAL	2.9
18	2W	85	VAL	2.9
32	2a	1531	A	2.9
40	2i	119	ALA	2.9
35	2d	158	ILE	2.9
1	2A	2144	U	2.9
33	2b	144	ARG	2.9
54	1w	72	C	2.9
7	2H	98	LEU	2.9
38	1g	38	LEU	2.9
46	2o	67	LEU	2.9
40	2i	41	VAL	2.9
47	1p	41	PRO	2.9
21	2Z	154	ASP	2.9
40	2i	42	ARG	2.9
43	1l	91	LYS	2.9
40	1i	115	GLY	2.9
41	2j	10	GLY	2.9
54	2w	47	U	2.9
6	2G	149	VAL	2.9
33	1b	165	VAL	2.9
43	1l	90	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
39	2h	136	GLU	2.9
1	1A	2152	G	2.9
10	2O	2	ILE	2.9
35	2d	47	ARG	2.9
38	1g	153	HIS	2.9
51	1t	22	ARG	2.9
40	2i	126	SER	2.9
19	2X	66	LEU	2.9
46	2o	56	LEU	2.9
48	2q	22	LEU	2.9
7	2H	24	VAL	2.9
33	1b	126	GLU	2.9
48	2q	42	TYR	2.9
35	2d	134	ASP	2.9
51	2t	9	ASN	2.9
40	2i	117	HIS	2.9
36	2e	129	ILE	2.9
39	2h	134	ILE	2.9
50	2s	49	ILE	2.9
33	2b	17	PHE	2.9
22	20	75	LEU	2.9
32	2a	570	G	2.9
1	2A	229	A	2.9
43	2l	47	LYS	2.9
52	1u	12	LYS	2.9
20	2Y	7	VAL	2.9
20	2Y	78	ALA	2.9
26	24	68	ARG	2.9
38	2g	32	ARG	2.9
39	2h	82	HIS	2.9
40	2i	124	GLN	2.9
11	2P	73	GLY	2.9
32	2a	879	C	2.9
39	2h	86	ILE	2.9
47	2p	9	PHE	2.9
51	1t	29	LYS	2.9
50	2s	5	LEU	2.9
1	1A	2190	G	2.9
14	2S	13	ARG	2.9
40	1i	119	ALA	2.9
38	1g	82	GLY	2.8
43	2l	27	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
21	2Z	82	ARG	2.8
47	1p	8	ARG	2.8
12	2Q	102	VAL	2.8
48	2q	87	LYS	2.8
54	1y	39	G	2.8
30	28	58	ILE	2.8
36	2e	109	ILE	2.8
42	2k	29	ILE	2.8
47	1p	36	ILE	2.8
11	2P	79	ARG	2.8
12	2Q	17	LEU	2.8
32	2a	89	C	2.8
34	1c	15	THR	2.8
20	2Y	29	GLU	2.8
30	28	10	ALA	2.8
40	2i	61	ALA	2.8
43	1l	43	VAL	2.8
48	2q	28	PRO	2.8
10	2O	25	LEU	2.8
48	2q	6	LEU	2.8
51	1t	20	LEU	2.8
51	1t	84	LEU	2.8
47	1p	29	ASP	2.8
1	2A	2143	C	2.8
4	2E	116	VAL	2.8
23	21	28	GLY	2.8
36	2e	134	ALA	2.8
28	26	21	TYR	2.8
36	2e	11	ILE	2.8
39	1h	83	ILE	2.8
40	2i	105	ASP	2.8
11	2P	32	THR	2.8
22	20	52	GLY	2.8
12	2Q	36	ALA	2.8
28	26	52	VAL	2.8
1	1A	2145	C	2.8
1	2A	2803	C	2.8
7	2H	3	ARG	2.8
38	1g	32	ARG	2.8
44	2m	94	ARG	2.8
54	1y	32	C	2.8
54	2y	61	C	2.8

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Mol	Chain	Res	Type	RSRZ
17	2V	80	GLN	2.8
33	1b	222	ILE	2.8
33	2b	80	ILE	2.8
35	2d	206	PHE	2.8
1	1A	2189	U	2.8
20	2Y	12	THR	2.8
8	2I	3	VAL	2.8
24	12	69	ARG	2.8
31	29	1	MET	2.8
36	2e	21	ALA	2.8
43	2l	48	PRO	2.8
44	1m	117	VAL	2.8
38	1g	3	ARG	2.8
46	2o	65	ARG	2.8
8	2I	29	TYR	2.8
54	2y	39	G	2.8
26	24	51	ASP	2.8
8	2I	35	LEU	2.8
33	1b	61	LEU	2.8
39	2h	135	CYS	2.8
46	1o	34	LEU	2.8
48	1q	90	ILE	2.8
34	2c	158	GLY	2.8
39	1h	90	GLY	2.8
44	1m	105	THR	2.8
4	2E	131	ALA	2.8
16	2U	42	ALA	2.8
25	23	21	ALA	2.8
34	2c	7	PRO	2.8
38	2g	156	TRP	2.8
32	2a	1117	G	2.8
34	2c	39	ILE	2.8
39	1h	112	LEU	2.8
3	2D	217	ARG	2.8
6	2G	115	ARG	2.8
15	2T	60	THR	2.8
50	2s	36	ARG	2.8
34	2c	37	GLN	2.7
12	2Q	32	TYR	2.7
3	2D	5	LYS	2.7
33	2b	55	PHE	2.7
33	2b	98	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
33	2b	145	LEU	2.7
36	2e	121	LYS	2.7
39	1h	119	LEU	2.7
41	2j	57	LYS	2.7
47	2p	80	PHE	2.7
7	2H	95	ARG	2.7
39	2h	92	ARG	2.7
48	2q	38	ARG	2.7
54	2y	57	G	2.7
29	17	45	ALA	2.7
47	1p	16	HIS	2.7
14	2S	57	LYS	2.7
33	1b	132	LYS	2.7
52	1u	3	LYS	2.7
26	24	45	GLY	2.7
31	29	24	TYR	2.7
44	1m	87	TYR	2.7
34	2c	30	ARG	2.7
51	2t	83	ARG	2.7
35	2d	146	ILE	2.7
17	2V	77	ALA	2.7
30	28	2	PRO	2.7
33	1b	232	PRO	2.7
1	2A	2585	U	2.7
14	2S	29	PHE	2.7
14	2S	92	TYR	2.7
21	2Z	155	LEU	2.7
32	2a	1150	U	2.7
34	2c	167	TRP	2.7
30	28	63	PRO	2.7
45	2n	14	PRO	2.7
18	2W	47	VAL	2.7
6	2G	48	GLU	2.7
46	1o	81	LEU	2.7
47	2p	6	LEU	2.7
54	1w	47	U	2.7
18	2W	96	ILE	2.7
44	2m	105	THR	2.7
16	2U	2	PRO	2.7
31	29	12	ASP	2.7
45	2n	60	SER	2.7
52	2u	23	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
45	2n	18	VAL	2.7
34	2c	190	ARG	2.7
41	1j	46	ARG	2.7
44	2m	88	ARG	2.7
4	1E	195	LEU	2.7
12	2Q	18	LYS	2.7
12	2Q	63	LYS	2.7
40	2i	78	LYS	2.7
47	1p	73	LEU	2.7
51	1t	14	LYS	2.7
32	2a	1321	C	2.7
17	2V	70	ILE	2.7
16	2U	50	ARG	2.7
23	21	68	PRO	2.7
33	1b	13	ALA	2.7
36	2e	24	ARG	2.7
40	2i	93	ARG	2.7
45	1n	57	ARG	2.7
50	2s	50	ALA	2.7
40	2i	108	VAL	2.7
19	2X	33	LYS	2.7
36	2e	88	LYS	2.7
40	2i	8	GLY	2.7
4	2E	151	TYR	2.7
35	2d	54	TYR	2.7
6	2G	39	ILE	2.7
34	1c	39	ILE	2.7
39	2h	4	ASP	2.7
45	2n	57	ARG	2.7
1	2A	2173	A	2.7
38	2g	152	ALA	2.7
45	2n	4	LYS	2.7
4	2E	125	GLY	2.7
1	2A	2149	G	2.7
25	23	6	VAL	2.7
25	23	50	VAL	2.7
32	2a	1001(A)	G	2.7
54	2w	5	G	2.7
54	2w	22	G	2.7
4	2E	195	LEU	2.7
24	22	60	LEU	2.7
33	2b	69	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
36	2e	119	LEU	2.7
39	2h	127	LEU	2.7
43	2l	10	LEU	2.7
10	2O	19	ILE	2.7
46	1o	87	ILE	2.7
12	2Q	129	THR	2.7
22	20	9	SER	2.7
30	28	37	SER	2.7
1	2A	2128	C	2.6
21	2Z	172	ALA	2.6
30	18	2	PRO	2.6
54	1w	4	U	2.6
39	1h	93	VAL	2.6
1	2A	896	A	2.6
12	2Q	79	LEU	2.6
35	1d	19	LEU	2.6
36	1e	139	LEU	2.6
40	2i	85	LEU	2.6
50	2s	16	LEU	2.6
32	2a	1516	G	2.6
20	2Y	55	TYR	2.6
39	2h	94	TYR	2.6
46	1o	36	ILE	2.6
51	2t	55	ILE	2.6
34	1c	78	GLY	2.6
34	2c	81	GLY	2.6
40	1i	117	HIS	2.6
50	2s	45	VAL	2.6
54	2y	64	U	2.6
32	2a	795	C	2.6
39	2h	133	LEU	2.6
41	2j	61	GLU	2.6
1	1A	1077	A	2.6
33	1b	137	ARG	2.6
29	27	27	GLY	2.6
54	1w	1	G	2.6
10	2O	41	ALA	2.6
48	2q	29	HIS	2.6
4	2E	52	LEU	2.6
44	2m	99	ARG	2.6
50	1s	78	ARG	2.6
49	2r	43	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
6	1G	88	ILE	2.6
31	29	17	ILE	2.6
34	2c	23	TYR	2.6
35	1d	158	ILE	2.6
40	1i	125	TYR	2.6
43	2l	64	TYR	2.6
30	28	15	LYS	2.6
41	1j	20	ALA	2.6
7	2H	115	VAL	2.6
30	28	23	VAL	2.6
32	2a	973	G	2.6
40	2i	121	ARG	2.6
47	1p	25	ARG	2.6
48	2q	10	VAL	2.6
7	2H	88	LEU	2.6
12	2Q	125	LEU	2.6
19	2X	92	LEU	2.6
51	1t	72	LEU	2.6
36	2e	45	PHE	2.6
44	2m	69	GLU	2.6
45	1n	50	LYS	2.6
48	2q	40	LYS	2.6
54	2w	38	A	2.6
5	1F	89	VAL	2.6
40	1i	109	VAL	2.6
9	2N	112	LEU	2.6
12	2Q	2	LEU	2.6
29	17	1	MET	2.6
35	2d	19	LEU	2.6
44	2m	82	MET	2.6
39	2h	87	SER	2.6
21	2Z	57	ILE	2.6
46	1o	68	ARG	2.6
51	1t	71	THR	2.6
54	1y	56	C	2.6
21	2Z	141	VAL	2.6
46	2o	27	VAL	2.6
47	1p	76	GLN	2.6
40	2i	102	LEU	2.6
50	2s	12	ASP	2.6
23	21	29	GLY	2.6
34	2c	194	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
38	1g	26	PHE	2.6
52	1u	16	GLY	2.6
1	1A	2125	G	2.6
33	2b	111	ARG	2.6
38	1g	155	ARG	2.6
34	1c	202	ILE	2.6
34	2c	14	ILE	2.6
47	1p	13	HIS	2.6
1	1A	884	C	2.6
3	2D	155	LEU	2.6
35	1d	78	LEU	2.6
43	2l	16	GLU	2.6
40	2i	37	PHE	2.6
50	2s	66	MET	2.6
29	27	23	ARG	2.6
45	1n	23	ARG	2.6
46	1o	65	ARG	2.6
3	1D	203	ASN	2.5
7	2H	89	ILE	2.5
16	1U	17	ILE	2.5
41	2j	42	THR	2.5
33	2b	186	ALA	2.5
36	1e	17	ALA	2.5
6	1G	146	TYR	2.5
32	2a	1021	G	2.5
13	2R	69	ASP	2.5
15	2T	114	LEU	2.5
22	20	67	VAL	2.5
31	29	16	VAL	2.5
35	2d	64	LEU	2.5
11	2P	1	MET	2.5
22	20	44	ARG	2.5
48	2q	91	ARG	2.5
43	2l	91	LYS	2.5
34	2c	174	PRO	2.5
41	2j	15	THR	2.5
42	2k	117	ASN	2.5
6	2G	169	ALA	2.5
54	1y	35	A	2.5
7	2H	52	VAL	2.5
12	2Q	34	LEU	2.5
27	25	58	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
22	20	55	ARG	2.5
12	2Q	69	PHE	2.5
32	1a	1030(C)	G	2.5
41	1j	60	ARG	2.5
32	2a	1320	C	2.5
7	2H	145	ALA	2.5
30	28	59	LYS	2.5
32	2a	1358	U	2.5
33	1b	221	LEU	2.5
44	1m	60	VAL	2.5
49	2r	66	LEU	2.5
51	2t	84	LEU	2.5
52	2u	12	LYS	2.5
55	2x	76	A	2.5
5	2F	56	GLU	2.5
32	2a	823	G	2.5
1	1A	1064	C	2.5
38	2g	24	THR	2.5
45	2n	54	PRO	2.5
52	2u	24	ARG	2.5
10	2O	8	LEU	2.5
16	2U	24	TYR	2.5
33	2b	184	VAL	2.5
35	2d	157	LEU	2.5
51	1t	18	GLN	2.5
48	2q	58	GLU	2.5
34	2c	164	ARG	2.5
1	2A	2100	G	2.5
16	2U	41	ALA	2.5
35	2d	209	ARG	2.5
38	2g	83	ALA	2.5
40	1i	82	ALA	2.5
52	1u	15	ARG	2.5
18	2W	103	ILE	2.5
40	2i	68	GLY	2.5
35	1d	11	LEU	2.5
35	1d	135	LEU	2.5
30	28	65	GLU	2.5
36	2e	115	VAL	2.5
47	1p	39	TYR	2.5
3	2D	6	PHE	2.5
33	2b	122	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
48	2q	82	MET	2.5
3	2D	38	LYS	2.5
47	1p	5	ARG	2.5
51	1t	79	ARG	2.5
9	2N	43	THR	2.5
27	15	2	ALA	2.5
40	2i	81	ILE	2.5
1	1A	1509	C	2.5
7	2H	43	VAL	2.5
42	2k	109	VAL	2.5
47	2p	2	VAL	2.5
1	1A	2112	G	2.5
26	24	43	TYR	2.5
32	2a	112	G	2.5
47	2p	17	TYR	2.5
14	2S	9	ARG	2.5
34	2c	179	ARG	2.5
41	1j	45	ARG	2.5
47	1p	66	PRO	2.5
48	1q	28	PRO	2.5
1	2A	2170	A	2.5
21	2Z	124	ILE	2.5
32	2a	969	A	2.5
41	2j	71	LEU	2.5
48	2q	84	LEU	2.5
54	2y	66	A	2.5
3	1D	113	VAL	2.5
36	2e	105	VAL	2.5
21	2Z	99	TYR	2.5
37	2f	59	TYR	2.5
42	1k	125	PHE	2.5
45	1n	16	PHE	2.5
41	1j	66	ARG	2.5
32	2a	1222	G	2.5
1	1A	271(K)	U	2.4
10	2O	27	GLY	2.4
14	2S	8	GLU	2.4
35	1d	7	PRO	2.4
3	2D	59	LYS	2.4
36	1e	134	ALA	2.4
5	2F	78	ILE	2.4
28	26	7	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
38	1g	120	ILE	2.4
47	1p	33	ILE	2.4
6	1G	149	VAL	2.4
26	14	56	VAL	2.4
35	2d	198	VAL	2.4
40	1i	108	VAL	2.4
9	2N	1	MET	2.4
33	2b	227	GLY	2.4
34	2c	80	GLY	2.4
35	1d	62	GLN	2.4
55	2x	3	C	2.4
12	2Q	114	ALA	2.4
32	1a	204	U	2.4
34	2c	176	HIS	2.4
42	2k	31	THR	2.4
54	2y	19	G	2.4
11	2P	6	LEU	2.4
14	1S	4	LEU	2.4
23	21	94	LEU	2.4
44	2m	78	ILE	2.4
48	2q	31	LEU	2.4
49	2r	85	LEU	2.4
35	1d	139	ARG	2.4
43	2l	96	VAL	2.4
48	1q	11	VAL	2.4
38	2g	26	PHE	2.4
17	2V	78	LYS	2.4
53	2v	15	A	2.4
33	2b	202	PRO	2.4
42	2k	115	PRO	2.4
46	2o	46	HIS	2.4
1	2A	2150	U	2.4
10	1O	47	ILE	2.4
15	2T	102	ILE	2.4
16	1U	18	LEU	2.4
26	14	62	ARG	2.4
38	2g	22	LEU	2.4
15	1T	109	GLU	2.4
33	1b	75	LYS	2.4
54	1w	3	G	2.4
7	2H	164	TYR	2.4
35	2d	165	MET	2.4

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Mol	Chain	Res	Type	RSRZ
3	1D	263	ARG	2.4
16	2U	33	ARG	2.4
21	2Z	122	ARG	2.4
54	1w	69	A	2.4
39	1h	39	LEU	2.4
1	1A	885	C	2.4
8	1I	4	ILE	2.4
11	2P	29	LYS	2.4
33	1b	127	ILE	2.4
33	2b	8	LYS	2.4
36	1e	88	LYS	2.4
48	2q	24	GLU	2.4
22	20	71	ASP	2.4
33	1b	93	VAL	2.4
20	2Y	89	PHE	2.4
1	2A	2116	G	2.4
3	2D	4	LYS	2.4
9	2N	10	GLU	2.4
14	2S	34	HIS	2.4
41	1j	57	LYS	2.4
3	2D	37	LEU	2.4
9	2N	23	LEU	2.4
38	1g	22	LEU	2.4
9	2N	71	ILE	2.4
11	2P	40	SER	2.4
41	1j	58	ASP	2.4
54	1y	23	A	2.4
54	2y	35	A	2.4
6	2G	89	GLY	2.4
20	2Y	80	GLY	2.4
32	1a	1532	U	2.4
48	1q	71	PHE	2.4
48	2q	80	GLY	2.4
55	2x	69	C	2.4
17	2V	84	LYS	2.4
44	1m	121	LYS	2.4
48	2q	92	ARG	2.4
1	2A	2319	G	2.4
11	2P	35	HIS	2.4
42	2k	35	PRO	2.4
3	2D	240	ALA	2.4
46	2o	57	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
10	2O	81	ASP	2.4
30	28	20	GLY	2.4
35	2d	2	GLY	2.4
31	29	25	VAL	2.4
39	1h	31	PHE	2.4
1	2A	2114	A	2.4
38	2g	78	ARG	2.4
47	1p	27	LYS	2.4
7	2H	58	GLU	2.4
44	1m	23	TYR	2.4
21	2Z	167	PRO	2.4
48	1q	45	HIS	2.4
16	2U	31	SER	2.4
22	10	75	LEU	2.4
23	21	98	LEU	2.4
36	1e	91	LEU	2.4
44	2m	96	LEU	2.4
46	2o	81	LEU	2.4
20	2Y	61	ILE	2.4
33	2b	18	GLY	2.4
35	2d	161	ASN	2.4
40	2i	6	GLY	2.4
40	2i	112	LYS	2.4
41	1j	50	ILE	2.4
54	1y	1	G	2.4
54	2w	15	G	2.4
11	2P	50	ARG	2.4
12	2Q	41	TRP	2.4
18	2W	14	PRO	2.3
35	2d	106	TYR	2.3
39	1h	5	PRO	2.3
42	2k	121	PRO	2.3
4	1E	28	ALA	2.3
16	2U	48	ALA	2.3
18	2W	13	SER	2.3
39	2h	124	ALA	2.3
40	1i	7	THR	2.3
40	1i	116	LYS	2.3
40	1i	126	SER	2.3
41	1j	32	ALA	2.3
51	1t	24	LEU	2.3
52	1u	11	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	1D	204	ILE	2.3
15	1T	108	ARG	2.3
33	2b	68	ILE	2.3
43	2l	100	ILE	2.3
46	1o	12	ILE	2.3
48	2q	78	GLU	2.3
20	2Y	13	VAL	2.3
34	2c	138	VAL	2.3
32	2a	1220	G	2.3
47	1p	59	TRP	2.3
15	2T	113	LYS	2.3
32	2a	90	U	2.3
41	2j	68	HIS	2.3
48	1q	34	LYS	2.3
50	2s	42	PRO	2.3
6	2G	173	LEU	2.3
9	2N	26	LEU	2.3
9	2N	120	LEU	2.3
1	2A	885	C	2.3
11	2P	22	GLY	2.3
33	1b	124	SER	2.3
22	20	12	ASN	2.3
32	1a	1030	C	2.3
40	1i	61	ALA	2.3
51	2t	79	ARG	2.3
24	22	57	ILE	2.3
33	2b	41	ILE	2.3
33	2b	162	ILE	2.3
21	2Z	88	PHE	2.3
38	2g	23	VAL	2.3
42	1k	14	VAL	2.3
26	14	46	GLN	2.3
38	2g	151	TYR	2.3
43	2l	94	PRO	2.3
4	2E	20	ALA	2.3
7	2H	102	ALA	2.3
21	2Z	76	LEU	2.3
34	1c	19	GLU	2.3
26	14	58	ARG	2.3
30	28	32	LEU	2.3
46	1o	56	LEU	2.3
54	2y	5	G	2.3

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Mol	Chain	Res	Type	RSRZ
30	28	17	THR	2.3
38	2g	2	ALA	2.3
32	2a	924	C	2.3
1	2A	735	A	2.3
33	2b	211	ILE	2.3
34	2c	134	ILE	2.3
12	2Q	109	VAL	2.3
21	1Z	141	VAL	2.3
22	20	69	PHE	2.3
35	1d	198	VAL	2.3
36	1e	55	VAL	2.3
38	2g	33	ASP	2.3
50	2s	14	HIS	2.3
33	1b	118	LEU	2.3
51	2t	10	LEU	2.3
52	1u	22	ARG	2.3
39	2h	58	TYR	2.3
5	1F	48	THR	2.3
18	2W	60	ASN	2.3
53	1v	23	U	2.3
1	2A	2148	G	2.3
32	2a	1061	G	2.3
40	2i	38	GLN	2.3
10	2O	43	VAL	2.3
12	1Q	81	VAL	2.3
33	2b	15	VAL	2.3
33	2b	105	PHE	2.3
46	2o	82	ILE	2.3
39	2h	95	VAL	2.3
20	2Y	62	GLU	2.3
28	26	42	TRP	2.3
35	2d	73	ARG	2.3
40	2i	39	GLY	2.3
8	2I	30	LEU	2.3
25	23	23	LEU	2.3
34	2c	12	LEU	2.3
9	2N	117	PHE	2.3
12	2Q	29	PHE	2.3
48	2q	65	ILE	2.3
44	2m	67	GLU	2.3
1	2A	2110	G	2.3
16	2U	36	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
26	24	55	ARG	2.3
35	2d	57	ARG	2.3
39	2h	122	ARG	2.3
40	2i	75	ASP	2.3
6	2G	177	GLY	2.3
3	2D	275	LYS	2.3
20	2Y	26	LYS	2.3
32	2a	794	A	2.3
33	1b	95	GLN	2.3
7	2H	106	THR	2.3
40	1i	114	TYR	2.3
45	2n	40	CYS	2.3
34	2c	206	GLU	2.3
1	2A	2172	U	2.3
21	2Z	44	PHE	2.3
26	24	14	ILE	2.3
43	2l	101	VAL	2.3
50	2s	9	VAL	2.3
11	2P	76	LYS	2.3
7	2H	65	HIS	2.3
7	2H	84	SER	2.3
16	1U	27	LEU	2.3
33	1b	233	SER	2.3
32	2a	1030	C	2.3
32	2a	1149	C	2.3
44	1m	107	ALA	2.3
21	1Z	170	THR	2.3
5	2F	64	ILE	2.3
5	2F	82	ILE	2.3
9	2N	118	LYS	2.3
12	2Q	64	ILE	2.3
45	2n	16	PHE	2.3
30	28	38	GLY	2.2
54	2w	33	U	2.2
33	2b	78	GLN	2.2
43	2l	9	GLN	2.2
15	1T	114	LEU	2.2
36	2e	138	ALA	2.2
38	2g	25	ALA	2.2
40	2i	122	ALA	2.2
6	1G	75	LYS	2.2
19	1X	65	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
30	28	52	LYS	2.2
33	2b	130	ARG	2.2
35	2d	68	TYR	2.2
46	2o	88	ARG	2.2
6	2G	134	GLY	2.2
33	2b	203	GLY	2.2
34	2c	153	VAL	2.2
41	2j	34	VAL	2.2
46	2o	3	ILE	2.2
36	2e	130	ASN	2.2
40	1i	110	GLU	2.2
51	2t	70	SER	2.2
21	2Z	125	LEU	2.2
40	2i	19	LEU	2.2
44	2m	64	TRP	2.2
3	1D	50	THR	2.2
7	2H	132	ARG	2.2
22	20	77	ARG	2.2
27	25	11	THR	2.2
40	2i	111	ARG	2.2
34	2c	17	ASP	2.2
1	2A	2175	C	2.2
36	2e	124	GLY	2.2
6	2G	160	VAL	2.2
25	23	9	VAL	2.2
40	2i	53	VAL	2.2
47	1p	4	ILE	2.2
48	2q	56	VAL	2.2
54	2y	18	G	2.2
11	2P	74	GLU	2.2
30	28	19	SER	2.2
2	2B	90	A	2.2
17	2V	76	LYS	2.2
31	29	33	LYS	2.2
32	1a	389	A	2.2
43	2l	52	LEU	2.2
47	1p	35	LYS	2.2
34	2c	22	TRP	2.2
50	2s	76	PRO	2.2
50	2s	44	MET	2.2
52	1u	10	ARG	2.2
18	2W	93	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
33	2b	79	ASP	2.2
38	2g	140	ASP	2.2
22	20	45	PHE	2.2
35	2d	167	GLY	2.2
41	1j	11	PHE	2.2
42	2k	86	GLY	2.2
48	1q	26	GLN	2.2
21	2Z	161	VAL	2.2
36	1e	80	ILE	2.2
43	2l	43	VAL	2.2
8	1I	9	LEU	2.2
35	1d	101	LEU	2.2
47	2p	73	LEU	2.2
33	2b	90	MET	2.2
1	1A	1095	A	2.2
8	1I	20	ASP	2.2
49	2r	47	THR	2.2
38	2g	85	TYR	2.2
42	1k	25	TYR	2.2
3	1D	51	VAL	2.2
3	2D	106	ILE	2.2
5	2F	57	VAL	2.2
12	2Q	97	VAL	2.2
36	2e	101	ILE	2.2
39	1h	61	VAL	2.2
49	2r	50	ILE	2.2
35	1d	209	ARG	2.2
47	2p	8	ARG	2.2
7	2H	71	LEU	2.2
14	2S	54	LEU	2.2
17	2V	87	HIS	2.2
23	21	46	LEU	2.2
35	1d	40	PRO	2.2
36	2e	139	LEU	2.2
46	2o	66	LEU	2.2
48	2q	43	LEU	2.2
1	2A	2142	C	2.2
34	2c	162	GLN	2.2
35	1d	102	ASP	2.2
47	1p	44	THR	2.2
32	2a	977	A	2.2
38	2g	43	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	2D	54	ARG	2.2
14	2S	31	SER	2.2
18	2W	24	ILE	2.2
34	2c	8	ILE	2.2
3	2D	206	LEU	2.2
22	20	59	LEU	2.2
25	23	12	PRO	2.2
25	23	16	PRO	2.2
34	1c	196	LEU	2.2
37	1f	61	LEU	2.2
49	1r	44	LEU	2.2
7	2H	90	LYS	2.2
11	2P	36	LYS	2.2
39	2h	116	LYS	2.2
43	2l	14	GLY	2.2
51	1t	59	ALA	2.2
27	25	29	THR	2.2
5	2F	83	PHE	2.2
32	2a	1062	U	2.2
35	1d	118	ARG	2.2
46	2o	15	PHE	2.2
1	2A	2583	G	2.2
40	2i	5	TYR	2.2
28	26	5	VAL	2.2
30	18	22	VAL	2.2
36	2e	33	VAL	2.2
39	1h	109	ILE	2.2
39	2h	109	ILE	2.2
48	2q	73	VAL	2.2
49	2r	22	VAL	2.2
1	2A	2169	A	2.2
32	2a	1357	A	2.2
16	2U	18	LEU	2.2
20	2Y	82	PRO	2.2
34	2c	47	LEU	2.2
43	1l	27	LEU	2.2
46	1o	31	LEU	2.2
5	2F	76	GLY	2.2
19	2X	1	MET	2.2
10	2O	6	THR	2.2
48	2q	7	THR	2.2
17	2V	82	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
38	2g	76	ARG	2.2
51	2t	17	ARG	2.2
40	1i	59	PHE	2.2
10	2O	29	ASN	2.1
22	20	19	LYS	2.1
35	1d	138	TYR	2.1
43	1l	98	TYR	2.1
42	2k	108	ILE	2.1
47	1p	62	VAL	2.1
4	2E	132	HIS	2.1
11	2P	27	HIS	2.1
45	2n	52	GLN	2.1
35	2d	29	PRO	2.1
47	1p	49	LEU	2.1
34	1c	205	GLY	2.1
36	2e	22	GLY	2.1
36	2e	114	GLY	2.1
8	1I	27	ARG	2.1
29	27	45	ALA	2.1
39	2h	91	ARG	2.1
44	2m	72	ALA	2.1
15	2T	1	MET	2.1
42	1k	87	THR	2.1
47	2p	22	THR	2.1
50	2s	33	THR	2.1
11	2P	46	LYS	2.1
17	2V	85	LYS	2.1
48	1q	78	GLU	2.1
36	2e	60	TYR	2.1
54	1w	13	C	2.1
7	2H	151	ILE	2.1
14	2S	40	ILE	2.1
41	2j	72	VAL	2.1
51	2t	33	ILE	2.1
7	2H	111	HIS	2.1
47	2p	74	LEU	2.1
48	2q	33	GLY	2.1
10	1O	17	ARG	2.1
25	23	30	ARG	2.1
35	2d	3	ARG	2.1
1	2A	2894	G	2.1
24	22	8	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
30	28	12	LYS	2.1
32	2a	1034	G	2.1
34	1c	72	LYS	2.1
35	1d	166	LYS	2.1
36	1e	95	ALA	2.1
40	1i	118	LYS	2.1
40	1i	127	LYS	2.1
1	2A	2801(A)	A	2.1
45	2n	43	CYS	2.1
6	1G	26	GLN	2.1
4	2E	26	ILE	2.1
18	2W	9	TYR	2.1
18	2W	10	VAL	2.1
48	2q	19	VAL	2.1
1	2A	2138	C	2.1
12	2Q	23	GLY	2.1
32	2a	1354	C	2.1
35	2d	108	LEU	2.1
35	2d	168	ARG	2.1
44	1m	119	GLY	2.1
54	1w	31	C	2.1
34	1c	206	GLU	2.1
36	1e	86	ALA	2.1
38	1g	150	ALA	2.1
23	21	34	THR	2.1
3	1D	15	PHE	2.1
35	2d	75	PHE	2.1
1	1A	1093	G	2.1
1	2A	910	A	2.1
32	2a	1225	A	2.1
32	2a	1363(A)	A	2.1
9	1N	140	VAL	2.1
9	2N	52	VAL	2.1
9	2N	87	LEU	2.1
11	2P	59	LEU	2.1
20	2Y	67	LEU	2.1
25	23	53	LEU	2.1
34	1c	201	TYR	2.1
34	2c	204	LEU	2.1
36	1e	121	LYS	2.1
44	2m	108	ARG	2.1
6	2G	142	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
9	2N	90	MET	2.1
11	2P	58	THR	2.1
7	1H	2	SER	2.1
14	2S	12	PHE	2.1
21	1Z	149	SER	2.1
51	2t	21	LYS	2.1
15	1T	87	ASP	2.1
6	2G	140	ILE	2.1
30	18	14	VAL	2.1
1	1A	2131	G	2.1
20	2Y	35	TYR	2.1
33	2b	58	ILE	2.1
34	1c	152	ILE	2.1
36	1e	13	ILE	2.1
46	2o	43	LEU	2.1
50	1s	67	VAL	2.1
50	2s	15	LEU	2.1
32	2a	978	A	2.1
36	2e	83	GLU	2.1
54	1w	10	G	2.1
54	1w	14	A	2.1
53	2v	23	U	2.1
3	1D	214	TRP	2.1
36	1e	18	ARG	2.1
36	1e	24	ARG	2.1
51	1t	8	ARG	2.1
4	2E	158	GLY	2.1
8	2I	20	ASP	2.1
20	2Y	58	GLY	2.1
12	2Q	105	GLU	2.1
20	1Y	31	LEU	2.1
21	2Z	91	LEU	2.1
22	20	37	LEU	2.1
24	22	61	LEU	2.1
4	1E	77	ILE	2.1
7	2H	37	VAL	2.1
36	1e	123	LEU	2.1
38	1g	91	VAL	2.1
49	2r	44	LEU	2.1
33	2b	148	TYR	2.1
11	2P	38	GLN	2.1
1	2A	2141	G	2.1

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Mol	Chain	Res	Type	RSRZ
34	1c	160	ALA	2.1
35	1d	111	ALA	2.1
36	2e	47	LYS	2.1
42	2k	123	LYS	2.1
1	2A	1963	U	2.1
40	2i	27	THR	2.1
27	25	12	SER	2.1
39	1h	136	GLU	2.1
46	1o	61	GLY	2.1
54	2w	30	C	2.1
13	2R	18	LEU	2.1
3	1D	49	ILE	2.1
7	2H	162	ILE	2.1
9	2N	85	ILE	2.1
20	2Y	51	VAL	2.1
21	2Z	174	VAL	2.1
31	29	3	VAL	2.1
34	1c	115	LEU	2.1
35	2d	148	VAL	2.1
48	2q	89	LEU	2.1
50	2s	11	VAL	2.1
50	2s	62	ILE	2.1
28	26	53	LYS	2.1
12	2Q	121	ALA	2.1
11	2P	33	ARG	2.1
35	2d	115	ARG	2.1
44	2m	93	ARG	2.1
46	2o	38	ARG	2.1
51	1t	15	ARG	2.1
41	2j	64	GLU	2.1
1	2A	2506	U	2.0
6	2G	141	PHE	2.1
12	2Q	100	GLY	2.1
32	2a	1287	A	2.1
39	1h	4	ASP	2.1
1	1A	1092	C	2.0
14	2S	4	LEU	2.0
16	2U	16	LYS	2.0
16	2U	19	LYS	2.0
21	1Z	102	LEU	2.0
34	1c	12	LEU	2.0
35	2d	135	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
38	2g	38	LEU	2.0
48	2q	4	LYS	2.0
12	2Q	132	VAL	2.0
36	1e	49	PRO	2.0
36	2e	118	ILE	2.0
8	1I	36	ALA	2.0
36	2e	140	ARG	2.0
39	1h	85	ARG	2.0
39	1h	91	ARG	2.0
7	2H	109	PHE	2.0
37	1f	92	LYS	2.0
40	2i	70	LYS	2.0
43	2l	46	LYS	2.0
33	2b	196	LEU	2.0
38	2g	99	LEU	2.0
48	2q	98	LEU	2.0
1	2A	734	A	2.0
1	2A	2151	G	2.0
4	1E	196	VAL	2.0
9	2N	140	VAL	2.0
12	2Q	96	VAL	2.0
21	2Z	86	VAL	2.0
32	1a	1503	A	2.0
33	2b	112	VAL	2.0
34	1c	106	VAL	2.0
6	2G	157	ILE	2.0
36	2e	106	PRO	2.0
49	2r	80	PRO	2.0
46	1o	64	ARG	2.0
3	1D	62	TYR	2.0
6	2G	164	GLU	2.0
22	20	68	GLU	2.0
30	28	64	TYR	2.0
5	2F	166	ALA	2.0
36	2e	108	ALA	2.0
9	2N	104	LYS	2.0
41	1j	93	GLY	2.0
48	1q	87	LYS	2.0
50	2s	32	LYS	2.0
10	2O	79	PHE	2.0
3	2D	182	LEU	2.0
5	1F	41	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	1D	3	VAL	2.0
4	2E	189	PRO	2.0
7	2H	76	VAL	2.0
11	2P	72	PRO	2.0
11	2P	125	VAL	2.0
18	1W	92	ARG	2.0
22	20	79	VAL	2.0
23	11	51	VAL	2.0
30	28	14	VAL	2.0
30	28	22	VAL	2.0
33	2b	136	VAL	2.0
40	2i	86	VAL	2.0
50	2s	51	VAL	2.0
9	1N	71	ILE	2.0
46	1o	3	ILE	2.0
1	2A	968	G	2.0
3	2D	144	ALA	2.0
21	2Z	9	TYR	2.0
32	2a	1035	A	2.0
27	25	14	ALA	2.0
37	2f	55	ASP	2.0
54	2y	56	C	2.0
47	1p	67	THR	2.0
4	2E	51	PHE	2.0
6	1G	82	LEU	2.0
22	20	11	ARG	2.0
17	2V	5	VAL	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	2w	55	20/21	0.59	0.37	74,91,97,99	0
54	4SU	2y	8	20/21	0.68	0.19	92,97,104,113	0
54	7MG	2y	46	24/25	0.71	0.22	87,98,104,119	0
54	PSU	1w	55	20/21	0.72	0.28	63,85,89,91	0
54	CM0	2y	34	25/26	0.73	0.49	82,94,105,114	0
54	7MG	2w	46	24/25	0.75	0.18	80,90,102,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	6MZ	2y	37	23/24	0.76	0.31	82,87,100,116	0
54	4SU	2w	8	20/21	0.77	0.22	84,94,99,102	0
54	4SU	1y	8	20/21	0.79	0.20	82,91,101,109	0
54	7MG	1y	46	24/25	0.79	0.23	82,91,96,99	0
54	PSU	2y	55	20/21	0.79	0.34	85,91,95,96	0
54	7MG	1w	46	24/25	0.80	0.18	74,82,92,94	0
54	PSU	1y	55	20/21	0.81	0.25	79,88,95,98	0
54	CM0	1y	34	25/26	0.82	0.51	79,86,99,109	0
54	5MU	2w	54	21/22	0.84	0.23	74,81,87,90	0
54	5MU	1y	54	21/22	0.85	0.21	70,80,88,93	0
54	6MZ	1y	37	23/24	0.86	0.32	77,82,92,107	0
54	5MU	2y	54	21/22	0.86	0.28	82,90,102,115	0
55	PSU	2x	55	20/21	0.86	0.16	67,73,86,93	0
54	4SU	1w	8	20/21	0.89	0.19	72,81,90,90	0
32	PSU	2a	516	20/21	0.91	0.18	63,68,72,80	0
55	4SU	2x	8	20/21	0.91	0.13	71,76,79,87	0
32	2MG	2a	1207	24/25	0.91	0.17	54,77,82,86	0
54	6MZ	2w	37	23/24	0.92	0.31	62,69,76,77	0
32	5MC	2a	967	21/22	0.92	0.27	58,65,74,77	0
54	CM0	2w	34	25/26	0.92	0.23	60,71,78,90	0
1	5MU	2A	1915	21/22	0.92	0.17	62,68,77,81	0
32	M2G	2a	966	25/26	0.92	0.26	53,63,72,76	0
55	4SU	1x	8	20/21	0.93	0.18	47,62,75,77	0
43	0TD	2l	92	10/11	0.93	0.30	56,61,66,79	0
43	0TD	1l	92	10/11	0.93	0.21	35,41,44,49	0
1	5MU	1A	1915	21/22	0.94	0.21	46,52,58,60	0
32	7MG	2a	527	24/25	0.94	0.19	54,62,69,71	0
32	5MC	2a	1400	21/22	0.94	0.29	56,62,67,67	0
54	5MU	1w	54	21/22	0.94	0.18	52,67,79,83	0
32	5MC	2a	1407	21/22	0.94	0.26	46,54,61,74	0
54	CM0	1w	34	25/26	0.94	0.20	53,60,68,73	0
55	5MU	2x	54	21/22	0.94	0.17	72,76,83,85	0
1	PSU	2A	1917	20/21	0.94	0.18	48,58,66,68	0
54	6MZ	1w	37	23/24	0.95	0.23	40,46,53,54	0
1	PSU	2A	1911	20/21	0.95	0.19	53,58,60,63	0
32	MA6	2a	1518	24/25	0.95	0.32	43,54,61,63	0
55	5MC	2x	32	21/22	0.95	0.26	60,67,74,75	0
55	5MU	1x	54	21/22	0.95	0.15	54,62,70,75	0
32	MA6	2a	1519	24/25	0.95	0.35	43,57,63,65	0
55	PSU	1x	55	20/21	0.95	0.16	50,62,65,72	0
32	4OC	2a	1402	22/23	0.95	0.22	45,58,61,62	0
32	5MC	2a	1404	21/22	0.96	0.22	46,51,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	2A	2605	20/21	0.96	0.20	29,38,42,46	0
32	PSU	1a	516	20/21	0.96	0.17	40,49,51,54	0
32	7MG	1a	527	24/25	0.96	0.21	28,38,44,47	0
32	5MC	1a	1400	21/22	0.96	0.21	30,40,46,48	0
32	4OC	1a	1402	22/23	0.96	0.22	27,41,47,53	0
1	OMC	2A	1920	21/22	0.96	0.23	49,58,60,62	0
1	5MC	2A	1942	21/22	0.96	0.19	47,56,62,68	0
1	5MC	2A	1962	21/22	0.96	0.17	39,50,54,56	0
1	5MC	1A	1962	21/22	0.97	0.19	26,32,35,45	0
32	UR3	2a	1498	21/22	0.97	0.26	39,53,60,64	0
1	OMG	2A	2251	24/25	0.97	0.22	33,39,43,46	0
32	5MC	1a	1404	21/22	0.97	0.21	28,31,36,37	0
32	MA6	1a	1518	24/25	0.97	0.23	26,33,37,43	0
32	MA6	1a	1519	24/25	0.97	0.23	28,33,42,44	0
1	PSU	1A	1911	20/21	0.97	0.20	37,44,51,53	0
55	5MC	1x	32	21/22	0.97	0.21	36,49,52,56	0
1	PSU	1A	1917	20/21	0.97	0.18	37,47,51,52	0
32	M2G	1a	966	25/26	0.97	0.22	37,45,51,55	0
32	5MC	1a	967	21/22	0.97	0.23	40,46,50,53	0
32	2MG	1a	1207	24/25	0.97	0.17	51,59,62,69	0
1	5MC	1A	1942	21/22	0.97	0.19	32,38,44,52	0
1	OMC	1A	1920	21/22	0.98	0.21	30,40,46,51	0
1	5MU	1A	1939	21/22	0.98	0.21	15,23,26,36	0
32	5MC	1a	1407	21/22	0.98	0.23	31,35,39,44	0
1	5MU	2A	1939	21/22	0.98	0.20	38,40,42,50	0
32	UR3	1a	1498	21/22	0.98	0.23	26,33,37,41	0
1	OMG	1A	2251	24/25	0.98	0.19	14,19,20,21	0
1	2MA	1A	2503	23/24	0.98	0.21	11,14,17,18	0
1	2MA	2A	2503	23/24	0.98	0.23	25,29,36,40	0
1	OMU	2A	2552	21/22	0.98	0.21	27,37,43,48	0
1	OMU	1A	2552	21/22	0.98	0.20	18,26,30,31	0
1	PSU	1A	2605	20/21	0.98	0.20	16,22,30,30	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

median, 95^{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
56	MG	1a	1786	1/1	-0.11	0.28	84,84,84,84	0
56	MG	1A	3993	1/1	0.18	0.60	86,86,86,86	0
56	MG	1l	202	1/1	0.24	0.41	82,82,82,82	0
56	MG	2a	3173	1/1	0.24	0.21	86,86,86,86	0
56	MG	2a	3106	1/1	0.30	0.19	74,74,74,74	0
56	MG	1A	3975	1/1	0.34	0.31	66,66,66,66	0
56	MG	1A	3973	1/1	0.35	0.21	72,72,72,72	0
56	MG	1A	4036	1/1	0.42	0.28	60,60,60,60	0
56	MG	1A	4075	1/1	0.42	0.21	40,40,40,40	0
56	MG	1A	4027	1/1	0.44	0.22	80,80,80,80	0
56	MG	2B	209	1/1	0.44	0.19	72,72,72,72	0
56	MG	2a	3077	1/1	0.47	0.18	66,66,66,66	0
56	MG	1A	3912	1/1	0.48	0.24	64,64,64,64	0
56	MG	2A	3824	1/1	0.48	0.20	76,76,76,76	0
56	MG	1A	4045	1/1	0.48	0.22	51,51,51,51	0
56	MG	1A	4028	1/1	0.50	0.11	59,59,59,59	0
56	MG	2a	3097	1/1	0.52	0.28	66,66,66,66	0
56	MG	1A	4044	1/1	0.52	0.25	46,46,46,46	0
56	MG	1A	3990	1/1	0.52	0.21	45,45,45,45	0
56	MG	1a	1760	1/1	0.53	0.09	50,50,50,50	0
56	MG	1x	114	1/1	0.53	0.35	74,74,74,74	0
56	MG	2Q	202	1/1	0.54	0.33	60,60,60,60	0
56	MG	2a	3141	1/1	0.55	0.21	55,55,55,55	0
56	MG	1A	3881	1/1	0.56	0.17	18,18,18,18	0
56	MG	1A	4014	1/1	0.56	0.10	41,41,41,41	0
56	MG	2A	3318	1/1	0.56	0.21	77,77,77,77	0
56	MG	2A	3781	1/1	0.56	0.14	70,70,70,70	0
56	MG	1A	3888	1/1	0.57	0.12	54,54,54,54	0
56	MG	2a	3135	1/1	0.58	0.10	78,78,78,78	0
56	MG	1A	3591	1/1	0.59	0.18	28,28,28,28	0
56	MG	2A	3784	1/1	0.60	0.12	56,56,56,56	0
56	MG	1a	1793	1/1	0.60	0.15	69,69,69,69	0
56	MG	1B	218	1/1	0.61	0.17	60,60,60,60	0
56	MG	1A	3947	1/1	0.61	0.09	44,44,44,44	0
56	MG	1A	4061	1/1	0.62	0.13	57,57,57,57	0
56	MG	2a	3100	1/1	0.62	0.38	61,61,61,61	0
56	MG	2B	212	1/1	0.62	0.19	70,70,70,70	0
56	MG	2A	3177	1/1	0.62	0.70	62,62,62,62	0
56	MG	1a	1612	1/1	0.62	0.18	62,62,62,62	0
56	MG	2a	3095	1/1	0.62	0.20	69,69,69,69	0
56	MG	1a	1790	1/1	0.63	0.16	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	3948	1/1	0.63	0.41	69,69,69,69	0
56	MG	2a	3043	1/1	0.63	0.20	49,49,49,49	0
56	MG	2a	3046	1/1	0.63	0.20	72,72,72,72	0
56	MG	2A	3416	1/1	0.63	0.18	57,57,57,57	0
56	MG	2a	3148	1/1	0.63	0.15	70,70,70,70	0
56	MG	2a	3161	1/1	0.63	0.12	65,65,65,65	0
56	MG	2a	3164	1/1	0.63	0.16	83,83,83,83	0
56	MG	2A	3613	1/1	0.63	0.16	32,32,32,32	0
56	MG	2a	3219	1/1	0.63	0.31	68,68,68,68	0
56	MG	1A	4060	1/1	0.64	0.15	51,51,51,51	0
56	MG	1A	4017	1/1	0.64	0.41	75,75,75,75	0
56	MG	1A	4040	1/1	0.64	0.35	59,59,59,59	0
56	MG	2A	3835	1/1	0.64	0.21	59,59,59,59	0
56	MG	2A	3538	1/1	0.64	0.17	42,42,42,42	0
56	MG	1A	4083	1/1	0.64	0.15	70,70,70,70	0
56	MG	2A	3624	1/1	0.64	0.25	37,37,37,37	0
56	MG	2a	3020	1/1	0.65	0.17	60,60,60,60	0
56	MG	2A	3769	1/1	0.65	0.14	45,45,45,45	0
56	MG	1a	1784	1/1	0.65	0.20	51,51,51,51	0
56	MG	1A	4098	1/1	0.65	0.45	66,66,66,66	0
56	MG	1A	3368	1/1	0.65	0.36	58,58,58,58	0
56	MG	1A	3657	1/1	0.66	0.18	18,18,18,18	0
56	MG	1A	3356	1/1	0.66	0.17	46,46,46,46	0
56	MG	2A	3424	1/1	0.66	0.23	62,62,62,62	0
56	MG	1E	302	1/1	0.66	0.74	52,52,52,52	0
56	MG	1Q	205	1/1	0.66	0.30	65,65,65,65	0
56	MG	1A	3949	1/1	0.66	0.12	58,58,58,58	0
56	MG	2A	3720	1/1	0.66	0.16	62,62,62,62	0
56	MG	1a	1627	1/1	0.66	0.15	50,50,50,50	0
56	MG	1A	4048	1/1	0.66	0.12	41,41,41,41	0
56	MG	2A	3314	1/1	0.66	0.13	60,60,60,60	0
56	MG	1a	1792	1/1	0.67	0.12	56,56,56,56	0
56	MG	2A	3503	1/1	0.67	0.43	50,50,50,50	0
56	MG	1a	1781	1/1	0.67	0.08	64,64,64,64	0
56	MG	2A	3571	1/1	0.67	0.16	56,56,56,56	0
56	MG	2A	3411	1/1	0.67	0.23	64,64,64,64	0
56	MG	1a	1825	1/1	0.67	0.12	58,58,58,58	0
56	MG	2A	3241	1/1	0.68	0.23	55,55,55,55	0
56	MG	1a	1815	1/1	0.68	0.19	59,59,59,59	0
56	MG	1A	4024	1/1	0.68	0.16	70,70,70,70	0
56	MG	1A	3943	1/1	0.68	0.21	69,69,69,69	0
56	MG	1v	101	1/1	0.68	0.49	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	1A	4054	1/1	0.68	0.17	50,50,50,50	0
56	MG	1A	3072	1/1	0.68	0.20	54,54,54,54	0
56	MG	2A	3062	1/1	0.69	0.25	50,50,50,50	0
56	MG	2A	3251	1/1	0.69	0.58	53,53,53,53	0
56	MG	1A	3750	1/1	0.69	0.20	13,13,13,13	0
56	MG	2y	103	1/1	0.69	0.18	65,65,65,65	0
56	MG	2A	3821	1/1	0.70	0.12	61,61,61,61	0
56	MG	1x	108	1/1	0.70	0.24	61,61,61,61	0
56	MG	2a	3091	1/1	0.70	0.82	66,66,66,66	0
56	MG	1a	1675	1/1	0.70	0.21	68,68,68,68	0
56	MG	2y	102	1/1	0.70	0.11	84,84,84,84	0
56	MG	2A	3355	1/1	0.70	0.27	63,63,63,63	0
56	MG	1A	3940	1/1	0.71	0.09	42,42,42,42	0
56	MG	1A	4021	1/1	0.71	0.09	60,60,60,60	0
56	MG	2A	3271	1/1	0.71	0.15	66,66,66,66	0
56	MG	1a	1712	1/1	0.71	0.32	49,49,49,49	0
56	MG	2a	3133	1/1	0.71	0.09	76,76,76,76	0
56	MG	1A	3801	1/1	0.71	0.13	35,35,35,35	0
56	MG	2A	3620	1/1	0.71	0.10	34,34,34,34	0
56	MG	1A	3970	1/1	0.71	0.30	67,67,67,67	0
56	MG	2a	3015	1/1	0.71	0.56	61,61,61,61	0
56	MG	2A	3669	1/1	0.71	0.14	55,55,55,55	0
56	MG	2a	3165	1/1	0.71	0.28	73,73,73,73	0
56	MG	2A	3373	1/1	0.71	0.19	46,46,46,46	0
56	MG	2A	3065	1/1	0.71	0.17	55,55,55,55	0
56	MG	2A	3775	1/1	0.71	0.36	77,77,77,77	0
56	MG	1A	3292	1/1	0.71	0.26	39,39,39,39	0
56	MG	2y	105	1/1	0.71	0.12	85,85,85,85	0
56	MG	1a	1606	1/1	0.72	0.21	53,53,53,53	0
56	MG	1A	3489	1/1	0.72	0.36	55,55,55,55	0
56	MG	2A	3849	1/1	0.72	0.19	70,70,70,70	0
56	MG	2a	3218	1/1	0.72	0.14	69,69,69,69	0
56	MG	1A	3433	1/1	0.73	0.16	52,52,52,52	0
56	MG	2A	3789	1/1	0.73	0.17	66,66,66,66	0
56	MG	2a	3104	1/1	0.73	0.35	60,60,60,60	0
56	MG	2A	3500	1/1	0.73	0.14	42,42,42,42	0
56	MG	2A	3232	1/1	0.73	0.40	65,65,65,65	0
56	MG	1B	227	1/1	0.73	0.12	46,46,46,46	0
56	MG	2A	3567	1/1	0.73	0.15	30,30,30,30	0
56	MG	1A	3478	1/1	0.73	0.17	50,50,50,50	0
56	MG	1A	3945	1/1	0.73	0.22	49,49,49,49	0
56	MG	2a	3162	1/1	0.73	0.13	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	1A	3360	1/1	0.73	0.78	46,46,46,46	0
56	MG	1x	112	1/1	0.73	0.19	67,67,67,67	0
56	MG	2A	3649	1/1	0.73	0.17	50,50,50,50	0
56	MG	2a	3216	1/1	0.73	0.15	61,61,61,61	0
56	MG	1A	3392	1/1	0.73	0.21	46,46,46,46	0
56	MG	1y	105	1/1	0.73	0.44	73,73,73,73	0
56	MG	1A	3625	1/1	0.73	0.15	36,36,36,36	0
56	MG	1A	3627	1/1	0.73	0.13	15,15,15,15	0
56	MG	2A	3419	1/1	0.73	0.20	54,54,54,54	0
56	MG	1a	1718	1/1	0.74	0.17	56,56,56,56	0
56	MG	1A	3911	1/1	0.74	0.18	64,64,64,64	0
56	MG	2A	3641	1/1	0.74	0.10	70,70,70,70	0
56	MG	2A	3253	1/1	0.74	0.15	53,53,53,53	0
56	MG	1A	3992	1/1	0.74	0.35	64,64,64,64	0
56	MG	2A	3080	1/1	0.74	0.15	63,63,63,63	0
56	MG	1A	3942	1/1	0.74	0.12	52,52,52,52	0
56	MG	2A	3346	1/1	0.74	0.12	59,59,59,59	0
56	MG	2a	3224	1/1	0.74	0.09	69,69,69,69	0
56	MG	2e	201	1/1	0.74	0.13	64,64,64,64	0
56	MG	1A	4032	1/1	0.74	0.14	65,65,65,65	0
56	MG	2A	3370	1/1	0.74	0.15	57,57,57,57	0
56	MG	2A	3238	1/1	0.74	0.35	42,42,42,42	0
56	MG	1A	3652	1/1	0.75	0.09	34,34,34,34	0
56	MG	2A	3722	1/1	0.75	0.29	53,53,53,53	0
56	MG	2A	3759	1/1	0.75	0.34	68,68,68,68	0
56	MG	1A	3878	1/1	0.75	0.15	13,13,13,13	0
56	MG	1A	3565	1/1	0.75	0.33	45,45,45,45	0
56	MG	1a	1801	1/1	0.75	0.23	65,65,65,65	0
56	MG	1a	1808	1/1	0.75	0.12	46,46,46,46	0
56	MG	1A	4006	1/1	0.75	0.08	76,76,76,76	0
56	MG	2A	3797	1/1	0.75	0.16	34,34,34,34	0
56	MG	1a	1639	1/1	0.75	0.23	41,41,41,41	0
56	MG	2A	3280	1/1	0.75	0.21	53,53,53,53	0
56	MG	2A	3647	1/1	0.75	0.58	62,62,62,62	0
56	MG	2A	3288	1/1	0.75	0.82	60,60,60,60	0
56	MG	2A	3857	1/1	0.75	0.15	56,56,56,56	0
56	MG	1A	3266	1/1	0.75	0.27	43,43,43,43	0
56	MG	1A	3834	1/1	0.76	0.10	28,28,28,28	0
56	MG	2A	3319	1/1	0.76	0.15	60,60,60,60	0
56	MG	2A	3121	1/1	0.76	0.16	63,63,63,63	0
56	MG	1A	3982	1/1	0.76	0.14	10,10,10,10	0
56	MG	2B	210	1/1	0.76	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	3278	1/1	0.76	0.13	58,58,58,58	0
56	MG	1A	3354	1/1	0.76	0.57	44,44,44,44	0
56	MG	2a	3003	1/1	0.76	0.15	66,66,66,66	0
56	MG	1A	3629	1/1	0.76	0.15	77,77,77,77	0
56	MG	1A	4101	1/1	0.76	0.21	44,44,44,44	0
56	MG	2a	3027	1/1	0.76	0.63	67,67,67,67	0
56	MG	2A	3749	1/1	0.76	0.12	68,68,68,68	0
56	MG	2a	3149	1/1	0.76	0.10	57,57,57,57	0
56	MG	2A	3674	1/1	0.77	0.09	52,52,52,52	0
56	MG	1a	1812	1/1	0.77	0.09	63,63,63,63	0
56	MG	1A	3978	1/1	0.77	0.20	48,48,48,48	0
56	MG	2F	303	1/1	0.77	0.82	56,56,56,56	0
56	MG	2G	201	1/1	0.77	0.13	56,56,56,56	0
56	MG	2A	3106	1/1	0.77	0.20	60,60,60,60	0
56	MG	1A	3962	1/1	0.77	0.23	37,37,37,37	0
56	MG	2A	3512	1/1	0.77	0.11	64,64,64,64	0
56	MG	1A	3996	1/1	0.77	0.09	31,31,31,31	0
56	MG	1a	1689	1/1	0.77	0.21	35,35,35,35	0
56	MG	2A	3321	1/1	0.77	0.36	58,58,58,58	0
56	MG	1a	1706	1/1	0.77	0.25	57,57,57,57	0
56	MG	2a	3049	1/1	0.77	0.52	73,73,73,73	0
56	MG	1B	209	1/1	0.77	0.21	46,46,46,46	0
56	MG	2A	3359	1/1	0.77	0.24	61,61,61,61	0
56	MG	1A	3869	1/1	0.77	0.13	29,29,29,29	0
56	MG	1a	1807	1/1	0.77	0.09	52,52,52,52	0
56	MG	2A	3268	1/1	0.77	0.11	69,69,69,69	0
56	MG	1a	1622	1/1	0.77	0.42	53,53,53,53	0
56	MG	1A	3837	1/1	0.78	0.22	48,48,48,48	0
56	MG	2A	3519	1/1	0.78	0.10	37,37,37,37	0
56	MG	1I	201	1/1	0.78	0.12	54,54,54,54	0
56	MG	1A	3756	1/1	0.78	0.13	43,43,43,43	0
56	MG	2A	3812	1/1	0.78	0.18	63,63,63,63	0
56	MG	1a	1810	1/1	0.78	0.28	76,76,76,76	0
56	MG	1a	1751	1/1	0.78	0.07	41,41,41,41	0
56	MG	1a	1759	1/1	0.78	0.15	42,42,42,42	0
56	MG	2A	3845	1/1	0.78	0.20	50,50,50,50	0
56	MG	2A	3218	1/1	0.78	0.32	52,52,52,52	0
56	MG	1a	1823	1/1	0.78	0.16	76,76,76,76	0
56	MG	1A	3721	1/1	0.78	0.14	56,56,56,56	0
56	MG	1A	3995	1/1	0.78	0.08	36,36,36,36	0
56	MG	1A	4111	1/1	0.78	0.31	59,59,59,59	0
56	MG	1A	3936	1/1	0.78	0.37	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3690	1/1	0.78	0.12	29,29,29,29	0
56	MG	1A	3618	1/1	0.78	0.19	22,22,22,22	0
56	MG	2a	3001	1/1	0.78	0.16	57,57,57,57	0
56	MG	1A	3941	1/1	0.78	0.09	46,46,46,46	0
56	MG	2a	3007	1/1	0.78	0.20	66,66,66,66	0
56	MG	2A	3449	1/1	0.78	0.17	49,49,49,49	0
56	MG	2a	3016	1/1	0.78	0.47	73,73,73,73	0
56	MG	1B	231	1/1	0.78	0.22	49,49,49,49	0
56	MG	2A	3048	1/1	0.78	0.14	48,48,48,48	0
56	MG	2A	3507	1/1	0.78	0.14	31,31,31,31	0
56	MG	2A	3780	1/1	0.78	0.07	60,60,60,60	0
56	MG	1A	3951	1/1	0.79	0.15	47,47,47,47	0
56	MG	1E	305	1/1	0.79	0.14	49,49,49,49	0
56	MG	1G	202	1/1	0.79	0.22	53,53,53,53	0
56	MG	2a	3053	1/1	0.79	0.23	67,67,67,67	0
56	MG	2a	3071	1/1	0.79	0.14	51,51,51,51	0
56	MG	2A	3534	1/1	0.79	0.13	54,54,54,54	0
56	MG	1x	101	1/1	0.79	0.16	49,49,49,49	0
56	MG	1A	4030	1/1	0.79	0.07	62,62,62,62	0
56	MG	1A	3414	1/1	0.79	0.30	44,44,44,44	0
56	MG	1a	1603	1/1	0.79	0.48	65,65,65,65	0
56	MG	1a	1605	1/1	0.79	0.67	54,54,54,54	0
56	MG	1A	3426	1/1	0.79	0.38	49,49,49,49	0
56	MG	2A	3854	1/1	0.79	0.58	39,39,39,39	0
56	MG	2A	3331	1/1	0.79	0.33	56,56,56,56	0
56	MG	1A	3886	1/1	0.79	0.39	50,50,50,50	0
56	MG	1A	4103	1/1	0.79	0.15	17,17,17,17	0
56	MG	1A	3525	1/1	0.79	0.83	44,44,44,44	0
56	MG	2a	3151	1/1	0.79	0.10	50,50,50,50	0
56	MG	2F	301	1/1	0.79	0.14	41,41,41,41	0
56	MG	1a	1796	1/1	0.79	0.10	47,47,47,47	0
56	MG	1a	1628	1/1	0.79	0.12	52,52,52,52	0
56	MG	1A	3386	1/1	0.79	0.19	34,34,34,34	0
56	MG	1a	1662	1/1	0.79	0.16	66,66,66,66	0
56	MG	2a	3177	1/1	0.79	0.21	59,59,59,59	0
56	MG	1A	3453	1/1	0.79	0.41	37,37,37,37	0
56	MG	2A	3750	1/1	0.79	0.29	58,58,58,58	0
56	MG	2a	3011	1/1	0.79	0.20	58,58,58,58	0
56	MG	1A	3917	1/1	0.79	0.15	64,64,64,64	0
56	MG	1a	1699	1/1	0.79	0.24	48,48,48,48	0
56	MG	1a	1822	1/1	0.79	0.17	58,58,58,58	0
56	MG	1A	3466	1/1	0.79	0.19	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	3028	1/1	0.79	0.13	71,71,71,71	0
56	MG	1A	3702	1/1	0.80	0.19	54,54,54,54	0
56	MG	1A	3457	1/1	0.80	0.14	53,53,53,53	0
56	MG	1A	3539	1/1	0.80	0.24	49,49,49,49	0
56	MG	1A	3225	1/1	0.80	0.27	54,54,54,54	0
56	MG	2A	3326	1/1	0.80	0.33	52,52,52,52	0
56	MG	1A	4053	1/1	0.80	1.07	62,62,62,62	0
56	MG	2A	3335	1/1	0.80	0.21	53,53,53,53	0
56	MG	2A	3725	1/1	0.80	0.14	50,50,50,50	0
56	MG	2A	3737	1/1	0.80	0.14	38,38,38,38	0
56	MG	2A	3747	1/1	0.80	0.11	56,56,56,56	0
56	MG	1A	3761	1/1	0.80	0.12	19,19,19,19	0
56	MG	2A	3070	1/1	0.80	0.21	54,54,54,54	0
56	MG	2a	3070	1/1	0.80	0.48	55,55,55,55	0
56	MG	1A	3969	1/1	0.80	0.17	43,43,43,43	0
56	MG	2A	3086	1/1	0.80	0.25	59,59,59,59	0
56	MG	2A	3103	1/1	0.80	0.13	38,38,38,38	0
56	MG	2A	3776	1/1	0.80	0.16	63,63,63,63	0
56	MG	1A	3788	1/1	0.80	0.18	31,31,31,31	0
56	MG	2A	3413	1/1	0.80	0.09	53,53,53,53	0
56	MG	1A	3148	1/1	0.80	0.27	28,28,28,28	0
56	MG	2A	3173	1/1	0.80	0.28	55,55,55,55	0
56	MG	1a	1601	1/1	0.80	0.18	50,50,50,50	0
56	MG	2A	3809	1/1	0.80	0.30	50,50,50,50	0
56	MG	2A	3178	1/1	0.80	0.42	48,48,48,48	0
56	MG	1a	1817	1/1	0.80	0.16	72,72,72,72	0
56	MG	1a	1818	1/1	0.80	0.12	68,68,68,68	0
56	MG	1A	3807	1/1	0.80	0.37	45,45,45,45	0
56	MG	2a	3154	1/1	0.80	0.12	77,77,77,77	0
56	MG	2A	3844	1/1	0.80	0.14	61,61,61,61	0
56	MG	1A	3425	1/1	0.80	0.18	34,34,34,34	0
56	MG	2A	3246	1/1	0.80	0.32	43,43,43,43	0
56	MG	2A	3853	1/1	0.80	0.20	36,36,36,36	0
56	MG	2A	3522	1/1	0.80	0.10	39,39,39,39	0
56	MG	1A	3670	1/1	0.80	0.17	45,45,45,45	0
56	MG	2a	3204	1/1	0.80	0.17	57,57,57,57	0
56	MG	1a	1761	1/1	0.80	0.17	50,50,50,50	0
56	MG	2A	3259	1/1	0.80	0.36	53,53,53,53	0
56	MG	1A	3680	1/1	0.80	0.13	20,20,20,20	0
56	MG	2A	3604	1/1	0.80	0.11	40,40,40,40	0
56	MG	2a	3229	1/1	0.80	0.08	52,52,52,52	0
56	MG	1w	106	1/1	0.80	0.19	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	1615	1/1	0.80	0.24	51,51,51,51	0
56	MG	1A	3700	1/1	0.80	0.16	31,31,31,31	0
56	MG	1x	109	1/1	0.80	0.21	55,55,55,55	0
56	MG	2A	3684	1/1	0.81	0.14	64,64,64,64	0
56	MG	1B	201	1/1	0.81	0.43	42,42,42,42	0
56	MG	2A	3098	1/1	0.81	0.11	46,46,46,46	0
56	MG	1A	3988	1/1	0.81	0.09	75,75,75,75	0
56	MG	1A	3711	1/1	0.81	0.10	54,54,54,54	0
56	MG	1A	3640	1/1	0.81	0.29	36,36,36,36	0
56	MG	2A	3298	1/1	0.81	0.24	60,60,60,60	0
56	MG	2A	3306	1/1	0.81	0.57	49,49,49,49	0
56	MG	1A	3240	1/1	0.81	0.30	57,57,57,57	0
56	MG	1A	3271	1/1	0.81	0.15	41,41,41,41	0
56	MG	1A	3621	1/1	0.81	0.19	26,26,26,26	0
56	MG	2A	3320	1/1	0.81	0.11	58,58,58,58	0
56	MG	2A	3184	1/1	0.81	0.16	53,53,53,53	0
56	MG	2A	3191	1/1	0.81	0.38	43,43,43,43	0
56	MG	2A	3202	1/1	0.81	0.41	56,56,56,56	0
56	MG	1A	4095	1/1	0.81	0.31	44,44,44,44	0
56	MG	2A	3047	1/1	0.81	0.13	63,63,63,63	0
56	MG	1A	3777	1/1	0.81	0.14	39,39,39,39	0
56	MG	2a	3197	1/1	0.81	0.08	72,72,72,72	0
56	MG	1a	1672	1/1	0.81	0.34	51,51,51,51	0
56	MG	1A	3420	1/1	0.81	0.56	45,45,45,45	0
56	MG	2A	3646	1/1	0.81	0.22	47,47,47,47	0
56	MG	2A	3069	1/1	0.81	0.13	52,52,52,52	0
56	MG	2A	3407	1/1	0.81	0.10	40,40,40,40	0
56	MG	2A	3665	1/1	0.81	0.07	40,40,40,40	0
56	MG	1A	3469	1/1	0.81	0.28	61,61,61,61	0
56	MG	1A	3477	1/1	0.81	0.13	31,31,31,31	0
56	MG	2a	3085	1/1	0.81	0.16	63,63,63,63	0
56	MG	2A	3850	1/1	0.81	0.63	70,70,70,70	0
56	MG	2A	3425	1/1	0.82	0.11	70,70,70,70	0
56	MG	2A	3256	1/1	0.82	0.18	60,60,60,60	0
56	MG	1A	3842	1/1	0.82	0.15	61,61,61,61	0
56	MG	1a	1633	1/1	0.82	0.14	57,57,57,57	0
56	MG	2A	3269	1/1	0.82	0.19	49,49,49,49	0
56	MG	2a	3075	1/1	0.82	0.10	53,53,53,53	0
56	MG	1A	3755	1/1	0.82	0.22	16,16,16,16	0
56	MG	1a	1641	1/1	0.82	0.21	49,49,49,49	0
56	MG	1A	3110	1/1	0.82	0.32	33,33,33,33	0
56	MG	2A	3281	1/1	0.82	0.17	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	3445	1/1	0.82	0.36	51,51,51,51	0
56	MG	1A	3534	1/1	0.82	0.15	52,52,52,52	0
56	MG	2A	3830	1/1	0.82	0.12	45,45,45,45	0
56	MG	1A	3470	1/1	0.82	0.30	46,46,46,46	0
56	MG	2A	3594	1/1	0.82	0.16	71,71,71,71	0
56	MG	1A	3910	1/1	0.82	0.06	67,67,67,67	0
56	MG	1A	4057	1/1	0.82	0.10	34,34,34,34	0
56	MG	1A	3316	1/1	0.82	0.19	27,27,27,27	0
56	MG	2A	3144	1/1	0.82	0.20	56,56,56,56	0
56	MG	2A	3159	1/1	0.82	0.10	66,66,66,66	0
56	MG	2A	3325	1/1	0.82	0.34	60,60,60,60	0
56	MG	2a	3156	1/1	0.82	0.12	49,49,49,49	0
56	MG	1A	3213	1/1	0.82	0.24	32,32,32,32	0
56	MG	1A	4064	1/1	0.82	0.14	54,54,54,54	0
56	MG	1a	1827	1/1	0.82	0.11	51,51,51,51	0
56	MG	1A	3913	1/1	0.82	0.15	61,61,61,61	0
56	MG	2a	3167	1/1	0.82	0.07	67,67,67,67	0
56	MG	1A	3916	1/1	0.82	0.09	56,56,56,56	0
56	MG	2A	3357	1/1	0.82	0.24	48,48,48,48	0
56	MG	2a	3178	1/1	0.82	0.11	42,42,42,42	0
56	MG	2A	3199	1/1	0.82	0.17	50,50,50,50	0
56	MG	2A	3699	1/1	0.82	0.12	52,52,52,52	0
56	MG	1A	3821	1/1	0.82	0.20	41,41,41,41	0
56	MG	1a	1776	1/1	0.82	0.19	62,62,62,62	0
56	MG	2A	3405	1/1	0.82	0.14	47,47,47,47	0
56	MG	1A	3919	1/1	0.82	0.13	25,25,25,25	0
56	MG	1a	1782	1/1	0.82	0.08	70,70,70,70	0
56	MG	1A	4029	1/1	0.82	0.13	31,31,31,31	0
56	MG	1a	1619	1/1	0.82	0.11	43,43,43,43	0
56	MG	1A	3741	1/1	0.82	0.16	32,32,32,32	0
56	MG	2y	104	1/1	0.82	0.13	59,59,59,59	0
56	MG	1A	3488	1/1	0.82	0.82	36,36,36,36	0
56	MG	1A	3395	1/1	0.83	0.39	29,29,29,29	0
56	MG	2A	3092	1/1	0.83	0.10	44,44,44,44	0
56	MG	2a	3037	1/1	0.83	0.18	50,50,50,50	0
56	MG	1A	3632	1/1	0.83	0.15	33,33,33,33	0
56	MG	2A	3760	1/1	0.83	0.07	57,57,57,57	0
56	MG	2A	3766	1/1	0.83	0.08	76,76,76,76	0
56	MG	1A	3809	1/1	0.83	0.18	12,12,12,12	0
56	MG	1A	3819	1/1	0.83	0.18	47,47,47,47	0
56	MG	2A	3521	1/1	0.83	0.15	33,33,33,33	0
56	MG	2A	3112	1/1	0.83	0.23	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	10	105	1/1	0.83	0.24	56,56,56,56	0
56	MG	1A	3731	1/1	0.83	0.19	13,13,13,13	0
56	MG	2A	3539	1/1	0.83	0.19	40,40,40,40	0
56	MG	2A	3545	1/1	0.83	0.18	27,27,27,27	0
56	MG	2A	3798	1/1	0.83	0.10	25,25,25,25	0
56	MG	1A	4023	1/1	0.83	0.24	70,70,70,70	0
56	MG	2A	3165	1/1	0.83	0.12	60,60,60,60	0
56	MG	2A	3582	1/1	0.83	0.07	51,51,51,51	0
56	MG	2A	3591	1/1	0.83	0.17	35,35,35,35	0
56	MG	1A	4079	1/1	0.83	0.09	30,30,30,30	0
56	MG	2a	3136	1/1	0.83	0.23	70,70,70,70	0
56	MG	2A	3597	1/1	0.83	0.06	66,66,66,66	0
56	MG	1f	202	1/1	0.83	0.12	59,59,59,59	0
56	MG	1A	3827	1/1	0.83	0.21	55,55,55,55	0
56	MG	1A	3398	1/1	0.83	0.31	45,45,45,45	0
56	MG	1A	3934	1/1	0.83	0.23	49,49,49,49	0
56	MG	2a	3155	1/1	0.83	0.20	65,65,65,65	0
56	MG	1A	3411	1/1	0.83	0.50	52,52,52,52	0
56	MG	1A	3448	1/1	0.83	0.18	41,41,41,41	0
56	MG	1A	3983	1/1	0.83	0.15	21,21,21,21	0
56	MG	2B	204	1/1	0.83	0.13	68,68,68,68	0
56	MG	1A	3168	1/1	0.83	0.34	31,31,31,31	0
56	MG	2a	3166	1/1	0.83	0.15	59,59,59,59	0
56	MG	1A	3313	1/1	0.83	0.14	60,60,60,60	0
56	MG	1a	1636	1/1	0.83	0.16	45,45,45,45	0
56	MG	2A	3024	1/1	0.83	0.14	67,67,67,67	0
56	MG	1a	1637	1/1	0.83	0.22	49,49,49,49	0
56	MG	2A	3252	1/1	0.83	0.19	54,54,54,54	0
56	MG	1A	3501	1/1	0.83	0.39	46,46,46,46	0
56	MG	2V	202	1/1	0.83	0.14	47,47,47,47	0
56	MG	20	102	1/1	0.83	0.14	59,59,59,59	0
56	MG	25	101	1/1	0.83	0.29	37,37,37,37	0
56	MG	2A	3710	1/1	0.83	0.12	52,52,52,52	0
56	MG	1A	3779	1/1	0.83	0.14	59,59,59,59	0
56	MG	1a	1645	1/1	0.83	0.34	54,54,54,54	0
56	MG	1A	3994	1/1	0.83	0.12	40,40,40,40	0
56	MG	2A	3735	1/1	0.83	0.17	59,59,59,59	0
56	MG	1a	1809	1/1	0.83	0.44	69,69,69,69	0
56	MG	1A	3361	1/1	0.83	0.57	50,50,50,50	0
59	ZN	24	501	1/1	0.83	0.05	113,113,113,113	0
56	MG	1A	3344	1/1	0.84	0.18	32,32,32,32	0
56	MG	2A	3119	1/1	0.84	0.28	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3276	1/1	0.84	0.13	49,49,49,49	0
56	MG	2A	3504	1/1	0.84	0.25	63,63,63,63	0
56	MG	1A	3585	1/1	0.84	0.15	35,35,35,35	0
56	MG	2A	3140	1/1	0.84	0.23	54,54,54,54	0
56	MG	2A	3142	1/1	0.84	0.36	57,57,57,57	0
56	MG	2a	3055	1/1	0.84	0.10	58,58,58,58	0
56	MG	1x	103	1/1	0.84	0.11	57,57,57,57	0
56	MG	1A	3390	1/1	0.84	0.24	45,45,45,45	0
56	MG	1A	3220	1/1	0.84	0.23	34,34,34,34	0
56	MG	2A	3782	1/1	0.84	0.26	50,50,50,50	0
56	MG	2A	3536	1/1	0.84	0.14	30,30,30,30	0
56	MG	2A	3310	1/1	0.84	0.23	63,63,63,63	0
56	MG	2A	3311	1/1	0.84	0.20	49,49,49,49	0
56	MG	1a	1683	1/1	0.84	0.20	60,60,60,60	0
56	MG	2A	3549	1/1	0.84	0.08	39,39,39,39	0
56	MG	2A	3175	1/1	0.84	0.12	59,59,59,59	0
56	MG	2A	3176	1/1	0.84	0.37	54,54,54,54	0
56	MG	1A	3026	1/1	0.84	0.42	56,56,56,56	0
56	MG	2A	3827	1/1	0.84	0.16	57,57,57,57	0
56	MG	1A	3490	1/1	0.84	0.30	28,28,28,28	0
56	MG	2A	3322	1/1	0.84	0.34	64,64,64,64	0
56	MG	2a	3146	1/1	0.84	0.19	72,72,72,72	0
56	MG	2A	3596	1/1	0.84	0.14	61,61,61,61	0
56	MG	2A	3006	1/1	0.84	0.18	49,49,49,49	0
56	MG	2A	3847	1/1	0.84	0.17	50,50,50,50	0
56	MG	2A	3020	1/1	0.84	0.19	54,54,54,54	0
56	MG	1A	3722	1/1	0.84	0.12	52,52,52,52	0
56	MG	2A	3334	1/1	0.84	0.10	49,49,49,49	0
56	MG	1a	1709	1/1	0.84	0.55	56,56,56,56	0
56	MG	2A	3628	1/1	0.84	0.12	35,35,35,35	0
56	MG	2A	3861	1/1	0.84	0.33	46,46,46,46	0
56	MG	1A	3459	1/1	0.84	0.17	44,44,44,44	0
56	MG	2A	3349	1/1	0.84	0.87	49,49,49,49	0
56	MG	2A	3230	1/1	0.84	0.37	56,56,56,56	0
56	MG	1A	4011	1/1	0.84	0.14	23,23,23,23	0
56	MG	1A	4012	1/1	0.84	0.17	17,17,17,17	0
56	MG	2A	3367	1/1	0.84	0.12	47,47,47,47	0
56	MG	1A	3514	1/1	0.84	0.18	38,38,38,38	0
56	MG	2A	3243	1/1	0.84	0.40	47,47,47,47	0
56	MG	1A	3370	1/1	0.84	0.36	40,40,40,40	0
56	MG	1B	236	1/1	0.84	0.13	31,31,31,31	0
56	MG	21	101	1/1	0.84	0.78	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	1A	3432	1/1	0.84	0.17	55,55,55,55	0
56	MG	1A	3651	1/1	0.84	0.12	39,39,39,39	0
56	MG	1A	3405	1/1	0.84	0.17	35,35,35,35	0
56	MG	2r	101	1/1	0.84	0.12	62,62,62,62	0
56	MG	1a	1640	1/1	0.84	0.29	59,59,59,59	0
56	MG	2A	3261	1/1	0.84	0.25	52,52,52,52	0
56	MG	1A	3541	1/1	0.84	0.17	46,46,46,46	0
56	MG	2A	3739	1/1	0.84	0.26	39,39,39,39	0
56	MG	2A	3439	1/1	0.84	0.36	63,63,63,63	0
56	MG	1A	3876	1/1	0.85	0.40	49,49,49,49	0
56	MG	1A	3518	1/1	0.85	0.15	43,43,43,43	0
56	MG	1A	3752	1/1	0.85	0.15	16,16,16,16	0
56	MG	2B	202	1/1	0.85	0.27	44,44,44,44	0
56	MG	2A	3260	1/1	0.85	0.60	59,59,59,59	0
56	MG	1F	308	1/1	0.85	0.23	37,37,37,37	0
56	MG	1A	3754	1/1	0.85	0.14	22,22,22,22	0
56	MG	1y	103	1/1	0.85	0.12	72,72,72,72	0
56	MG	2A	3586	1/1	0.85	0.25	55,55,55,55	0
56	MG	1a	1727	1/1	0.85	0.43	58,58,58,58	0
56	MG	2A	3273	1/1	0.85	0.21	57,57,57,57	0
56	MG	1a	1730	1/1	0.85	0.19	52,52,52,52	0
56	MG	2T	202	1/1	0.85	0.12	46,46,46,46	0
56	MG	2T	204	1/1	0.85	0.29	57,57,57,57	0
56	MG	2A	3016	1/1	0.85	0.10	41,41,41,41	0
56	MG	2A	3600	1/1	0.85	0.23	52,52,52,52	0
56	MG	1a	1749	1/1	0.85	0.32	57,57,57,57	0
56	MG	1A	3207	1/1	0.85	0.16	47,47,47,47	0
56	MG	2A	3615	1/1	0.85	0.17	42,42,42,42	0
56	MG	1N	206	1/1	0.85	0.19	40,40,40,40	0
56	MG	1P	202	1/1	0.85	0.11	22,22,22,22	0
56	MG	2A	3052	1/1	0.85	0.18	52,52,52,52	0
56	MG	1A	3267	1/1	0.85	0.38	47,47,47,47	0
56	MG	1a	1767	1/1	0.85	0.09	60,60,60,60	0
56	MG	1a	1771	1/1	0.85	0.17	45,45,45,45	0
56	MG	2a	3024	1/1	0.85	1.25	57,57,57,57	0
56	MG	2a	3025	1/1	0.85	0.95	57,57,57,57	0
56	MG	1Z	304	1/1	0.85	0.21	52,52,52,52	0
56	MG	2A	3078	1/1	0.85	0.11	54,54,54,54	0
56	MG	2A	3667	1/1	0.85	0.22	56,56,56,56	0
56	MG	1a	1777	1/1	0.85	0.31	61,61,61,61	0
56	MG	1A	3082	1/1	0.85	0.22	28,28,28,28	0
56	MG	1A	3472	1/1	0.85	0.39	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	3556	1/1	0.85	0.37	40,40,40,40	0
56	MG	1a	1604	1/1	0.85	0.15	53,53,53,53	0
56	MG	2A	3329	1/1	0.85	0.58	58,58,58,58	0
56	MG	1A	3914	1/1	0.85	0.18	41,41,41,41	0
56	MG	2A	3108	1/1	0.85	0.35	49,49,49,49	0
56	MG	1A	3781	1/1	0.85	0.20	48,48,48,48	0
56	MG	2A	3343	1/1	0.85	0.11	63,63,63,63	0
56	MG	1A	3665	1/1	0.85	0.15	19,19,19,19	0
56	MG	1a	1795	1/1	0.85	0.13	58,58,58,58	0
56	MG	2A	3744	1/1	0.85	0.14	38,38,38,38	0
56	MG	2A	3139	1/1	0.85	0.49	53,53,53,53	0
56	MG	1a	1614	1/1	0.85	0.12	46,46,46,46	0
56	MG	1a	1797	1/1	0.85	0.14	46,46,46,46	0
56	MG	2a	3124	1/1	0.85	0.20	68,68,68,68	0
56	MG	2A	3752	1/1	0.85	0.12	59,59,59,59	0
56	MG	1A	3359	1/1	0.85	0.30	37,37,37,37	0
56	MG	2A	3155	1/1	0.85	0.27	56,56,56,56	0
56	MG	1A	4071	1/1	0.85	0.10	38,38,38,38	0
56	MG	2A	3403	1/1	0.85	0.18	45,45,45,45	0
56	MG	2A	3770	1/1	0.85	0.20	77,77,77,77	0
56	MG	1A	3921	1/1	0.85	0.16	39,39,39,39	0
56	MG	1A	3442	1/1	0.85	0.30	55,55,55,55	0
56	MG	2A	3779	1/1	0.85	0.49	55,55,55,55	0
56	MG	1A	3694	1/1	0.85	0.18	21,21,21,21	0
56	MG	1A	3007	1/1	0.85	0.16	33,33,33,33	0
56	MG	1A	3598	1/1	0.85	0.18	20,20,20,20	0
56	MG	1A	3615	1/1	0.85	0.16	29,29,29,29	0
56	MG	2A	3786	1/1	0.85	0.13	65,65,65,65	0
56	MG	2A	3788	1/1	0.85	0.07	48,48,48,48	0
56	MG	2A	3421	1/1	0.85	0.17	43,43,43,43	0
56	MG	2A	3792	1/1	0.85	0.07	63,63,63,63	0
56	MG	2A	3793	1/1	0.85	0.18	31,31,31,31	0
56	MG	1A	3307	1/1	0.85	0.27	49,49,49,49	0
56	MG	1A	3367	1/1	0.85	0.16	51,51,51,51	0
56	MG	2a	3187	1/1	0.85	0.13	57,57,57,57	0
56	MG	1A	3064	1/1	0.85	0.19	42,42,42,42	0
56	MG	2A	3448	1/1	0.85	0.13	36,36,36,36	0
56	MG	2a	3205	1/1	0.85	0.12	61,61,61,61	0
56	MG	1B	206	1/1	0.85	0.19	46,46,46,46	0
56	MG	1A	3861	1/1	0.85	0.31	30,30,30,30	0
56	MG	1a	1834	1/1	0.85	0.09	54,54,54,54	0
56	MG	1A	3018	1/1	0.85	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3233	1/1	0.85	0.11	55,55,55,55	0
56	MG	2d	301	1/1	0.85	0.16	48,48,48,48	0
56	MG	2A	3840	1/1	0.85	0.09	47,47,47,47	0
56	MG	1B	225	1/1	0.85	0.14	31,31,31,31	0
56	MG	1A	3872	1/1	0.85	0.14	19,19,19,19	0
56	MG	1w	102	1/1	0.85	0.31	60,60,60,60	0
56	MG	1w	105	1/1	0.85	0.13	62,62,62,62	0
56	MG	1A	3956	1/1	0.85	0.41	61,61,61,61	0
56	MG	1a	1693	1/1	0.85	0.40	66,66,66,66	0
56	MG	2A	3263	1/1	0.86	0.18	51,51,51,51	0
56	MG	1A	3803	1/1	0.86	0.15	55,55,55,55	0
56	MG	2A	3541	1/1	0.86	0.13	38,38,38,38	0
56	MG	1A	3681	1/1	0.86	0.07	56,56,56,56	0
56	MG	2A	3053	1/1	0.86	0.10	44,44,44,44	0
56	MG	1A	4066	1/1	0.86	0.33	62,62,62,62	0
56	MG	1A	3688	1/1	0.86	0.20	39,39,39,39	0
56	MG	2A	3572	1/1	0.86	0.19	75,75,75,75	0
56	MG	1a	1788	1/1	0.86	0.18	65,65,65,65	0
56	MG	2E	307	1/1	0.86	0.14	57,57,57,57	0
56	MG	1A	3250	1/1	0.86	0.17	31,31,31,31	0
56	MG	1A	3251	1/1	0.86	0.19	28,28,28,28	0
56	MG	2A	3286	1/1	0.86	0.42	56,56,56,56	0
56	MG	1A	3400	1/1	0.86	0.12	30,30,30,30	0
56	MG	2A	3296	1/1	0.86	0.23	53,53,53,53	0
56	MG	2A	3081	1/1	0.86	0.11	56,56,56,56	0
56	MG	2A	3603	1/1	0.86	0.18	39,39,39,39	0
56	MG	1A	3998	1/1	0.86	0.20	49,49,49,49	0
56	MG	2A	3307	1/1	0.86	0.33	51,51,51,51	0
56	MG	2A	3308	1/1	0.86	0.33	55,55,55,55	0
56	MG	1A	3447	1/1	0.86	0.37	63,63,63,63	0
56	MG	2a	3002	1/1	0.86	0.16	44,44,44,44	0
56	MG	1A	4007	1/1	0.86	0.14	54,54,54,54	0
56	MG	1a	1799	1/1	0.86	0.09	54,54,54,54	0
56	MG	2a	3009	1/1	0.86	0.38	64,64,64,64	0
56	MG	1A	3216	1/1	0.86	0.73	32,32,32,32	0
56	MG	1A	3332	1/1	0.86	0.16	34,34,34,34	0
56	MG	1A	3944	1/1	0.86	0.07	41,41,41,41	0
56	MG	1A	3623	1/1	0.86	0.12	33,33,33,33	0
56	MG	1A	4020	1/1	0.86	0.22	59,59,59,59	0
56	MG	1A	3865	1/1	0.86	0.69	42,42,42,42	0
56	MG	1a	1667	1/1	0.86	0.17	48,48,48,48	0
56	MG	1A	3059	1/1	0.86	0.13	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3033	1/1	0.86	0.09	55,55,55,55	0
56	MG	2A	3679	1/1	0.86	0.18	53,53,53,53	0
56	MG	1A	3626	1/1	0.86	0.14	42,42,42,42	0
56	MG	2A	3333	1/1	0.86	0.34	63,63,63,63	0
56	MG	2A	3149	1/1	0.86	0.05	52,52,52,52	0
56	MG	2A	3150	1/1	0.86	0.12	40,40,40,40	0
56	MG	2A	3712	1/1	0.86	0.17	55,55,55,55	0
56	MG	2a	3058	1/1	0.86	0.10	55,55,55,55	0
56	MG	2a	3065	1/1	0.86	0.12	38,38,38,38	0
56	MG	1A	3353	1/1	0.86	0.15	56,56,56,56	0
56	MG	1A	3953	1/1	0.86	0.09	25,25,25,25	0
56	MG	1A	3107	1/1	0.86	0.29	40,40,40,40	0
56	MG	2A	3727	1/1	0.86	0.15	58,58,58,58	0
56	MG	2A	3734	1/1	0.86	0.16	51,51,51,51	0
56	MG	2A	3354	1/1	0.86	0.14	45,45,45,45	0
56	MG	2A	3172	1/1	0.86	0.22	61,61,61,61	0
56	MG	1A	3528	1/1	0.86	0.16	37,37,37,37	0
56	MG	1A	3965	1/1	0.86	0.12	52,52,52,52	0
56	MG	2A	3364	1/1	0.86	0.19	40,40,40,40	0
56	MG	1A	3532	1/1	0.86	0.15	39,39,39,39	0
56	MG	1A	3161	1/1	0.86	0.25	40,40,40,40	0
56	MG	2a	3129	1/1	0.86	0.18	51,51,51,51	0
56	MG	1a	1714	1/1	0.86	0.24	44,44,44,44	0
56	MG	2A	3376	1/1	0.86	0.14	55,55,55,55	0
56	MG	2A	3380	1/1	0.86	0.23	63,63,63,63	0
56	MG	2a	3137	1/1	0.86	0.05	64,64,64,64	0
56	MG	2A	3761	1/1	0.86	0.16	54,54,54,54	0
56	MG	2A	3384	1/1	0.86	0.18	47,47,47,47	0
56	MG	2A	3180	1/1	0.86	0.89	61,61,61,61	0
56	MG	1w	101	1/1	0.86	0.17	49,49,49,49	0
56	MG	2A	3771	1/1	0.86	0.15	53,53,53,53	0
56	MG	1N	204	1/1	0.86	0.72	41,41,41,41	0
56	MG	1a	1720	1/1	0.86	0.26	39,39,39,39	0
56	MG	1a	1722	1/1	0.86	0.21	42,42,42,42	0
56	MG	1A	4042	1/1	0.86	0.45	47,47,47,47	0
56	MG	2A	3219	1/1	0.86	0.28	45,45,45,45	0
56	MG	1O	201	1/1	0.86	0.16	51,51,51,51	0
56	MG	1a	1739	1/1	0.86	0.09	51,51,51,51	0
56	MG	1A	3971	1/1	0.86	0.17	35,35,35,35	0
56	MG	2A	3431	1/1	0.86	0.18	54,54,54,54	0
56	MG	2a	3171	1/1	0.86	0.15	61,61,61,61	0
56	MG	1A	3430	1/1	0.86	0.44	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	3442	1/1	0.86	0.35	44,44,44,44	0
56	MG	2A	3445	1/1	0.86	1.56	49,49,49,49	0
56	MG	2A	3795	1/1	0.86	0.12	39,39,39,39	0
56	MG	1x	113	1/1	0.86	0.20	61,61,61,61	0
56	MG	1Y	203	1/1	0.86	0.19	43,43,43,43	0
56	MG	2A	3483	1/1	0.86	0.15	34,34,34,34	0
56	MG	2A	3244	1/1	0.86	0.26	49,49,49,49	0
56	MG	1A	3358	1/1	0.86	0.20	43,43,43,43	0
56	MG	1y	104	1/1	0.86	0.12	70,70,70,70	0
56	MG	1A	4052	1/1	0.86	0.20	21,21,21,21	0
56	MG	2A	3829	1/1	0.86	0.10	34,34,34,34	0
56	MG	1A	3475	1/1	0.86	0.26	30,30,30,30	0
56	MG	1A	3787	1/1	0.86	0.15	25,25,25,25	0
56	MG	2A	3257	1/1	0.86	0.13	46,46,46,46	0
56	MG	1A	3476	1/1	0.86	0.16	37,37,37,37	0
56	MG	2A	3523	1/1	0.86	0.07	28,28,28,28	0
56	MG	2A	3524	1/1	0.86	0.18	62,62,62,62	0
56	MG	1A	3577	1/1	0.86	0.23	47,47,47,47	0
56	MG	1a	1780	1/1	0.86	0.16	56,56,56,56	0
56	MG	2A	3609	1/1	0.87	0.12	43,43,43,43	0
56	MG	2a	3034	1/1	0.87	0.10	54,54,54,54	0
56	MG	2a	3035	1/1	0.87	0.17	62,62,62,62	0
56	MG	2A	3794	1/1	0.87	0.09	52,52,52,52	0
56	MG	2a	3041	1/1	0.87	0.15	55,55,55,55	0
56	MG	1A	3285	1/1	0.87	0.13	61,61,61,61	0
56	MG	1A	3017	1/1	0.87	0.50	49,49,49,49	0
56	MG	1A	3563	1/1	0.87	0.27	50,50,50,50	0
56	MG	2A	3162	1/1	0.87	0.20	56,56,56,56	0
56	MG	2a	3054	1/1	0.87	0.10	60,60,60,60	0
56	MG	2A	3810	1/1	0.87	0.17	58,58,58,58	0
56	MG	1A	3759	1/1	0.87	0.10	14,14,14,14	0
56	MG	1N	205	1/1	0.87	0.36	52,52,52,52	0
56	MG	1A	3259	1/1	0.87	0.12	36,36,36,36	0
56	MG	1A	3481	1/1	0.87	0.17	46,46,46,46	0
56	MG	2A	3433	1/1	0.87	0.61	44,44,44,44	0
56	MG	1A	3238	1/1	0.87	0.20	50,50,50,50	0
56	MG	2A	3832	1/1	0.87	0.36	46,46,46,46	0
56	MG	1Q	204	1/1	0.87	0.14	53,53,53,53	0
56	MG	1a	1695	1/1	0.87	0.21	37,37,37,37	0
56	MG	2A	3841	1/1	0.87	0.16	42,42,42,42	0
56	MG	1A	3454	1/1	0.87	0.68	33,33,33,33	0
56	MG	2A	3044	1/1	0.87	0.17	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	3467	1/1	0.87	0.21	53,53,53,53	0
56	MG	2A	3474	1/1	0.87	0.20	43,43,43,43	0
56	MG	1a	1703	1/1	0.87	0.22	51,51,51,51	0
56	MG	2a	3130	1/1	0.87	0.15	62,62,62,62	0
56	MG	2A	3499	1/1	0.87	0.23	54,54,54,54	0
56	MG	2A	3193	1/1	0.87	0.18	59,59,59,59	0
56	MG	2A	3856	1/1	0.87	0.77	45,45,45,45	0
56	MG	2A	3196	1/1	0.87	0.15	48,48,48,48	0
56	MG	1A	3954	1/1	0.87	0.08	60,60,60,60	0
56	MG	1A	3894	1/1	0.87	0.10	52,52,52,52	0
56	MG	1A	3424	1/1	0.87	0.12	39,39,39,39	0
56	MG	2B	206	1/1	0.87	0.10	56,56,56,56	0
56	MG	2A	3516	1/1	0.87	0.16	38,38,38,38	0
56	MG	14	101	1/1	0.87	0.14	60,60,60,60	0
56	MG	1A	3601	1/1	0.87	0.15	20,20,20,20	0
56	MG	1A	3968	1/1	0.87	0.10	66,66,66,66	0
56	MG	1A	4097	1/1	0.87	0.15	50,50,50,50	0
56	MG	2A	3071	1/1	0.87	0.85	47,47,47,47	0
56	MG	2F	305	1/1	0.87	0.19	53,53,53,53	0
56	MG	1A	3602	1/1	0.87	0.14	26,26,26,26	0
56	MG	2A	3535	1/1	0.87	0.13	43,43,43,43	0
56	MG	1A	3500	1/1	0.87	0.14	45,45,45,45	0
56	MG	1A	3198	1/1	0.87	0.11	17,17,17,17	0
56	MG	2U	203	1/1	0.87	0.44	42,42,42,42	0
56	MG	1a	1743	1/1	0.87	0.08	48,48,48,48	0
56	MG	1A	3465	1/1	0.87	0.14	56,56,56,56	0
56	MG	2A	3097	1/1	0.87	0.09	42,42,42,42	0
56	MG	1A	3810	1/1	0.87	0.12	25,25,25,25	0
56	MG	2A	3553	1/1	0.87	0.10	48,48,48,48	0
56	MG	1e	201	1/1	0.87	0.66	48,48,48,48	0
56	MG	1A	3088	1/1	0.87	0.17	20,20,20,20	0
56	MG	2a	3004	1/1	0.87	0.10	56,56,56,56	0
56	MG	1A	4035	1/1	0.87	0.34	44,44,44,44	0
56	MG	1A	3468	1/1	0.87	0.11	41,41,41,41	0
56	MG	2a	3010	1/1	0.87	0.30	61,61,61,61	0
56	MG	1A	4037	1/1	0.87	0.09	47,47,47,47	0
56	MG	1A	3338	1/1	0.87	0.18	35,35,35,35	0
56	MG	2j	202	1/1	0.87	0.12	70,70,70,70	0
56	MG	1A	3342	1/1	0.87	0.98	30,30,30,30	0
56	MG	1A	3364	1/1	0.87	0.39	38,38,38,38	0
56	MG	2A	3396	1/1	0.87	0.13	18,18,18,18	0
56	MG	1a	1779	1/1	0.87	0.12	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	1A	3751	1/1	0.87	0.12	28,28,28,28	0
56	MG	1A	3403	1/1	0.87	0.13	32,32,32,32	0
56	MG	2A	3352	1/1	0.88	0.11	36,36,36,36	0
56	MG	2F	302	1/1	0.88	0.21	52,52,52,52	0
56	MG	1A	3633	1/1	0.88	0.19	26,26,26,26	0
56	MG	1F	304	1/1	0.88	0.34	41,41,41,41	0
56	MG	1A	3634	1/1	0.88	0.16	26,26,26,26	0
56	MG	1A	3482	1/1	0.88	0.20	44,44,44,44	0
56	MG	1A	3907	1/1	0.88	0.55	55,55,55,55	0
56	MG	2A	3668	1/1	0.88	0.13	52,52,52,52	0
56	MG	1N	202	1/1	0.88	0.12	29,29,29,29	0
56	MG	1a	1711	1/1	0.88	0.20	48,48,48,48	0
56	MG	2A	3675	1/1	0.88	0.14	51,51,51,51	0
56	MG	2A	3189	1/1	0.88	0.13	39,39,39,39	0
56	MG	2A	3374	1/1	0.88	0.15	48,48,48,48	0
56	MG	2A	3686	1/1	0.88	0.14	48,48,48,48	0
56	MG	1A	3323	1/1	0.88	0.12	42,42,42,42	0
56	MG	1A	3770	1/1	0.88	0.14	34,34,34,34	0
56	MG	2A	3702	1/1	0.88	0.12	29,29,29,29	0
56	MG	2a	3006	1/1	0.88	0.09	63,63,63,63	0
56	MG	2A	3382	1/1	0.88	0.20	48,48,48,48	0
56	MG	1A	3462	1/1	0.88	0.41	49,49,49,49	0
56	MG	2A	3716	1/1	0.88	0.14	65,65,65,65	0
56	MG	2A	3718	1/1	0.88	0.22	42,42,42,42	0
56	MG	2a	3014	1/1	0.88	0.15	39,39,39,39	0
56	MG	2A	3719	1/1	0.88	0.09	64,64,64,64	0
56	MG	1A	3061	1/1	0.88	0.13	40,40,40,40	0
56	MG	2a	3017	1/1	0.88	0.13	66,66,66,66	0
56	MG	2A	3401	1/1	0.88	0.18	46,46,46,46	0
56	MG	1A	4050	1/1	0.88	0.12	30,30,30,30	0
56	MG	2A	3210	1/1	0.88	0.27	50,50,50,50	0
56	MG	1A	3662	1/1	0.88	0.10	10,10,10,10	0
56	MG	1a	1728	1/1	0.88	0.09	45,45,45,45	0
56	MG	1A	3495	1/1	0.88	0.16	37,37,37,37	0
56	MG	1a	1735	1/1	0.88	0.16	62,62,62,62	0
56	MG	1x	115	1/1	0.88	0.26	53,53,53,53	0
56	MG	1Y	202	1/1	0.88	0.23	53,53,53,53	0
56	MG	2A	3239	1/1	0.88	0.28	52,52,52,52	0
56	MG	1A	3205	1/1	0.88	0.22	26,26,26,26	0
56	MG	1a	1747	1/1	0.88	0.12	30,30,30,30	0
56	MG	1A	4056	1/1	0.88	0.11	44,44,44,44	0
56	MG	2A	3245	1/1	0.88	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	10	103	1/1	0.88	0.12	44,44,44,44	0
56	MG	1a	1756	1/1	0.88	0.16	67,67,67,67	0
56	MG	1A	3592	1/1	0.88	0.13	39,39,39,39	0
56	MG	1A	3152	1/1	0.88	0.52	31,31,31,31	0
56	MG	2a	3068	1/1	0.88	0.19	56,56,56,56	0
56	MG	1A	3922	1/1	0.88	0.21	46,46,46,46	0
56	MG	2A	3774	1/1	0.88	0.13	59,59,59,59	0
56	MG	1A	3923	1/1	0.88	0.12	32,32,32,32	0
56	MG	2A	3049	1/1	0.88	0.17	60,60,60,60	0
56	MG	2a	3081	1/1	0.88	0.20	59,59,59,59	0
56	MG	1A	3930	1/1	0.88	0.12	31,31,31,31	0
56	MG	1A	3683	1/1	0.88	0.14	26,26,26,26	0
56	MG	1A	3504	1/1	0.88	0.32	37,37,37,37	0
56	MG	1A	3062	1/1	0.88	0.19	30,30,30,30	0
56	MG	2a	3099	1/1	0.88	0.16	57,57,57,57	0
56	MG	1A	3609	1/1	0.88	0.14	20,20,20,20	0
56	MG	2a	3103	1/1	0.88	0.07	63,63,63,63	0
56	MG	1A	4086	1/1	0.88	0.23	59,59,59,59	0
56	MG	1A	4010	1/1	0.88	0.14	27,27,27,27	0
56	MG	2a	3116	1/1	0.88	0.14	65,65,65,65	0
56	MG	1A	3365	1/1	0.88	0.41	39,39,39,39	0
56	MG	2a	3126	1/1	0.88	0.16	50,50,50,50	0
56	MG	2A	3790	1/1	0.88	0.16	42,42,42,42	0
56	MG	2A	3277	1/1	0.88	0.48	61,61,61,61	0
56	MG	1a	1625	1/1	0.88	0.17	50,50,50,50	0
56	MG	1A	3616	1/1	0.88	0.09	28,28,28,28	0
56	MG	1A	3718	1/1	0.88	0.14	40,40,40,40	0
56	MG	2A	3528	1/1	0.88	0.14	51,51,51,51	0
56	MG	2A	3090	1/1	0.88	0.10	50,50,50,50	0
56	MG	2A	3807	1/1	0.88	0.08	64,64,64,64	0
56	MG	1A	3522	1/1	0.88	0.11	28,28,28,28	0
56	MG	2A	3094	1/1	0.88	0.19	48,48,48,48	0
56	MG	1A	3346	1/1	0.88	0.12	38,38,38,38	0
56	MG	2a	3153	1/1	0.88	0.07	61,61,61,61	0
56	MG	2A	3817	1/1	0.88	0.11	58,58,58,58	0
56	MG	1a	1794	1/1	0.88	0.21	60,60,60,60	0
56	MG	2A	3101	1/1	0.88	0.12	47,47,47,47	0
56	MG	2a	3157	1/1	0.88	0.10	58,58,58,58	0
56	MG	2a	3158	1/1	0.88	0.10	67,67,67,67	0
56	MG	2A	3543	1/1	0.88	0.13	31,31,31,31	0
56	MG	1A	4116	1/1	0.88	0.52	31,31,31,31	0
56	MG	2A	3309	1/1	0.88	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	2A	3831	1/1	0.88	0.16	49,49,49,49	0
56	MG	2A	3104	1/1	0.88	0.18	52,52,52,52	0
56	MG	2A	3560	1/1	0.88	0.09	30,30,30,30	0
56	MG	1A	3408	1/1	0.88	0.32	49,49,49,49	0
56	MG	1A	3733	1/1	0.88	0.11	28,28,28,28	0
56	MG	1A	3111	1/1	0.88	0.12	37,37,37,37	0
56	MG	1A	3190	1/1	0.88	0.12	49,49,49,49	0
56	MG	1a	1652	1/1	0.88	0.10	49,49,49,49	0
56	MG	2a	3188	1/1	0.88	0.14	71,71,71,71	0
56	MG	1a	1657	1/1	0.88	0.20	54,54,54,54	0
56	MG	2a	3199	1/1	0.88	0.10	56,56,56,56	0
56	MG	1a	1658	1/1	0.88	0.10	51,51,51,51	0
56	MG	2A	3324	1/1	0.88	0.15	50,50,50,50	0
56	MG	2a	3214	1/1	0.88	0.13	57,57,57,57	0
56	MG	1A	3379	1/1	0.88	0.21	27,27,27,27	0
56	MG	1a	1664	1/1	0.88	0.10	59,59,59,59	0
56	MG	1a	1666	1/1	0.88	0.27	56,56,56,56	0
56	MG	2A	3860	1/1	0.88	0.36	44,44,44,44	0
56	MG	1A	3224	1/1	0.88	0.18	34,34,34,34	0
56	MG	1A	3554	1/1	0.88	0.13	32,32,32,32	0
56	MG	1B	234	1/1	0.88	0.18	65,65,65,65	0
56	MG	2A	3160	1/1	0.88	0.09	54,54,54,54	0
56	MG	2q	201	1/1	0.88	0.11	56,56,56,56	0
56	MG	2B	208	1/1	0.88	0.24	56,56,56,56	0
56	MG	1A	4031	1/1	0.88	0.09	42,42,42,42	0
56	MG	1A	3964	1/1	0.88	0.30	36,36,36,36	0
56	MG	1a	1690	1/1	0.88	0.13	33,33,33,33	0
56	MG	2A	3632	1/1	0.88	0.10	54,54,54,54	0
56	MG	2E	308	1/1	0.88	0.10	48,48,48,48	0
56	MG	1A	3860	1/1	0.89	0.08	27,27,27,27	0
56	MG	1w	108	1/1	0.89	0.61	52,52,52,52	0
56	MG	1A	3619	1/1	0.89	0.14	17,17,17,17	0
56	MG	1A	3728	1/1	0.89	0.18	41,41,41,41	0
56	MG	1A	3730	1/1	0.89	0.18	25,25,25,25	0
56	MG	2A	3377	1/1	0.89	0.18	58,58,58,58	0
56	MG	2A	3379	1/1	0.89	0.63	52,52,52,52	0
56	MG	1A	3515	1/1	0.89	0.18	54,54,54,54	0
56	MG	1A	3136	1/1	0.89	0.15	31,31,31,31	0
56	MG	2A	3204	1/1	0.89	0.51	46,46,46,46	0
56	MG	2A	3207	1/1	0.89	0.14	44,44,44,44	0
56	MG	1A	3735	1/1	0.89	0.09	68,68,68,68	0
56	MG	2A	3212	1/1	0.89	0.28	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	3214	1/1	0.89	0.31	54,54,54,54	0
56	MG	2A	3406	1/1	0.89	0.20	53,53,53,53	0
56	MG	2a	3018	1/1	0.89	0.18	59,59,59,59	0
56	MG	1A	3140	1/1	0.89	0.18	33,33,33,33	0
56	MG	1A	3143	1/1	0.89	0.26	35,35,35,35	0
56	MG	2A	3229	1/1	0.89	0.74	46,46,46,46	0
56	MG	1a	1729	1/1	0.89	0.26	42,42,42,42	0
56	MG	1A	4049	1/1	0.89	0.10	31,31,31,31	0
56	MG	1A	3146	1/1	0.89	0.45	25,25,25,25	0
56	MG	1A	3328	1/1	0.89	0.18	36,36,36,36	0
56	MG	10	102	1/1	0.89	0.17	42,42,42,42	0
56	MG	2A	3754	1/1	0.89	0.15	46,46,46,46	0
56	MG	1A	3904	1/1	0.89	0.20	11,11,11,11	0
56	MG	2A	3021	1/1	0.89	0.15	52,52,52,52	0
56	MG	2a	3045	1/1	0.89	0.28	67,67,67,67	0
56	MG	1A	3977	1/1	0.89	0.14	42,42,42,42	0
56	MG	2A	3040	1/1	0.89	0.12	53,53,53,53	0
56	MG	13	101	1/1	0.89	0.16	46,46,46,46	0
56	MG	2A	3447	1/1	0.89	0.25	34,34,34,34	0
56	MG	1A	3906	1/1	0.89	0.10	28,28,28,28	0
56	MG	1A	3981	1/1	0.89	0.13	51,51,51,51	0
56	MG	1A	3105	1/1	0.89	0.61	26,26,26,26	0
56	MG	2A	3255	1/1	0.89	0.12	58,58,58,58	0
56	MG	2A	3050	1/1	0.89	0.26	49,49,49,49	0
56	MG	1A	3265	1/1	0.89	0.11	30,30,30,30	0
56	MG	1A	3090	1/1	0.89	0.11	55,55,55,55	0
56	MG	1A	3636	1/1	0.89	0.19	63,63,63,63	0
56	MG	2a	3078	1/1	0.89	0.15	56,56,56,56	0
56	MG	2a	3079	1/1	0.89	0.10	40,40,40,40	0
56	MG	1A	3991	1/1	0.89	0.17	47,47,47,47	0
56	MG	2A	3785	1/1	0.89	0.14	56,56,56,56	0
56	MG	2A	3066	1/1	0.89	0.65	44,44,44,44	0
56	MG	2A	3510	1/1	0.89	0.16	64,64,64,64	0
56	MG	2A	3267	1/1	0.89	0.12	44,44,44,44	0
56	MG	1A	3553	1/1	0.89	0.14	47,47,47,47	0
56	MG	1A	3474	1/1	0.89	0.57	30,30,30,30	0
56	MG	1A	3117	1/1	0.89	0.26	33,33,33,33	0
56	MG	2A	3076	1/1	0.89	0.22	42,42,42,42	0
56	MG	1A	3427	1/1	0.89	0.55	45,45,45,45	0
56	MG	2a	3111	1/1	0.89	0.12	60,60,60,60	0
56	MG	1A	3270	1/1	0.89	0.56	39,39,39,39	0
56	MG	1A	3785	1/1	0.89	0.14	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3801	1/1	0.89	0.11	41,41,41,41	0
56	MG	2A	3805	1/1	0.89	0.10	50,50,50,50	0
56	MG	2A	3082	1/1	0.89	0.42	36,36,36,36	0
56	MG	1A	3999	1/1	0.89	0.16	27,27,27,27	0
56	MG	1A	4004	1/1	0.89	0.31	73,73,73,73	0
56	MG	1A	4005	1/1	0.89	0.21	69,69,69,69	0
56	MG	2A	3815	1/1	0.89	0.08	59,59,59,59	0
56	MG	2A	3290	1/1	0.89	0.15	59,59,59,59	0
56	MG	2a	3144	1/1	0.89	0.09	74,74,74,74	0
56	MG	2A	3291	1/1	0.89	0.13	43,43,43,43	0
56	MG	2a	3147	1/1	0.89	0.09	71,71,71,71	0
56	MG	1A	3663	1/1	0.89	0.14	17,17,17,17	0
56	MG	1A	3569	1/1	0.89	0.80	36,36,36,36	0
56	MG	2A	3548	1/1	0.89	0.10	39,39,39,39	0
56	MG	1A	4118	1/1	0.89	1.01	35,35,35,35	0
56	MG	1A	3791	1/1	0.89	0.19	31,31,31,31	0
56	MG	1B	204	1/1	0.89	0.19	50,50,50,50	0
56	MG	1a	1648	1/1	0.89	0.15	54,54,54,54	0
56	MG	2A	3568	1/1	0.89	0.13	44,44,44,44	0
56	MG	1A	3380	1/1	0.89	0.14	33,33,33,33	0
56	MG	1a	1654	1/1	0.89	0.13	35,35,35,35	0
56	MG	1A	3382	1/1	0.89	0.16	31,31,31,31	0
56	MG	2A	3317	1/1	0.89	0.12	49,49,49,49	0
56	MG	1A	3440	1/1	0.89	0.49	33,33,33,33	0
56	MG	1A	3349	1/1	0.89	0.18	41,41,41,41	0
56	MG	1A	3352	1/1	0.89	0.18	37,37,37,37	0
56	MG	1B	230	1/1	0.89	0.11	53,53,53,53	0
56	MG	2A	3599	1/1	0.89	0.14	44,44,44,44	0
56	MG	1A	3391	1/1	0.89	0.23	58,58,58,58	0
56	MG	1B	232	1/1	0.89	0.11	48,48,48,48	0
56	MG	2a	3183	1/1	0.89	0.12	41,41,41,41	0
56	MG	1a	1674	1/1	0.89	0.16	55,55,55,55	0
56	MG	2B	201	1/1	0.89	0.21	64,64,64,64	0
56	MG	1A	3165	1/1	0.89	0.20	44,44,44,44	0
56	MG	2A	3153	1/1	0.89	0.09	36,36,36,36	0
56	MG	2a	3201	1/1	0.89	0.08	58,58,58,58	0
56	MG	2A	3330	1/1	0.89	0.20	49,49,49,49	0
56	MG	2A	3618	1/1	0.89	0.09	44,44,44,44	0
56	MG	1a	1678	1/1	0.89	0.10	43,43,43,43	0
56	MG	2A	3622	1/1	0.89	0.08	40,40,40,40	0
56	MG	1a	1682	1/1	0.89	0.09	50,50,50,50	0
56	MG	1A	3451	1/1	0.89	0.12	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	1A	3946	1/1	0.89	0.09	53,53,53,53	0
56	MG	2A	3341	1/1	0.89	0.13	49,49,49,49	0
56	MG	1b	301	1/1	0.89	0.16	76,76,76,76	0
56	MG	2A	3171	1/1	0.89	0.12	38,38,38,38	0
56	MG	2A	3348	1/1	0.89	0.33	63,63,63,63	0
56	MG	2l	202	1/1	0.89	0.14	50,50,50,50	0
56	MG	1A	3134	1/1	0.89	0.58	23,23,23,23	0
56	MG	1A	3355	1/1	0.89	0.23	34,34,34,34	0
56	MG	2x	103	1/1	0.89	0.10	62,62,62,62	0
56	MG	1F	305	1/1	0.89	0.24	31,31,31,31	0
56	MG	1F	306	1/1	0.89	0.36	17,17,17,17	0
56	MG	1a	1702	1/1	0.89	0.15	49,49,49,49	0
56	MG	1A	3234	1/1	0.89	0.29	40,40,40,40	0
56	MG	2y	106	1/1	0.89	0.14	72,72,72,72	0
57	LUJ	2A	3851	42/44	0.89	0.32	50,62,75,82	0
57	LUJ	2A	3852	42/44	0.89	0.56	38,59,68,75	0
56	MG	1A	3843	1/1	0.89	0.07	38,38,38,38	0
56	MG	2T	203	1/1	0.90	0.13	52,52,52,52	0
56	MG	1S	201	1/1	0.90	0.17	38,38,38,38	0
56	MG	2A	3638	1/1	0.90	0.15	58,58,58,58	0
56	MG	1U	201	1/1	0.90	0.20	31,31,31,31	0
56	MG	1U	206	1/1	0.90	0.44	36,36,36,36	0
56	MG	1w	103	1/1	0.90	0.15	60,60,60,60	0
56	MG	1A	3611	1/1	0.90	0.09	38,38,38,38	0
56	MG	2A	3650	1/1	0.90	0.19	48,48,48,48	0
56	MG	2A	3653	1/1	0.90	0.14	38,38,38,38	0
56	MG	2A	3351	1/1	0.90	0.09	58,58,58,58	0
56	MG	1A	3260	1/1	0.90	0.45	35,35,35,35	0
56	MG	1a	1713	1/1	0.90	0.33	59,59,59,59	0
56	MG	2A	3179	1/1	0.90	0.25	44,44,44,44	0
56	MG	2A	3670	1/1	0.90	0.13	63,63,63,63	0
56	MG	1A	4067	1/1	0.90	0.21	35,35,35,35	0
56	MG	1x	102	1/1	0.90	0.16	54,54,54,54	0
56	MG	2A	3362	1/1	0.90	0.08	37,37,37,37	0
56	MG	2A	3363	1/1	0.90	0.68	52,52,52,52	0
56	MG	2A	3187	1/1	0.90	0.21	56,56,56,56	0
56	MG	10	101	1/1	0.90	0.18	24,24,24,24	0
56	MG	2A	3691	1/1	0.90	0.15	47,47,47,47	0
56	MG	1x	104	1/1	0.90	0.12	55,55,55,55	0
56	MG	1A	4068	1/1	0.90	0.22	38,38,38,38	0
56	MG	2A	3705	1/1	0.90	0.11	45,45,45,45	0
56	MG	1A	3927	1/1	0.90	0.07	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	2A	3197	1/1	0.90	0.10	50,50,50,50	0
56	MG	2a	3029	1/1	0.90	0.17	42,42,42,42	0
56	MG	1A	3121	1/1	0.90	0.77	29,29,29,29	0
56	MG	2A	3200	1/1	0.90	0.13	46,46,46,46	0
56	MG	1A	3932	1/1	0.90	0.11	41,41,41,41	0
56	MG	2a	3036	1/1	0.90	0.07	46,46,46,46	0
56	MG	1A	3704	1/1	0.90	0.20	52,52,52,52	0
56	MG	2A	3205	1/1	0.90	0.10	48,48,48,48	0
56	MG	1A	3531	1/1	0.90	0.14	43,43,43,43	0
56	MG	2A	3726	1/1	0.90	0.21	58,58,58,58	0
56	MG	2A	3208	1/1	0.90	0.46	57,57,57,57	0
56	MG	1A	3937	1/1	0.90	0.16	33,33,33,33	0
56	MG	2a	3052	1/1	0.90	0.10	43,43,43,43	0
56	MG	2A	3404	1/1	0.90	0.19	48,48,48,48	0
56	MG	1A	3939	1/1	0.90	0.38	49,49,49,49	0
56	MG	1A	3716	1/1	0.90	0.08	43,43,43,43	0
56	MG	2a	3057	1/1	0.90	0.09	41,41,41,41	0
56	MG	1A	3437	1/1	0.90	0.36	26,26,26,26	0
56	MG	2a	3060	1/1	0.90	0.24	61,61,61,61	0
56	MG	2a	3064	1/1	0.90	0.10	34,34,34,34	0
56	MG	2A	3010	1/1	0.90	0.14	41,41,41,41	0
56	MG	2A	3223	1/1	0.90	0.62	52,52,52,52	0
56	MG	2a	3069	1/1	0.90	0.18	64,64,64,64	0
56	MG	1A	3200	1/1	0.90	0.11	45,45,45,45	0
56	MG	1a	1750	1/1	0.90	0.13	49,49,49,49	0
56	MG	1A	3329	1/1	0.90	0.16	33,33,33,33	0
56	MG	2A	3756	1/1	0.90	0.09	52,52,52,52	0
56	MG	2A	3422	1/1	0.90	0.16	45,45,45,45	0
56	MG	1A	3083	1/1	0.90	0.14	23,23,23,23	0
56	MG	2A	3030	1/1	0.90	0.11	36,36,36,36	0
56	MG	2A	3035	1/1	0.90	0.12	35,35,35,35	0
56	MG	2A	3240	1/1	0.90	0.12	39,39,39,39	0
56	MG	1A	3542	1/1	0.90	0.19	28,28,28,28	0
56	MG	2A	3043	1/1	0.90	0.63	37,37,37,37	0
56	MG	1A	3544	1/1	0.90	0.13	51,51,51,51	0
56	MG	2A	3446	1/1	0.90	0.10	44,44,44,44	0
56	MG	1A	3848	1/1	0.90	0.69	26,26,26,26	0
56	MG	1a	1766	1/1	0.90	0.13	52,52,52,52	0
56	MG	1a	1626	1/1	0.90	0.13	40,40,40,40	0
56	MG	1A	3336	1/1	0.90	0.19	39,39,39,39	0
56	MG	2a	3112	1/1	0.90	0.11	39,39,39,39	0
56	MG	2a	3114	1/1	0.90	0.10	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	1a	1774	1/1	0.90	0.11	42,42,42,42	0
56	MG	2a	3122	1/1	0.90	0.29	52,52,52,52	0
56	MG	2A	3480	1/1	0.90	0.28	67,67,67,67	0
56	MG	1B	208	1/1	0.90	0.17	56,56,56,56	0
56	MG	2A	3489	1/1	0.90	0.21	64,64,64,64	0
56	MG	1a	1631	1/1	0.90	0.13	46,46,46,46	0
56	MG	2A	3064	1/1	0.90	0.15	49,49,49,49	0
56	MG	1A	3177	1/1	0.90	0.14	45,45,45,45	0
56	MG	1A	4026	1/1	0.90	0.44	52,52,52,52	0
56	MG	2A	3067	1/1	0.90	0.14	38,38,38,38	0
56	MG	2a	3138	1/1	0.90	0.12	77,77,77,77	0
56	MG	1A	3736	1/1	0.90	0.09	45,45,45,45	0
56	MG	2a	3143	1/1	0.90	0.10	73,73,73,73	0
56	MG	2A	3265	1/1	0.90	0.76	52,52,52,52	0
56	MG	1A	3184	1/1	0.90	0.23	30,30,30,30	0
56	MG	1A	3747	1/1	0.90	0.16	9,9,9,9	0
56	MG	1A	3874	1/1	0.90	0.17	22,22,22,22	0
56	MG	1A	3275	1/1	0.90	0.30	35,35,35,35	0
56	MG	1a	1789	1/1	0.90	0.28	66,66,66,66	0
56	MG	2A	3808	1/1	0.90	0.18	53,53,53,53	0
56	MG	1B	233	1/1	0.90	0.32	67,67,67,67	0
56	MG	1A	3215	1/1	0.90	0.40	47,47,47,47	0
56	MG	1A	3566	1/1	0.90	0.22	40,40,40,40	0
56	MG	1A	3568	1/1	0.90	0.85	30,30,30,30	0
56	MG	2A	3091	1/1	0.90	0.23	54,54,54,54	0
56	MG	1A	3415	1/1	0.90	0.39	46,46,46,46	0
56	MG	2A	3823	1/1	0.90	0.13	24,24,24,24	0
56	MG	1E	306	1/1	0.90	0.62	41,41,41,41	0
56	MG	1A	3416	1/1	0.90	0.33	42,42,42,42	0
56	MG	1A	3582	1/1	0.90	0.64	38,38,38,38	0
56	MG	1A	3044	1/1	0.90	0.08	26,26,26,26	0
56	MG	2a	3168	1/1	0.90	0.09	58,58,58,58	0
56	MG	1a	1802	1/1	0.90	0.10	56,56,56,56	0
56	MG	2A	3303	1/1	0.90	0.17	46,46,46,46	0
56	MG	2a	3176	1/1	0.90	0.12	46,46,46,46	0
56	MG	2A	3304	1/1	0.90	0.15	64,64,64,64	0
56	MG	1a	1670	1/1	0.90	0.60	59,59,59,59	0
56	MG	2a	3180	1/1	0.90	0.11	83,83,83,83	0
56	MG	2A	3105	1/1	0.90	0.14	57,57,57,57	0
56	MG	1A	3765	1/1	0.90	0.30	36,36,36,36	0
56	MG	1A	3252	1/1	0.90	0.21	39,39,39,39	0
56	MG	2A	3109	1/1	0.90	0.11	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	3578	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	3308	1/1	0.90	0.15	34,34,34,34	0
56	MG	2a	3203	1/1	0.90	0.14	59,59,59,59	0
56	MG	1A	3980	1/1	0.90	0.39	72,72,72,72	0
56	MG	2A	3588	1/1	0.90	0.11	36,36,36,36	0
56	MG	2A	3589	1/1	0.90	0.11	58,58,58,58	0
56	MG	2a	3215	1/1	0.90	0.38	71,71,71,71	0
56	MG	2A	3120	1/1	0.90	0.19	61,61,61,61	0
56	MG	1a	1813	1/1	0.90	0.13	38,38,38,38	0
56	MG	1A	3778	1/1	0.90	0.14	17,17,17,17	0
56	MG	2a	3220	1/1	0.90	0.15	56,56,56,56	0
56	MG	1A	3678	1/1	0.90	0.13	18,18,18,18	0
56	MG	1a	1687	1/1	0.90	0.17	46,46,46,46	0
56	MG	1A	3679	1/1	0.90	0.14	7,7,7,7	0
56	MG	2d	302	1/1	0.90	0.16	61,61,61,61	0
56	MG	2A	3148	1/1	0.90	0.12	56,56,56,56	0
56	MG	2i	201	1/1	0.90	0.15	49,49,49,49	0
56	MG	1A	3310	1/1	0.90	0.15	41,41,41,41	0
56	MG	2A	3608	1/1	0.90	0.17	33,33,33,33	0
56	MG	1a	1691	1/1	0.90	0.30	44,44,44,44	0
56	MG	1a	1692	1/1	0.90	0.18	34,34,34,34	0
56	MG	2v	103	1/1	0.90	0.39	69,69,69,69	0
56	MG	2A	3614	1/1	0.90	0.14	45,45,45,45	0
56	MG	1O	204	1/1	0.90	0.31	52,52,52,52	0
56	MG	1A	3389	1/1	0.90	0.12	35,35,35,35	0
56	MG	1a	1697	1/1	0.90	0.20	41,41,41,41	0
56	MG	1A	3521	1/1	0.90	0.15	29,29,29,29	0
56	MG	1A	3197	1/1	0.90	0.12	34,34,34,34	0
56	MG	2A	3625	1/1	0.90	0.27	43,43,43,43	0
56	MG	2A	3627	1/1	0.90	0.26	40,40,40,40	0
56	MG	2A	3338	1/1	0.90	0.32	56,56,56,56	0
56	MG	2A	3116	1/1	0.91	0.10	38,38,38,38	0
56	MG	2A	3316	1/1	0.91	0.30	45,45,45,45	0
56	MG	2A	3118	1/1	0.91	0.37	45,45,45,45	0
56	MG	1A	4009	1/1	0.91	0.17	14,14,14,14	0
56	MG	1A	3764	1/1	0.91	0.12	58,58,58,58	0
56	MG	1a	1671	1/1	0.91	0.25	58,58,58,58	0
56	MG	2A	3124	1/1	0.91	0.42	47,47,47,47	0
56	MG	2A	3129	1/1	0.91	0.12	30,30,30,30	0
56	MG	2A	3136	1/1	0.91	0.24	34,34,34,34	0
56	MG	1a	1816	1/1	0.91	0.08	38,38,38,38	0
56	MG	1A	3049	1/1	0.91	0.14	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3219	1/1	0.91	0.42	39,39,39,39	0
56	MG	1A	3406	1/1	0.91	0.15	44,44,44,44	0
56	MG	28	101	1/1	0.91	0.23	42,42,42,42	0
56	MG	2A	3146	1/1	0.91	0.37	44,44,44,44	0
56	MG	2A	3147	1/1	0.91	0.39	32,32,32,32	0
56	MG	1A	3057	1/1	0.91	0.15	30,30,30,30	0
56	MG	2A	3630	1/1	0.91	0.89	40,40,40,40	0
56	MG	1A	3926	1/1	0.91	0.08	33,33,33,33	0
56	MG	2A	3634	1/1	0.91	0.15	61,61,61,61	0
56	MG	2A	3336	1/1	0.91	0.15	49,49,49,49	0
56	MG	1A	3409	1/1	0.91	0.42	36,36,36,36	0
56	MG	2A	3643	1/1	0.91	0.08	52,52,52,52	0
56	MG	2a	3013	1/1	0.91	0.16	56,56,56,56	0
56	MG	1A	3063	1/1	0.91	0.15	23,23,23,23	0
56	MG	1a	1688	1/1	0.91	0.09	57,57,57,57	0
56	MG	2A	3158	1/1	0.91	0.52	60,60,60,60	0
56	MG	1b	302	1/1	0.91	0.09	64,64,64,64	0
56	MG	1A	3782	1/1	0.91	0.18	52,52,52,52	0
56	MG	2A	3659	1/1	0.91	0.16	40,40,40,40	0
56	MG	2A	3661	1/1	0.91	0.15	35,35,35,35	0
56	MG	2A	3662	1/1	0.91	0.06	67,67,67,67	0
56	MG	1A	3125	1/1	0.91	0.15	42,42,42,42	0
56	MG	2A	3666	1/1	0.91	0.10	59,59,59,59	0
56	MG	1A	3277	1/1	0.91	0.96	31,31,31,31	0
56	MG	2A	3167	1/1	0.91	0.15	39,39,39,39	0
56	MG	1A	3278	1/1	0.91	0.64	27,27,27,27	0
56	MG	1A	3938	1/1	0.91	0.12	30,30,30,30	0
56	MG	2A	3673	1/1	0.91	0.12	52,52,52,52	0
56	MG	1A	3281	1/1	0.91	0.25	37,37,37,37	0
56	MG	1N	201	1/1	0.91	0.78	42,42,42,42	0
56	MG	1w	104	1/1	0.91	0.39	70,70,70,70	0
56	MG	1A	3422	1/1	0.91	0.44	40,40,40,40	0
56	MG	1A	3583	1/1	0.91	0.52	32,32,32,32	0
56	MG	2A	3368	1/1	0.91	0.46	51,51,51,51	0
56	MG	2a	3051	1/1	0.91	0.13	54,54,54,54	0
56	MG	1A	3284	1/1	0.91	0.11	46,46,46,46	0
56	MG	2A	3692	1/1	0.91	0.10	53,53,53,53	0
56	MG	2A	3372	1/1	0.91	0.10	39,39,39,39	0
56	MG	1A	3692	1/1	0.91	0.26	45,45,45,45	0
56	MG	1a	1708	1/1	0.91	0.13	66,66,66,66	0
56	MG	1A	3587	1/1	0.91	0.10	37,37,37,37	0
56	MG	1A	4039	1/1	0.91	0.12	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	2a	3062	1/1	0.91	0.17	55,55,55,55	0
56	MG	1A	3811	1/1	0.91	0.18	28,28,28,28	0
56	MG	1A	3813	1/1	0.91	0.12	24,24,24,24	0
56	MG	1A	3696	1/1	0.91	0.14	37,37,37,37	0
56	MG	1A	3697	1/1	0.91	0.15	39,39,39,39	0
56	MG	2A	3390	1/1	0.91	0.22	32,32,32,32	0
56	MG	2A	3723	1/1	0.91	0.12	43,43,43,43	0
56	MG	2A	3198	1/1	0.91	0.29	47,47,47,47	0
56	MG	1S	203	1/1	0.91	0.14	63,63,63,63	0
56	MG	1A	3699	1/1	0.91	0.14	53,53,53,53	0
56	MG	2A	3733	1/1	0.91	0.12	42,42,42,42	0
56	MG	1A	3226	1/1	0.91	0.12	33,33,33,33	0
56	MG	1V	202	1/1	0.91	0.09	59,59,59,59	0
56	MG	2a	3088	1/1	0.91	0.12	53,53,53,53	0
56	MG	2a	3090	1/1	0.91	0.18	56,56,56,56	0
56	MG	1A	3836	1/1	0.91	0.08	44,44,44,44	0
56	MG	2a	3093	1/1	0.91	0.12	53,53,53,53	0
56	MG	2A	3004	1/1	0.91	0.13	48,48,48,48	0
56	MG	2A	3741	1/1	0.91	0.16	50,50,50,50	0
56	MG	2A	3742	1/1	0.91	0.09	53,53,53,53	0
56	MG	2A	3408	1/1	0.91	0.61	57,57,57,57	0
56	MG	1A	3701	1/1	0.91	0.20	48,48,48,48	0
56	MG	2A	3009	1/1	0.91	0.15	47,47,47,47	0
56	MG	1A	3048	1/1	0.91	0.16	21,21,21,21	0
56	MG	2A	3011	1/1	0.91	0.21	48,48,48,48	0
56	MG	2A	3015	1/1	0.91	0.13	38,38,38,38	0
56	MG	2A	3755	1/1	0.91	0.09	76,76,76,76	0
56	MG	1A	3593	1/1	0.91	0.15	18,18,18,18	0
56	MG	2A	3019	1/1	0.91	0.13	35,35,35,35	0
56	MG	1A	3844	1/1	0.91	0.15	18,18,18,18	0
56	MG	2A	3427	1/1	0.91	0.14	53,53,53,53	0
56	MG	2A	3428	1/1	0.91	0.80	50,50,50,50	0
56	MG	2A	3768	1/1	0.91	0.07	61,61,61,61	0
56	MG	2a	3132	1/1	0.91	0.12	53,53,53,53	0
56	MG	1A	3298	1/1	0.91	0.21	32,32,32,32	0
56	MG	1a	1748	1/1	0.91	0.13	45,45,45,45	0
56	MG	2A	3437	1/1	0.91	0.18	42,42,42,42	0
56	MG	1A	3856	1/1	0.91	0.14	22,22,22,22	0
56	MG	2A	3031	1/1	0.91	0.21	45,45,45,45	0
56	MG	1A	3429	1/1	0.91	0.26	19,19,19,19	0
56	MG	1A	3496	1/1	0.91	0.09	37,37,37,37	0
56	MG	1a	1752	1/1	0.91	0.15	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	18	101	1/1	0.91	0.58	38,38,38,38	0
56	MG	2A	3045	1/1	0.91	0.25	57,57,57,57	0
56	MG	2A	3465	1/1	0.91	0.17	37,37,37,37	0
56	MG	1a	1757	1/1	0.91	0.18	46,46,46,46	0
56	MG	1a	1758	1/1	0.91	0.10	43,43,43,43	0
56	MG	2A	3478	1/1	0.91	0.10	44,44,44,44	0
56	MG	2A	3479	1/1	0.91	0.27	56,56,56,56	0
56	MG	1A	3301	1/1	0.91	0.17	34,34,34,34	0
56	MG	2A	3481	1/1	0.91	0.17	32,32,32,32	0
56	MG	1A	3235	1/1	0.91	0.29	35,35,35,35	0
56	MG	2A	3487	1/1	0.91	0.12	42,42,42,42	0
56	MG	2a	3160	1/1	0.91	0.06	46,46,46,46	0
56	MG	1A	3870	1/1	0.91	0.09	29,29,29,29	0
56	MG	1A	3727	1/1	0.91	0.17	56,56,56,56	0
56	MG	1A	4074	1/1	0.91	0.07	27,27,27,27	0
56	MG	2A	3501	1/1	0.91	0.08	57,57,57,57	0
56	MG	1a	1607	1/1	0.91	0.18	46,46,46,46	0
56	MG	2A	3258	1/1	0.91	0.20	42,42,42,42	0
56	MG	1A	3091	1/1	0.91	0.14	14,14,14,14	0
56	MG	1A	3239	1/1	0.91	0.44	29,29,29,29	0
56	MG	2A	3511	1/1	0.91	0.10	37,37,37,37	0
56	MG	1A	3312	1/1	0.91	0.18	40,40,40,40	0
56	MG	2A	3515	1/1	0.91	0.12	60,60,60,60	0
56	MG	1A	3517	1/1	0.91	0.10	53,53,53,53	0
56	MG	2a	3179	1/1	0.91	0.11	46,46,46,46	0
56	MG	1A	3885	1/1	0.91	0.45	35,35,35,35	0
56	MG	2A	3266	1/1	0.91	0.33	37,37,37,37	0
56	MG	2a	3186	1/1	0.91	0.07	77,77,77,77	0
56	MG	1A	4096	1/1	0.91	0.17	36,36,36,36	0
56	MG	2A	3073	1/1	0.91	0.15	47,47,47,47	0
56	MG	2a	3194	1/1	0.91	0.07	49,49,49,49	0
56	MG	1A	3092	1/1	0.91	0.22	42,42,42,42	0
56	MG	1A	3241	1/1	0.91	0.36	27,27,27,27	0
56	MG	1A	3890	1/1	0.91	0.13	39,39,39,39	0
56	MG	1A	3099	1/1	0.91	0.38	37,37,37,37	0
56	MG	1A	3897	1/1	0.91	0.12	40,40,40,40	0
56	MG	1A	3144	1/1	0.91	0.55	32,32,32,32	0
56	MG	2a	3208	1/1	0.91	0.16	66,66,66,66	0
56	MG	1A	3060	1/1	0.91	0.11	59,59,59,59	0
56	MG	2A	3842	1/1	0.91	0.14	56,56,56,56	0
56	MG	1A	4129	1/1	0.91	0.18	33,33,33,33	0
56	MG	2A	3542	1/1	0.91	0.16	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	3284	1/1	0.91	0.19	53,53,53,53	0
56	MG	1A	3080	1/1	0.91	0.34	28,28,28,28	0
56	MG	2A	3287	1/1	0.91	0.16	50,50,50,50	0
56	MG	1B	202	1/1	0.91	0.20	26,26,26,26	0
56	MG	2A	3095	1/1	0.91	0.19	42,42,42,42	0
56	MG	1A	3334	1/1	0.91	0.30	47,47,47,47	0
56	MG	1A	3081	1/1	0.91	0.46	26,26,26,26	0
56	MG	1A	3261	1/1	0.91	0.27	28,28,28,28	0
56	MG	2A	3302	1/1	0.91	0.21	52,52,52,52	0
56	MG	1A	3340	1/1	0.91	0.27	57,57,57,57	0
56	MG	2A	3575	1/1	0.91	0.26	49,49,49,49	0
56	MG	1A	3157	1/1	0.91	0.24	21,21,21,21	0
56	MG	2A	3305	1/1	0.91	0.26	52,52,52,52	0
56	MG	1a	1804	1/1	0.91	0.14	40,40,40,40	0
56	MG	1B	220	1/1	0.91	0.22	46,46,46,46	0
56	MG	2A	3107	1/1	0.91	0.15	48,48,48,48	0
56	MG	1B	221	1/1	0.91	0.17	46,46,46,46	0
56	MG	2B	217	1/1	0.91	0.10	49,49,49,49	0
56	MG	2D	301	1/1	0.91	0.13	27,27,27,27	0
57	LUJ	1A	4100	42/44	0.91	0.35	23,39,54,62	0
56	MG	1A	3648	1/1	0.91	0.14	27,27,27,27	0
56	MG	1A	4008	1/1	0.91	0.10	25,25,25,25	0
59	ZN	14	102	1/1	0.91	0.10	94,94,94,94	0
56	MG	2A	3312	1/1	0.91	0.46	47,47,47,47	0
59	ZN	29	102	1/1	0.91	0.10	69,69,69,69	0
56	MG	1A	3073	1/1	0.92	0.10	27,27,27,27	0
56	MG	2A	3337	1/1	0.92	0.26	38,38,38,38	0
56	MG	2A	3610	1/1	0.92	0.14	28,28,28,28	0
56	MG	2A	3612	1/1	0.92	0.14	42,42,42,42	0
56	MG	1A	3535	1/1	0.92	0.16	20,20,20,20	0
56	MG	2A	3340	1/1	0.92	0.18	65,65,65,65	0
56	MG	2P	202	1/1	0.92	0.15	48,48,48,48	0
56	MG	2Q	201	1/1	0.92	0.07	51,51,51,51	0
56	MG	1A	3895	1/1	0.92	0.14	41,41,41,41	0
56	MG	1a	1677	1/1	0.92	0.37	56,56,56,56	0
56	MG	2A	3345	1/1	0.92	0.72	47,47,47,47	0
56	MG	1A	3078	1/1	0.92	0.11	28,28,28,28	0
56	MG	2A	3347	1/1	0.92	0.38	51,51,51,51	0
56	MG	1A	3418	1/1	0.92	0.30	37,37,37,37	0
56	MG	1A	3263	1/1	0.92	0.12	48,48,48,48	0
56	MG	1a	1685	1/1	0.92	0.13	51,51,51,51	0
56	MG	1A	3757	1/1	0.92	0.23	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	25	102	1/1	0.92	0.14	38,38,38,38	0
56	MG	1A	3319	1/1	0.92	0.23	42,42,42,42	0
56	MG	1A	3547	1/1	0.92	0.37	43,43,43,43	0
56	MG	1D	311	1/1	0.92	0.56	17,17,17,17	0
56	MG	2A	3358	1/1	0.92	0.08	49,49,49,49	0
56	MG	1A	3551	1/1	0.92	0.74	39,39,39,39	0
56	MG	1A	3166	1/1	0.92	0.13	34,34,34,34	0
56	MG	2A	3181	1/1	0.92	0.13	32,32,32,32	0
56	MG	2A	3648	1/1	0.92	0.21	39,39,39,39	0
56	MG	1A	3766	1/1	0.92	0.10	22,22,22,22	0
56	MG	1F	302	1/1	0.92	0.38	28,28,28,28	0
56	MG	1A	3767	1/1	0.92	0.20	22,22,22,22	0
56	MG	1A	3769	1/1	0.92	0.22	33,33,33,33	0
56	MG	1A	3135	1/1	0.92	0.13	30,30,30,30	0
56	MG	1A	3376	1/1	0.92	0.48	32,32,32,32	0
56	MG	1a	1705	1/1	0.92	0.15	43,43,43,43	0
56	MG	1F	310	1/1	0.92	0.23	40,40,40,40	0
56	MG	1A	4022	1/1	0.92	0.13	60,60,60,60	0
56	MG	2a	3022	1/1	0.92	0.19	40,40,40,40	0
56	MG	1y	106	1/1	0.92	0.12	48,48,48,48	0
56	MG	2A	3201	1/1	0.92	0.12	49,49,49,49	0
56	MG	2A	3381	1/1	0.92	0.19	44,44,44,44	0
56	MG	2A	3671	1/1	0.92	0.09	43,43,43,43	0
56	MG	1A	3664	1/1	0.92	0.15	13,13,13,13	0
56	MG	1A	3561	1/1	0.92	0.21	35,35,35,35	0
56	MG	1A	3924	1/1	0.92	0.11	31,31,31,31	0
56	MG	2A	3677	1/1	0.92	0.06	72,72,72,72	0
56	MG	2A	3394	1/1	0.92	0.27	34,34,34,34	0
56	MG	1A	3013	1/1	0.92	0.42	13,13,13,13	0
56	MG	2A	3400	1/1	0.92	0.25	49,49,49,49	0
56	MG	2A	3689	1/1	0.92	0.11	25,25,25,25	0
56	MG	1A	3480	1/1	0.92	0.11	42,42,42,42	0
56	MG	2A	3402	1/1	0.92	0.18	38,38,38,38	0
56	MG	2a	3047	1/1	0.92	0.32	48,48,48,48	0
56	MG	1A	3180	1/1	0.92	0.12	31,31,31,31	0
56	MG	1A	3100	1/1	0.92	0.13	52,52,52,52	0
56	MG	1A	3483	1/1	0.92	0.14	38,38,38,38	0
56	MG	2A	3217	1/1	0.92	0.39	47,47,47,47	0
56	MG	2A	3707	1/1	0.92	0.14	61,61,61,61	0
56	MG	2A	3708	1/1	0.92	0.09	53,53,53,53	0
56	MG	2a	3056	1/1	0.92	0.13	46,46,46,46	0
56	MG	1a	1723	1/1	0.92	0.17	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3790	1/1	0.92	0.06	34,34,34,34	0
56	MG	2A	3022	1/1	0.92	0.95	45,45,45,45	0
56	MG	2a	3061	1/1	0.92	0.10	58,58,58,58	0
56	MG	1A	3682	1/1	0.92	0.19	15,15,15,15	0
56	MG	1A	3575	1/1	0.92	0.51	28,28,28,28	0
56	MG	1A	3485	1/1	0.92	0.38	33,33,33,33	0
56	MG	2A	3034	1/1	0.92	0.25	31,31,31,31	0
56	MG	2A	3235	1/1	0.92	0.12	47,47,47,47	0
56	MG	2A	3724	1/1	0.92	0.32	37,37,37,37	0
56	MG	2A	3236	1/1	0.92	0.16	52,52,52,52	0
56	MG	1A	3805	1/1	0.92	0.10	37,37,37,37	0
56	MG	1A	3233	1/1	0.92	0.64	29,29,29,29	0
56	MG	2A	3731	1/1	0.92	0.12	65,65,65,65	0
56	MG	1a	1742	1/1	0.92	0.11	48,48,48,48	0
56	MG	1A	3006	1/1	0.92	0.18	34,34,34,34	0
56	MG	1U	207	1/1	0.92	1.38	71,71,71,71	0
56	MG	2a	3086	1/1	0.92	0.06	37,37,37,37	0
56	MG	2A	3436	1/1	0.92	0.16	35,35,35,35	0
56	MG	2A	3046	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3192	1/1	0.92	0.23	40,40,40,40	0
56	MG	1W	206	1/1	0.92	0.23	23,23,23,23	0
56	MG	2a	3094	1/1	0.92	0.13	54,54,54,54	0
56	MG	2A	3248	1/1	0.92	0.12	51,51,51,51	0
56	MG	2A	3745	1/1	0.92	0.17	49,49,49,49	0
56	MG	2a	3098	1/1	0.92	0.70	70,70,70,70	0
56	MG	1A	3494	1/1	0.92	0.17	48,48,48,48	0
56	MG	1A	4046	1/1	0.92	0.09	24,24,24,24	0
56	MG	2a	3101	1/1	0.92	0.09	65,65,65,65	0
56	MG	1Y	204	1/1	0.92	0.13	41,41,41,41	0
56	MG	1a	1754	1/1	0.92	0.07	29,29,29,29	0
56	MG	2A	3451	1/1	0.92	0.12	48,48,48,48	0
56	MG	2A	3455	1/1	0.92	0.22	42,42,42,42	0
56	MG	2A	3464	1/1	0.92	0.11	53,53,53,53	0
56	MG	2A	3758	1/1	0.92	0.16	54,54,54,54	0
56	MG	2A	3054	1/1	0.92	0.11	35,35,35,35	0
56	MG	2a	3121	1/1	0.92	0.20	48,48,48,48	0
56	MG	1A	4047	1/1	0.92	0.15	46,46,46,46	0
56	MG	2a	3123	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3473	1/1	0.92	0.27	39,39,39,39	0
56	MG	2A	3762	1/1	0.92	0.08	41,41,41,41	0
56	MG	2A	3763	1/1	0.92	0.14	62,62,62,62	0
56	MG	2A	3765	1/1	0.92	0.10	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	1A	3032	1/1	0.92	0.77	18,18,18,18	0
56	MG	2A	3477	1/1	0.92	0.16	59,59,59,59	0
56	MG	1A	3065	1/1	0.92	0.19	22,22,22,22	0
56	MG	1A	3066	1/1	0.92	0.12	36,36,36,36	0
56	MG	1A	3595	1/1	0.92	0.18	35,35,35,35	0
56	MG	1A	3833	1/1	0.92	0.11	29,29,29,29	0
56	MG	2a	3139	1/1	0.92	0.33	68,68,68,68	0
56	MG	1a	1763	1/1	0.92	0.12	34,34,34,34	0
56	MG	2A	3486	1/1	0.92	0.21	50,50,50,50	0
56	MG	1A	3288	1/1	0.92	0.10	36,36,36,36	0
56	MG	17	104	1/1	0.92	0.10	21,21,21,21	0
56	MG	2A	3496	1/1	0.92	0.14	52,52,52,52	0
56	MG	2A	3497	1/1	0.92	0.12	45,45,45,45	0
56	MG	1A	3835	1/1	0.92	0.09	35,35,35,35	0
56	MG	19	101	1/1	0.92	0.10	47,47,47,47	0
56	MG	1A	3089	1/1	0.92	0.19	39,39,39,39	0
56	MG	1A	3506	1/1	0.92	0.25	15,15,15,15	0
56	MG	2A	3275	1/1	0.92	0.12	53,53,53,53	0
56	MG	1A	3960	1/1	0.92	0.12	18,18,18,18	0
56	MG	1A	4062	1/1	0.92	0.15	15,15,15,15	0
56	MG	1A	3513	1/1	0.92	0.12	38,38,38,38	0
56	MG	2A	3279	1/1	0.92	0.18	48,48,48,48	0
56	MG	2A	3513	1/1	0.92	0.08	47,47,47,47	0
56	MG	1A	3449	1/1	0.92	0.32	36,36,36,36	0
56	MG	1A	3245	1/1	0.92	0.58	45,45,45,45	0
56	MG	2A	3799	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3283	1/1	0.92	0.24	39,39,39,39	0
56	MG	2A	3804	1/1	0.92	0.13	33,33,33,33	0
56	MG	1A	3967	1/1	0.92	0.27	64,64,64,64	0
56	MG	2a	3170	1/1	0.92	0.26	84,84,84,84	0
56	MG	1A	4070	1/1	0.92	0.09	19,19,19,19	0
56	MG	2a	3172	1/1	0.92	0.05	59,59,59,59	0
56	MG	1a	1617	1/1	0.92	0.09	36,36,36,36	0
56	MG	1A	3846	1/1	0.92	0.11	31,31,31,31	0
56	MG	2A	3527	1/1	0.92	0.33	57,57,57,57	0
56	MG	2A	3100	1/1	0.92	0.13	47,47,47,47	0
56	MG	1A	3723	1/1	0.92	0.18	31,31,31,31	0
56	MG	1a	1624	1/1	0.92	0.20	42,42,42,42	0
56	MG	2A	3818	1/1	0.92	0.10	47,47,47,47	0
56	MG	1A	3724	1/1	0.92	0.11	25,25,25,25	0
56	MG	1A	3857	1/1	0.92	0.18	40,40,40,40	0
56	MG	1A	3972	1/1	0.92	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	2a	3193	1/1	0.92	0.12	54,54,54,54	0
56	MG	2A	3826	1/1	0.92	0.16	36,36,36,36	0
56	MG	1A	3725	1/1	0.92	0.38	51,51,51,51	0
56	MG	2A	3828	1/1	0.92	0.12	57,57,57,57	0
56	MG	1a	1629	1/1	0.92	0.19	41,41,41,41	0
56	MG	1A	3726	1/1	0.92	0.26	55,55,55,55	0
56	MG	1A	3976	1/1	0.92	0.12	61,61,61,61	0
56	MG	1A	3862	1/1	0.92	0.29	31,31,31,31	0
56	MG	1A	3155	1/1	0.92	0.29	28,28,28,28	0
56	MG	2A	3837	1/1	0.92	0.14	48,48,48,48	0
56	MG	2A	3839	1/1	0.92	0.09	41,41,41,41	0
56	MG	1A	3979	1/1	0.92	0.30	52,52,52,52	0
56	MG	2A	3556	1/1	0.92	0.10	31,31,31,31	0
56	MG	2A	3557	1/1	0.92	0.09	55,55,55,55	0
56	MG	2A	3559	1/1	0.92	0.14	33,33,33,33	0
56	MG	1A	3305	1/1	0.92	0.13	32,32,32,32	0
56	MG	1A	3519	1/1	0.92	0.19	45,45,45,45	0
56	MG	2a	3231	1/1	0.92	0.08	73,73,73,73	0
56	MG	1A	3871	1/1	0.92	0.12	14,14,14,14	0
56	MG	2A	3569	1/1	0.92	0.09	24,24,24,24	0
56	MG	1A	3620	1/1	0.92	0.20	49,49,49,49	0
56	MG	2f	201	1/1	0.92	0.07	48,48,48,48	0
56	MG	1A	3985	1/1	0.92	0.14	16,16,16,16	0
56	MG	1a	1653	1/1	0.92	0.25	58,58,58,58	0
56	MG	2k	201	1/1	0.92	0.13	56,56,56,56	0
56	MG	2l	201	1/1	0.92	0.14	48,48,48,48	0
56	MG	1A	3986	1/1	0.92	0.16	18,18,18,18	0
56	MG	1A	3456	1/1	0.92	0.19	31,31,31,31	0
56	MG	2A	3143	1/1	0.92	0.11	37,37,37,37	0
56	MG	1a	1820	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	3209	1/1	0.92	0.18	40,40,40,40	0
56	MG	2y	101	1/1	0.92	0.12	67,67,67,67	0
56	MG	1a	1661	1/1	0.92	0.25	36,36,36,36	0
56	MG	1B	205	1/1	0.92	0.17	28,28,28,28	0
56	MG	1A	3211	1/1	0.92	0.46	32,32,32,32	0
56	MG	1A	3738	1/1	0.92	0.13	31,31,31,31	0
56	MG	2A	3598	1/1	0.92	0.10	50,50,50,50	0
56	MG	2A	3152	1/1	0.92	0.16	46,46,46,46	0
56	MG	2B	213	1/1	0.92	0.08	56,56,56,56	0
56	MG	2B	216	1/1	0.92	0.23	74,74,74,74	0
56	MG	1A	3309	1/1	0.92	0.17	34,34,34,34	0
56	MG	1A	3413	1/1	0.92	0.13	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	1A	3054	1/1	0.92	0.20	28,28,28,28	0
56	MG	2A	3242	1/1	0.93	0.26	61,61,61,61	0
56	MG	1a	1659	1/1	0.93	0.18	50,50,50,50	0
56	MG	1A	3783	1/1	0.93	0.16	14,14,14,14	0
56	MG	1A	4087	1/1	0.93	0.12	33,33,33,33	0
56	MG	1A	4089	1/1	0.93	0.17	47,47,47,47	0
56	MG	1a	1665	1/1	0.93	0.50	46,46,46,46	0
56	MG	2A	3249	1/1	0.93	0.11	48,48,48,48	0
56	MG	2A	3863	1/1	0.93	0.06	48,48,48,48	0
56	MG	2A	3531	1/1	0.93	0.09	39,39,39,39	0
56	MG	1A	3444	1/1	0.93	0.09	49,49,49,49	0
56	MG	1A	3653	1/1	0.93	0.13	29,29,29,29	0
56	MG	1a	1668	1/1	0.93	0.10	34,34,34,34	0
56	MG	2A	3254	1/1	0.93	0.10	43,43,43,43	0
56	MG	1A	3654	1/1	0.93	0.15	18,18,18,18	0
56	MG	2A	3002	1/1	0.93	0.17	44,44,44,44	0
56	MG	1A	3952	1/1	0.93	0.08	29,29,29,29	0
56	MG	1A	3655	1/1	0.93	0.14	20,20,20,20	0
56	MG	1a	1673	1/1	0.93	0.42	43,43,43,43	0
56	MG	1A	3112	1/1	0.93	0.23	39,39,39,39	0
56	MG	1A	4110	1/1	0.93	0.34	30,30,30,30	0
56	MG	2E	301	1/1	0.93	0.55	45,45,45,45	0
56	MG	2E	305	1/1	0.93	0.13	37,37,37,37	0
56	MG	2A	3014	1/1	0.93	0.15	55,55,55,55	0
56	MG	2A	3264	1/1	0.93	0.61	51,51,51,51	0
56	MG	1A	3955	1/1	0.93	0.12	19,19,19,19	0
56	MG	1A	4115	1/1	0.93	0.37	26,26,26,26	0
56	MG	1a	1681	1/1	0.93	0.09	32,32,32,32	0
56	MG	2A	3562	1/1	0.93	0.12	27,27,27,27	0
56	MG	1A	3661	1/1	0.93	0.12	13,13,13,13	0
56	MG	2N	201	1/1	0.93	0.58	57,57,57,57	0
56	MG	2O	202	1/1	0.93	0.09	48,48,48,48	0
56	MG	2P	201	1/1	0.93	0.17	52,52,52,52	0
56	MG	1A	3254	1/1	0.93	0.20	45,45,45,45	0
56	MG	1A	3255	1/1	0.93	0.14	50,50,50,50	0
56	MG	2A	3570	1/1	0.93	0.13	34,34,34,34	0
56	MG	2Q	204	1/1	0.93	0.12	49,49,49,49	0
56	MG	2T	201	1/1	0.93	0.17	57,57,57,57	0
56	MG	2A	3272	1/1	0.93	0.13	42,42,42,42	0
56	MG	1a	1686	1/1	0.93	0.22	49,49,49,49	0
56	MG	2A	3026	1/1	0.93	0.19	43,43,43,43	0
56	MG	2U	201	1/1	0.93	0.13	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2U	202	1/1	0.93	0.55	57,57,57,57	0
56	MG	2A	3028	1/1	0.93	0.12	38,38,38,38	0
56	MG	1A	3385	1/1	0.93	0.27	27,27,27,27	0
56	MG	2X	101	1/1	0.93	0.15	49,49,49,49	0
56	MG	20	101	1/1	0.93	0.10	55,55,55,55	0
56	MG	1A	3150	1/1	0.93	0.21	38,38,38,38	0
56	MG	2A	3587	1/1	0.93	0.17	44,44,44,44	0
56	MG	1A	3327	1/1	0.93	0.12	33,33,33,33	0
56	MG	1A	3671	1/1	0.93	0.15	14,14,14,14	0
56	MG	2A	3039	1/1	0.93	0.15	50,50,50,50	0
56	MG	2A	3282	1/1	0.93	0.08	42,42,42,42	0
56	MG	1A	3672	1/1	0.93	0.08	33,33,33,33	0
56	MG	1A	3814	1/1	0.93	0.17	37,37,37,37	0
56	MG	2A	3285	1/1	0.93	0.11	37,37,37,37	0
56	MG	1A	3817	1/1	0.93	0.11	33,33,33,33	0
56	MG	1B	212	1/1	0.93	0.10	27,27,27,27	0
56	MG	1A	3674	1/1	0.93	0.21	44,44,44,44	0
56	MG	1A	3820	1/1	0.93	0.10	49,49,49,49	0
56	MG	1a	1701	1/1	0.93	0.16	42,42,42,42	0
56	MG	1A	3113	1/1	0.93	0.46	36,36,36,36	0
56	MG	2A	3297	1/1	0.93	0.39	47,47,47,47	0
56	MG	1A	3824	1/1	0.93	0.15	33,33,33,33	0
56	MG	2A	3299	1/1	0.93	0.16	44,44,44,44	0
56	MG	1A	3455	1/1	0.93	0.12	39,39,39,39	0
56	MG	1A	3543	1/1	0.93	0.09	52,52,52,52	0
56	MG	2a	3019	1/1	0.93	0.17	58,58,58,58	0
56	MG	1A	3097	1/1	0.93	0.09	35,35,35,35	0
56	MG	2a	3021	1/1	0.93	0.32	45,45,45,45	0
56	MG	2A	3056	1/1	0.93	0.12	52,52,52,52	0
56	MG	2A	3057	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3058	1/1	0.93	0.15	51,51,51,51	0
56	MG	2A	3060	1/1	0.93	0.11	27,27,27,27	0
56	MG	2A	3061	1/1	0.93	0.36	48,48,48,48	0
56	MG	1A	3085	1/1	0.93	0.42	25,25,25,25	0
56	MG	2a	3032	1/1	0.93	0.15	40,40,40,40	0
56	MG	2A	3063	1/1	0.93	0.09	44,44,44,44	0
56	MG	1A	3548	1/1	0.93	0.20	25,25,25,25	0
56	MG	1A	3685	1/1	0.93	0.11	15,15,15,15	0
56	MG	2A	3315	1/1	0.93	0.19	63,63,63,63	0
56	MG	1A	3686	1/1	0.93	0.09	32,32,32,32	0
56	MG	2a	3040	1/1	0.93	0.24	59,59,59,59	0
56	MG	1A	3984	1/1	0.93	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3549	1/1	0.93	0.28	26,26,26,26	0
56	MG	1E	304	1/1	0.93	0.17	19,19,19,19	0
56	MG	1A	3689	1/1	0.93	0.14	22,22,22,22	0
56	MG	1A	3987	1/1	0.93	0.11	25,25,25,25	0
56	MG	1a	1724	1/1	0.93	0.20	56,56,56,56	0
56	MG	2a	3050	1/1	0.93	0.22	61,61,61,61	0
56	MG	2A	3651	1/1	0.93	0.15	51,51,51,51	0
56	MG	1a	1726	1/1	0.93	0.14	36,36,36,36	0
56	MG	1A	3458	1/1	0.93	0.23	20,20,20,20	0
56	MG	1A	3847	1/1	0.93	0.14	36,36,36,36	0
56	MG	1A	3552	1/1	0.93	0.20	27,27,27,27	0
56	MG	2A	3083	1/1	0.93	1.15	53,53,53,53	0
56	MG	1A	3849	1/1	0.93	0.10	36,36,36,36	0
56	MG	1a	1732	1/1	0.93	0.26	47,47,47,47	0
56	MG	1a	1734	1/1	0.93	0.24	45,45,45,45	0
56	MG	1A	3850	1/1	0.93	0.09	33,33,33,33	0
56	MG	1A	3394	1/1	0.93	0.31	27,27,27,27	0
56	MG	1A	3461	1/1	0.93	0.13	19,19,19,19	0
56	MG	2A	3672	1/1	0.93	0.12	34,34,34,34	0
56	MG	2a	3067	1/1	0.93	0.08	51,51,51,51	0
56	MG	1A	3264	1/1	0.93	0.19	40,40,40,40	0
56	MG	1a	1746	1/1	0.93	0.12	36,36,36,36	0
56	MG	2A	3099	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	3464	1/1	0.93	0.34	50,50,50,50	0
56	MG	2A	3678	1/1	0.93	0.15	59,59,59,59	0
56	MG	1A	3397	1/1	0.93	0.37	22,22,22,22	0
56	MG	2A	3682	1/1	0.93	0.24	48,48,48,48	0
56	MG	1A	3863	1/1	0.93	0.38	24,24,24,24	0
56	MG	2a	3080	1/1	0.93	0.13	47,47,47,47	0
56	MG	1A	3160	1/1	0.93	0.23	55,55,55,55	0
56	MG	1A	3218	1/1	0.93	0.22	28,28,28,28	0
56	MG	1A	3705	1/1	0.93	0.21	35,35,35,35	0
56	MG	1A	3402	1/1	0.93	0.30	32,32,32,32	0
56	MG	1A	3712	1/1	0.93	0.13	28,28,28,28	0
56	MG	2A	3696	1/1	0.93	0.07	38,38,38,38	0
56	MG	2A	3697	1/1	0.93	0.07	53,53,53,53	0
56	MG	1P	203	1/1	0.93	0.48	45,45,45,45	0
56	MG	1A	3714	1/1	0.93	0.23	49,49,49,49	0
56	MG	2A	3703	1/1	0.93	0.12	39,39,39,39	0
56	MG	2A	3113	1/1	0.93	0.16	29,29,29,29	0
56	MG	2A	3115	1/1	0.93	0.11	54,54,54,54	0
56	MG	1A	3339	1/1	0.93	0.12	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	1R	202	1/1	0.93	0.21	45,45,45,45	0
56	MG	1A	3028	1/1	0.93	0.16	25,25,25,25	0
56	MG	2A	3714	1/1	0.93	0.22	51,51,51,51	0
56	MG	1A	3879	1/1	0.93	0.08	16,16,16,16	0
56	MG	2a	3109	1/1	0.93	0.20	46,46,46,46	0
56	MG	1a	1764	1/1	0.93	0.14	47,47,47,47	0
56	MG	1A	3128	1/1	0.93	0.32	26,26,26,26	0
56	MG	1A	3407	1/1	0.93	0.09	44,44,44,44	0
56	MG	2A	3721	1/1	0.93	0.19	40,40,40,40	0
56	MG	2a	3117	1/1	0.93	0.07	50,50,50,50	0
56	MG	2a	3118	1/1	0.93	0.09	54,54,54,54	0
56	MG	1A	3343	1/1	0.93	0.39	24,24,24,24	0
56	MG	2A	3138	1/1	0.93	0.11	57,57,57,57	0
56	MG	1a	1773	1/1	0.93	0.09	59,59,59,59	0
56	MG	2A	3375	1/1	0.93	0.13	48,48,48,48	0
56	MG	1A	3584	1/1	0.93	0.15	44,44,44,44	0
56	MG	2a	3127	1/1	0.93	0.22	45,45,45,45	0
56	MG	1W	201	1/1	0.93	0.22	27,27,27,27	0
56	MG	2A	3730	1/1	0.93	0.12	39,39,39,39	0
56	MG	1A	3129	1/1	0.93	0.32	28,28,28,28	0
56	MG	1A	3410	1/1	0.93	0.13	42,42,42,42	0
56	MG	1A	3130	1/1	0.93	0.21	34,34,34,34	0
56	MG	1A	3896	1/1	0.93	0.11	38,38,38,38	0
56	MG	2A	3736	1/1	0.93	0.11	50,50,50,50	0
56	MG	1Z	302	1/1	0.93	0.17	45,45,45,45	0
56	MG	2A	3738	1/1	0.93	0.16	33,33,33,33	0
56	MG	1a	1783	1/1	0.93	0.07	38,38,38,38	0
56	MG	2a	3142	1/1	0.93	0.06	61,61,61,61	0
56	MG	2A	3393	1/1	0.93	0.17	46,46,46,46	0
56	MG	1A	3347	1/1	0.93	0.18	32,32,32,32	0
56	MG	1A	3900	1/1	0.93	0.29	31,31,31,31	0
56	MG	1A	3901	1/1	0.93	0.60	27,27,27,27	0
56	MG	1A	3101	1/1	0.93	0.38	21,21,21,21	0
56	MG	2A	3157	1/1	0.93	0.12	67,67,67,67	0
56	MG	1A	3905	1/1	0.93	0.20	17,17,17,17	0
56	MG	11	101	1/1	0.93	0.14	30,30,30,30	0
56	MG	2A	3753	1/1	0.93	0.24	51,51,51,51	0
56	MG	12	3701	1/1	0.93	0.16	25,25,25,25	0
56	MG	1A	4033	1/1	0.93	0.10	42,42,42,42	0
56	MG	2A	3164	1/1	0.93	0.06	36,36,36,36	0
56	MG	1A	3594	1/1	0.93	0.16	36,36,36,36	0
56	MG	2A	3409	1/1	0.93	0.09	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	2A	3410	1/1	0.93	0.16	43,43,43,43	0
56	MG	1A	3227	1/1	0.93	0.52	31,31,31,31	0
56	MG	2A	3412	1/1	0.93	0.17	48,48,48,48	0
56	MG	2A	3168	1/1	0.93	0.29	44,44,44,44	0
56	MG	2A	3414	1/1	0.93	0.13	55,55,55,55	0
56	MG	1A	3484	1/1	0.93	0.14	31,31,31,31	0
56	MG	18	104	1/1	0.93	0.30	47,47,47,47	0
56	MG	2a	3169	1/1	0.93	0.20	60,60,60,60	0
56	MG	1a	1800	1/1	0.93	0.14	28,28,28,28	0
56	MG	1A	3599	1/1	0.93	0.16	37,37,37,37	0
56	MG	1A	3737	1/1	0.93	0.25	30,30,30,30	0
56	MG	1a	1602	1/1	0.93	0.15	54,54,54,54	0
56	MG	1A	3232	1/1	0.93	0.31	22,22,22,22	0
56	MG	1A	3739	1/1	0.93	0.14	53,53,53,53	0
56	MG	2A	3777	1/1	0.93	0.17	58,58,58,58	0
56	MG	1A	3417	1/1	0.93	0.12	22,22,22,22	0
56	MG	2A	3432	1/1	0.93	0.12	48,48,48,48	0
56	MG	1A	3745	1/1	0.93	0.22	41,41,41,41	0
56	MG	1A	3103	1/1	0.93	0.24	19,19,19,19	0
56	MG	1A	3183	1/1	0.93	0.12	32,32,32,32	0
56	MG	2A	3188	1/1	0.93	0.09	31,31,31,31	0
56	MG	1A	3421	1/1	0.93	0.18	30,30,30,30	0
56	MG	1A	3009	1/1	0.93	0.10	16,16,16,16	0
56	MG	1A	3289	1/1	0.93	0.13	31,31,31,31	0
56	MG	2A	3194	1/1	0.93	0.13	46,46,46,46	0
56	MG	1A	3237	1/1	0.93	0.14	46,46,46,46	0
56	MG	1A	3068	1/1	0.93	0.14	13,13,13,13	0
56	MG	1A	3109	1/1	0.93	0.23	25,25,25,25	0
56	MG	1A	3931	1/1	0.93	0.10	38,38,38,38	0
56	MG	2A	3463	1/1	0.93	0.19	37,37,37,37	0
56	MG	2a	3211	1/1	0.93	0.15	60,60,60,60	0
56	MG	1A	4058	1/1	0.93	0.10	34,34,34,34	0
56	MG	1a	1826	1/1	0.93	0.07	66,66,66,66	0
56	MG	1A	4059	1/1	0.93	0.13	20,20,20,20	0
56	MG	1A	3043	1/1	0.93	0.25	33,33,33,33	0
56	MG	1A	3507	1/1	0.93	0.16	18,18,18,18	0
56	MG	2A	3475	1/1	0.93	0.06	44,44,44,44	0
56	MG	1a	1630	1/1	0.93	0.16	39,39,39,39	0
56	MG	1A	3508	1/1	0.93	0.24	18,18,18,18	0
56	MG	1f	201	1/1	0.93	0.16	32,32,32,32	0
56	MG	2A	3211	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3509	1/1	0.93	0.37	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3482	1/1	0.93	0.11	56,56,56,56	0
56	MG	1a	1635	1/1	0.93	0.23	52,52,52,52	0
56	MG	2A	3485	1/1	0.93	0.13	47,47,47,47	0
56	MG	2A	3215	1/1	0.93	0.42	58,58,58,58	0
56	MG	1A	3145	1/1	0.93	0.38	23,23,23,23	0
56	MG	2A	3488	1/1	0.93	0.20	42,42,42,42	0
56	MG	1A	3366	1/1	0.93	0.41	30,30,30,30	0
56	MG	1A	3050	1/1	0.93	0.12	30,30,30,30	0
56	MG	2A	3220	1/1	0.93	0.47	39,39,39,39	0
56	MG	2A	3222	1/1	0.93	0.42	44,44,44,44	0
56	MG	2x	102	1/1	0.93	0.07	62,62,62,62	0
56	MG	1A	3436	1/1	0.93	0.83	41,41,41,41	0
56	MG	1A	3249	1/1	0.93	0.21	23,23,23,23	0
56	MG	1A	4073	1/1	0.93	0.27	37,37,37,37	0
56	MG	1A	3438	1/1	0.93	0.71	49,49,49,49	0
56	MG	2A	3506	1/1	0.93	0.12	54,54,54,54	0
56	MG	1a	1651	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3646	1/1	0.93	0.16	28,28,28,28	0
57	LUJ	1A	4099	42/44	0.93	0.24	32,44,54,57	0
56	MG	1A	4077	1/1	0.93	0.13	46,46,46,46	0
56	MG	1A	3203	1/1	0.93	0.20	54,54,54,54	0
56	MG	1A	3147	1/1	0.93	0.35	21,21,21,21	0
57	LUJ	2a	3232	44/44	0.93	0.28	40,55,62,65	0
58	K	1A	4137	1/1	0.93	0.08	49,49,49,49	0
56	MG	1x	105	1/1	0.93	0.20	52,52,52,52	0
56	MG	2A	3848	1/1	0.93	0.15	55,55,55,55	0
56	MG	1A	4085	1/1	0.93	0.20	37,37,37,37	0
56	MG	2B	214	1/1	0.94	0.52	69,69,69,69	0
56	MG	1A	4088	1/1	0.94	0.07	47,47,47,47	0
56	MG	2A	3585	1/1	0.94	0.10	29,29,29,29	0
56	MG	2A	3313	1/1	0.94	0.13	59,59,59,59	0
56	MG	2D	303	1/1	0.94	0.26	29,29,29,29	0
56	MG	1A	3247	1/1	0.94	0.37	47,47,47,47	0
56	MG	2E	304	1/1	0.94	0.30	47,47,47,47	0
56	MG	2A	3114	1/1	0.94	0.14	60,60,60,60	0
56	MG	1A	4091	1/1	0.94	0.11	36,36,36,36	0
56	MG	1a	1621	1/1	0.94	0.09	44,44,44,44	0
56	MG	2A	3593	1/1	0.94	0.07	55,55,55,55	0
56	MG	1A	4093	1/1	0.94	0.14	45,45,45,45	0
56	MG	2A	3595	1/1	0.94	0.18	34,34,34,34	0
56	MG	1A	3859	1/1	0.94	0.22	20,20,20,20	0
56	MG	1A	3729	1/1	0.94	0.09	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	1A	3210	1/1	0.94	0.22	36,36,36,36	0
56	MG	2A	3123	1/1	0.94	0.16	43,43,43,43	0
56	MG	1A	3058	1/1	0.94	0.12	39,39,39,39	0
56	MG	1A	3523	1/1	0.94	0.15	23,23,23,23	0
56	MG	1A	3734	1/1	0.94	0.19	8,8,8,8	0
56	MG	2A	3607	1/1	0.94	0.13	34,34,34,34	0
56	MG	2A	3327	1/1	0.94	0.24	53,53,53,53	0
56	MG	2A	3137	1/1	0.94	0.21	38,38,38,38	0
56	MG	1a	1806	1/1	0.94	0.08	58,58,58,58	0
56	MG	1A	4107	1/1	0.94	0.41	21,21,21,21	0
56	MG	1A	3868	1/1	0.94	0.08	57,57,57,57	0
56	MG	2A	3141	1/1	0.94	0.20	42,42,42,42	0
56	MG	1A	3460	1/1	0.94	0.25	26,26,26,26	0
56	MG	1a	1634	1/1	0.94	0.25	59,59,59,59	0
56	MG	1A	4113	1/1	0.94	0.54	32,32,32,32	0
56	MG	2A	3145	1/1	0.94	0.43	33,33,33,33	0
56	MG	2A	3623	1/1	0.94	0.27	45,45,45,45	0
56	MG	2A	3339	1/1	0.94	0.13	48,48,48,48	0
56	MG	1A	3526	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	3302	1/1	0.94	0.19	35,35,35,35	0
56	MG	1A	3069	1/1	0.94	0.16	14,14,14,14	0
56	MG	1A	4120	1/1	0.94	0.62	33,33,33,33	0
56	MG	1A	4125	1/1	0.94	0.55	29,29,29,29	0
56	MG	2A	3151	1/1	0.94	0.27	63,63,63,63	0
56	MG	2A	3635	1/1	0.94	0.15	72,72,72,72	0
56	MG	2A	3636	1/1	0.94	0.24	57,57,57,57	0
56	MG	2a	3005	1/1	0.94	0.08	46,46,46,46	0
56	MG	1A	4126	1/1	0.94	0.16	25,25,25,25	0
56	MG	2A	3640	1/1	0.94	0.16	49,49,49,49	0
56	MG	2a	3008	1/1	0.94	0.15	58,58,58,58	0
56	MG	1a	1821	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3642	1/1	0.94	0.21	66,66,66,66	0
56	MG	2A	3154	1/1	0.94	0.10	53,53,53,53	0
56	MG	2a	3012	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3645	1/1	0.94	0.11	25,25,25,25	0
56	MG	1A	3463	1/1	0.94	0.46	42,42,42,42	0
56	MG	2A	3156	1/1	0.94	0.14	74,74,74,74	0
56	MG	1A	4134	1/1	0.94	0.13	31,31,31,31	0
56	MG	1A	3045	1/1	0.94	0.10	27,27,27,27	0
56	MG	1A	3743	1/1	0.94	0.08	27,27,27,27	0
56	MG	1A	3412	1/1	0.94	0.12	48,48,48,48	0
56	MG	1a	1830	1/1	0.94	0.34	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	3656	1/1	0.94	0.07	57,57,57,57	0
56	MG	2A	3657	1/1	0.94	0.20	58,58,58,58	0
56	MG	1a	1831	1/1	0.94	0.14	41,41,41,41	0
56	MG	2A	3660	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3645	1/1	0.94	0.06	30,30,30,30	0
56	MG	2A	3366	1/1	0.94	0.26	51,51,51,51	0
56	MG	1A	3748	1/1	0.94	0.17	44,44,44,44	0
56	MG	2a	3030	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3749	1/1	0.94	0.19	29,29,29,29	0
56	MG	2A	3369	1/1	0.94	0.36	46,46,46,46	0
56	MG	2A	3169	1/1	0.94	0.11	37,37,37,37	0
56	MG	2A	3170	1/1	0.94	0.14	35,35,35,35	0
56	MG	1a	1660	1/1	0.94	0.09	48,48,48,48	0
56	MG	1A	3537	1/1	0.94	0.07	25,25,25,25	0
56	MG	2a	3039	1/1	0.94	0.16	49,49,49,49	0
56	MG	1B	210	1/1	0.94	0.32	43,43,43,43	0
56	MG	2A	3174	1/1	0.94	0.12	45,45,45,45	0
56	MG	1A	3014	1/1	0.94	0.33	25,25,25,25	0
56	MG	1A	3892	1/1	0.94	0.45	37,37,37,37	0
56	MG	1A	3467	1/1	0.94	0.16	44,44,44,44	0
56	MG	1A	4003	1/1	0.94	0.09	24,24,24,24	0
56	MG	1B	223	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3680	1/1	0.94	0.11	60,60,60,60	0
56	MG	1B	224	1/1	0.94	0.19	55,55,55,55	0
56	MG	1A	3170	1/1	0.94	0.52	33,33,33,33	0
56	MG	2A	3182	1/1	0.94	0.27	51,51,51,51	0
56	MG	1A	3256	1/1	0.94	0.11	30,30,30,30	0
56	MG	2A	3185	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3397	1/1	0.94	0.43	38,38,38,38	0
56	MG	2A	3398	1/1	0.94	0.23	41,41,41,41	0
56	MG	2A	3186	1/1	0.94	0.39	38,38,38,38	0
56	MG	1w	107	1/1	0.94	0.06	59,59,59,59	0
56	MG	2A	3698	1/1	0.94	0.12	55,55,55,55	0
56	MG	1A	3362	1/1	0.94	0.13	42,42,42,42	0
56	MG	2A	3700	1/1	0.94	0.10	36,36,36,36	0
56	MG	1A	3471	1/1	0.94	0.18	34,34,34,34	0
56	MG	1A	3257	1/1	0.94	0.17	32,32,32,32	0
56	MG	1A	3658	1/1	0.94	0.10	28,28,28,28	0
56	MG	1A	3660	1/1	0.94	0.17	9,9,9,9	0
56	MG	2A	3195	1/1	0.94	0.13	35,35,35,35	0
56	MG	1A	3024	1/1	0.94	0.14	36,36,36,36	0
56	MG	2a	3072	1/1	0.94	0.11	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3073	1/1	0.94	0.24	49,49,49,49	0
56	MG	1D	301	1/1	0.94	0.13	34,34,34,34	0
56	MG	2a	3076	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3095	1/1	0.94	0.15	35,35,35,35	0
56	MG	2A	3715	1/1	0.94	0.07	47,47,47,47	0
56	MG	1E	301	1/1	0.94	0.27	20,20,20,20	0
56	MG	1A	3079	1/1	0.94	0.45	28,28,28,28	0
56	MG	1E	303	1/1	0.94	0.15	24,24,24,24	0
56	MG	2a	3083	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3322	1/1	0.94	0.10	36,36,36,36	0
56	MG	1y	101	1/1	0.94	0.19	30,30,30,30	0
56	MG	2A	3417	1/1	0.94	0.15	35,35,35,35	0
56	MG	1A	3120	1/1	0.94	0.13	23,23,23,23	0
56	MG	1A	3667	1/1	0.94	0.19	32,32,32,32	0
56	MG	1F	301	1/1	0.94	0.22	30,30,30,30	0
56	MG	2A	3209	1/1	0.94	0.10	39,39,39,39	0
56	MG	1A	3669	1/1	0.94	0.12	20,20,20,20	0
56	MG	2a	3096	1/1	0.94	0.10	46,46,46,46	0
56	MG	1A	3915	1/1	0.94	0.08	26,26,26,26	0
56	MG	1A	3324	1/1	0.94	0.23	41,41,41,41	0
56	MG	2A	3429	1/1	0.94	0.42	48,48,48,48	0
56	MG	2A	3005	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	3560	1/1	0.94	0.13	21,21,21,21	0
56	MG	1A	3377	1/1	0.94	0.17	12,12,12,12	0
56	MG	1A	3378	1/1	0.94	0.14	39,39,39,39	0
56	MG	1G	201	1/1	0.94	0.17	28,28,28,28	0
56	MG	2a	3107	1/1	0.94	0.10	48,48,48,48	0
56	MG	1A	3187	1/1	0.94	0.17	33,33,33,33	0
56	MG	2a	3110	1/1	0.94	0.17	41,41,41,41	0
56	MG	2A	3441	1/1	0.94	1.14	39,39,39,39	0
56	MG	1A	3042	1/1	0.94	0.16	25,25,25,25	0
56	MG	2A	3443	1/1	0.94	0.17	57,57,57,57	0
56	MG	1A	3229	1/1	0.94	0.25	10,10,10,10	0
56	MG	2A	3227	1/1	0.94	0.51	39,39,39,39	0
56	MG	2A	3748	1/1	0.94	0.09	48,48,48,48	0
56	MG	1A	3486	1/1	0.94	0.56	39,39,39,39	0
56	MG	1A	3573	1/1	0.94	0.56	18,18,18,18	0
56	MG	1A	4034	1/1	0.94	0.10	26,26,26,26	0
56	MG	1A	3929	1/1	0.94	0.07	19,19,19,19	0
56	MG	1A	3795	1/1	0.94	0.08	17,17,17,17	0
56	MG	2A	3456	1/1	0.94	0.10	39,39,39,39	0
56	MG	2A	3457	1/1	0.94	0.13	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	3458	1/1	0.94	0.23	48,48,48,48	0
56	MG	2A	3461	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3800	1/1	0.94	0.13	32,32,32,32	0
56	MG	2a	3134	1/1	0.94	0.22	60,60,60,60	0
56	MG	1a	1716	1/1	0.94	0.15	37,37,37,37	0
56	MG	1A	3487	1/1	0.94	0.50	38,38,38,38	0
56	MG	1a	1719	1/1	0.94	0.11	33,33,33,33	0
56	MG	2A	3469	1/1	0.94	0.26	52,52,52,52	0
56	MG	1A	3231	1/1	0.94	0.31	24,24,24,24	0
56	MG	2a	3140	1/1	0.94	0.35	77,77,77,77	0
56	MG	1a	1721	1/1	0.94	0.13	38,38,38,38	0
56	MG	2A	3036	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3037	1/1	0.94	0.25	47,47,47,47	0
56	MG	1Q	203	1/1	0.94	0.11	45,45,45,45	0
56	MG	2a	3145	1/1	0.94	0.06	53,53,53,53	0
56	MG	2A	3772	1/1	0.94	0.24	52,52,52,52	0
56	MG	1A	4041	1/1	0.94	0.08	24,24,24,24	0
56	MG	1A	3579	1/1	0.94	0.26	37,37,37,37	0
56	MG	1A	4043	1/1	0.94	0.07	31,31,31,31	0
56	MG	1R	204	1/1	0.94	0.25	32,32,32,32	0
56	MG	2A	3778	1/1	0.94	0.24	74,74,74,74	0
56	MG	1A	3806	1/1	0.94	0.58	22,22,22,22	0
56	MG	1A	3434	1/1	0.94	0.10	36,36,36,36	0
56	MG	1T	202	1/1	0.94	0.16	53,53,53,53	0
56	MG	1a	1731	1/1	0.94	0.19	45,45,45,45	0
56	MG	1A	3269	1/1	0.94	0.11	37,37,37,37	0
56	MG	1A	3492	1/1	0.94	0.08	43,43,43,43	0
56	MG	2A	3490	1/1	0.94	0.25	52,52,52,52	0
56	MG	2A	3787	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3693	1/1	0.94	0.12	9,9,9,9	0
56	MG	1a	1737	1/1	0.94	0.10	48,48,48,48	0
56	MG	1a	1738	1/1	0.94	0.20	44,44,44,44	0
56	MG	1V	201	1/1	0.94	0.22	37,37,37,37	0
56	MG	2A	3262	1/1	0.94	0.15	27,27,27,27	0
56	MG	2A	3502	1/1	0.94	0.06	37,37,37,37	0
56	MG	1A	3051	1/1	0.94	0.34	40,40,40,40	0
56	MG	1A	3586	1/1	0.94	0.55	39,39,39,39	0
56	MG	1A	3337	1/1	0.94	0.14	42,42,42,42	0
56	MG	1X	104	1/1	0.94	0.50	29,29,29,29	0
56	MG	2a	3174	1/1	0.94	0.13	51,51,51,51	0
56	MG	2a	3175	1/1	0.94	0.07	51,51,51,51	0
56	MG	2A	3508	1/1	0.94	0.19	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	1X	105	1/1	0.94	0.24	41,41,41,41	0
56	MG	1A	3439	1/1	0.94	0.49	30,30,30,30	0
56	MG	1A	3126	1/1	0.94	0.15	23,23,23,23	0
56	MG	2A	3270	1/1	0.94	0.14	38,38,38,38	0
56	MG	1A	4055	1/1	0.94	0.09	37,37,37,37	0
56	MG	1A	3025	1/1	0.94	0.26	38,38,38,38	0
56	MG	2A	3811	1/1	0.94	0.10	25,25,25,25	0
56	MG	2A	3518	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	3503	1/1	0.94	0.29	45,45,45,45	0
56	MG	2A	3520	1/1	0.94	0.11	48,48,48,48	0
56	MG	2a	3195	1/1	0.94	0.15	45,45,45,45	0
56	MG	1A	3153	1/1	0.94	0.17	15,15,15,15	0
56	MG	2A	3820	1/1	0.94	0.06	52,52,52,52	0
56	MG	1A	3950	1/1	0.94	0.12	32,32,32,32	0
56	MG	1A	3201	1/1	0.94	0.18	30,30,30,30	0
56	MG	2A	3074	1/1	0.94	0.44	49,49,49,49	0
56	MG	2A	3825	1/1	0.94	0.13	53,53,53,53	0
56	MG	1A	3154	1/1	0.94	0.15	32,32,32,32	0
56	MG	1A	3055	1/1	0.94	0.12	41,41,41,41	0
56	MG	2A	3079	1/1	0.94	0.22	26,26,26,26	0
56	MG	11	102	1/1	0.94	0.42	61,61,61,61	0
56	MG	1a	1762	1/1	0.94	0.15	60,60,60,60	0
56	MG	1A	3713	1/1	0.94	0.10	51,51,51,51	0
56	MG	1A	3399	1/1	0.94	0.14	37,37,37,37	0
56	MG	1A	3838	1/1	0.94	0.17	33,33,33,33	0
56	MG	2A	3836	1/1	0.94	0.16	49,49,49,49	0
56	MG	2a	3225	1/1	0.94	0.10	60,60,60,60	0
56	MG	2a	3228	1/1	0.94	0.11	60,60,60,60	0
56	MG	2A	3540	1/1	0.94	0.23	43,43,43,43	0
56	MG	17	102	1/1	0.94	0.28	37,37,37,37	0
56	MG	1A	3958	1/1	0.94	0.14	30,30,30,30	0
56	MG	1A	4069	1/1	0.94	0.28	27,27,27,27	0
56	MG	1A	3510	1/1	0.94	0.62	33,33,33,33	0
56	MG	2A	3843	1/1	0.94	0.12	35,35,35,35	0
56	MG	2A	3546	1/1	0.94	0.16	31,31,31,31	0
56	MG	2A	3293	1/1	0.94	0.22	52,52,52,52	0
56	MG	2A	3295	1/1	0.94	0.18	56,56,56,56	0
56	MG	2A	3550	1/1	0.94	0.22	34,34,34,34	0
56	MG	1A	3206	1/1	0.94	0.60	27,27,27,27	0
56	MG	2A	3096	1/1	0.94	0.20	65,65,65,65	0
56	MG	1A	3612	1/1	0.94	0.13	46,46,46,46	0
56	MG	2v	102	1/1	0.94	0.70	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	3558	1/1	0.94	0.14	27,27,27,27	0
56	MG	2x	101	1/1	0.94	0.12	45,45,45,45	0
56	MG	2A	3855	1/1	0.94	0.16	29,29,29,29	0
56	MG	1A	3613	1/1	0.94	0.18	16,16,16,16	0
56	MG	2x	104	1/1	0.94	0.14	57,57,57,57	0
56	MG	1A	3401	1/1	0.94	0.18	30,30,30,30	0
56	MG	2A	3859	1/1	0.94	0.16	39,39,39,39	0
56	MG	2A	3561	1/1	0.94	0.24	54,54,54,54	0
56	MG	1A	3001	1/1	0.94	0.17	32,32,32,32	0
56	MG	2A	3862	1/1	0.94	0.19	34,34,34,34	0
56	MG	2A	3564	1/1	0.94	0.23	49,49,49,49	0
56	MG	1A	3516	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3133	1/1	0.94	0.17	15,15,15,15	0
56	MG	1A	3852	1/1	0.94	0.21	44,44,44,44	0
56	MG	1a	1608	1/1	0.94	0.11	45,45,45,45	0
56	MG	1a	1787	1/1	0.94	0.23	49,49,49,49	0
56	MG	1a	1609	1/1	0.94	0.12	41,41,41,41	0
58	K	2A	3434	1/1	0.94	0.17	67,67,67,67	0
56	MG	2A	3573	1/1	0.94	0.10	22,22,22,22	0
56	MG	1A	3853	1/1	0.94	0.26	34,34,34,34	0
56	MG	1A	3350	1/1	0.94	0.34	38,38,38,38	0
59	ZN	2n	501	1/1	0.94	0.07	84,84,84,84	0
56	MG	1X	103	1/1	0.95	0.22	19,19,19,19	0
56	MG	1A	3053	1/1	0.95	0.12	25,25,25,25	0
56	MG	2A	3440	1/1	0.95	0.35	48,48,48,48	0
56	MG	1A	3188	1/1	0.95	0.39	30,30,30,30	0
56	MG	2A	3051	1/1	0.95	0.14	45,45,45,45	0
56	MG	1A	4076	1/1	0.95	0.18	8,8,8,8	0
56	MG	2A	3695	1/1	0.95	0.13	51,51,51,51	0
56	MG	2A	3444	1/1	0.95	0.22	38,38,38,38	0
56	MG	1A	3562	1/1	0.95	0.49	25,25,25,25	0
56	MG	1A	3290	1/1	0.95	0.15	32,32,32,32	0
56	MG	2A	3055	1/1	0.95	0.07	45,45,45,45	0
56	MG	2A	3247	1/1	0.95	0.31	48,48,48,48	0
56	MG	2A	3701	1/1	0.95	0.28	32,32,32,32	0
56	MG	1A	3446	1/1	0.95	0.40	35,35,35,35	0
56	MG	2A	3450	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3704	1/1	0.95	0.07	27,27,27,27	0
56	MG	1Z	303	1/1	0.95	0.20	26,26,26,26	0
56	MG	2A	3250	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3974	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3059	1/1	0.95	0.16	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	1A	3291	1/1	0.95	0.09	44,44,44,44	0
56	MG	2A	3713	1/1	0.95	0.18	69,69,69,69	0
56	MG	1A	3867	1/1	0.95	0.36	37,37,37,37	0
56	MG	1A	3567	1/1	0.95	0.13	36,36,36,36	0
56	MG	1A	3019	1/1	0.95	0.11	30,30,30,30	0
56	MG	2A	3717	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	4090	1/1	0.95	0.13	32,32,32,32	0
56	MG	2A	3466	1/1	0.95	0.22	39,39,39,39	0
56	MG	1A	3753	1/1	0.95	0.15	25,25,25,25	0
56	MG	1a	1755	1/1	0.95	0.08	29,29,29,29	0
56	MG	1A	4092	1/1	0.95	0.31	45,45,45,45	0
56	MG	2A	3068	1/1	0.95	0.17	24,24,24,24	0
56	MG	12	3702	1/1	0.95	0.22	30,30,30,30	0
56	MG	2A	3476	1/1	0.95	0.16	45,45,45,45	0
56	MG	1A	3294	1/1	0.95	0.25	47,47,47,47	0
56	MG	1A	4094	1/1	0.95	0.11	38,38,38,38	0
56	MG	2A	3728	1/1	0.95	0.09	54,54,54,54	0
56	MG	2A	3729	1/1	0.95	0.17	38,38,38,38	0
56	MG	15	101	1/1	0.95	0.53	31,31,31,31	0
56	MG	15	103	1/1	0.95	0.11	36,36,36,36	0
56	MG	16	102	1/1	0.95	0.47	47,47,47,47	0
56	MG	1A	3570	1/1	0.95	0.65	30,30,30,30	0
56	MG	1A	3873	1/1	0.95	0.13	22,22,22,22	0
56	MG	1A	3450	1/1	0.95	0.11	34,34,34,34	0
56	MG	1A	3295	1/1	0.95	0.29	47,47,47,47	0
56	MG	1A	3505	1/1	0.95	0.24	43,43,43,43	0
56	MG	1A	3452	1/1	0.95	0.18	27,27,27,27	0
56	MG	2A	3085	1/1	0.95	0.11	24,24,24,24	0
56	MG	1A	4105	1/1	0.95	0.11	31,31,31,31	0
56	MG	2A	3743	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3495	1/1	0.95	0.11	55,55,55,55	0
56	MG	2a	3066	1/1	0.95	0.24	40,40,40,40	0
56	MG	1A	3880	1/1	0.95	0.15	14,14,14,14	0
56	MG	1A	3404	1/1	0.95	0.40	34,34,34,34	0
56	MG	1A	3989	1/1	0.95	0.07	61,61,61,61	0
56	MG	1A	3883	1/1	0.95	0.20	56,56,56,56	0
56	MG	1A	3675	1/1	0.95	0.11	23,23,23,23	0
56	MG	1A	3114	1/1	0.95	0.39	22,22,22,22	0
56	MG	1A	4117	1/1	0.95	0.55	21,21,21,21	0
56	MG	1A	3887	1/1	0.95	0.21	29,29,29,29	0
56	MG	2A	3505	1/1	0.95	0.10	42,42,42,42	0
56	MG	1a	1613	1/1	0.95	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3196	1/1	0.95	0.12	21,21,21,21	0
56	MG	1A	3115	1/1	0.95	0.33	26,26,26,26	0
56	MG	1a	1616	1/1	0.95	0.11	46,46,46,46	0
56	MG	1A	3512	1/1	0.95	0.39	40,40,40,40	0
56	MG	1a	1618	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3997	1/1	0.95	0.10	31,31,31,31	0
56	MG	2A	3514	1/1	0.95	0.18	49,49,49,49	0
56	MG	2A	3294	1/1	0.95	0.16	55,55,55,55	0
56	MG	2A	3767	1/1	0.95	0.35	70,70,70,70	0
56	MG	1a	1620	1/1	0.95	0.19	40,40,40,40	0
56	MG	1A	4130	1/1	0.95	0.60	19,19,19,19	0
56	MG	1A	4132	1/1	0.95	0.42	24,24,24,24	0
56	MG	1A	3771	1/1	0.95	0.20	20,20,20,20	0
56	MG	1A	3772	1/1	0.95	0.14	61,61,61,61	0
56	MG	1A	4001	1/1	0.95	0.23	28,28,28,28	0
56	MG	1A	3034	1/1	0.95	0.36	25,25,25,25	0
56	MG	1A	3119	1/1	0.95	0.20	21,21,21,21	0
56	MG	2A	3525	1/1	0.95	0.28	46,46,46,46	0
56	MG	1a	1803	1/1	0.95	0.11	48,48,48,48	0
56	MG	2a	3102	1/1	0.95	0.06	56,56,56,56	0
56	MG	1A	3684	1/1	0.95	0.14	10,10,10,10	0
56	MG	1A	3258	1/1	0.95	0.13	37,37,37,37	0
56	MG	1A	3230	1/1	0.95	0.13	37,37,37,37	0
56	MG	1A	3021	1/1	0.95	0.11	28,28,28,28	0
56	MG	1A	3363	1/1	0.95	0.11	36,36,36,36	0
56	MG	2A	3126	1/1	0.95	0.18	29,29,29,29	0
56	MG	1A	3786	1/1	0.95	0.15	13,13,13,13	0
56	MG	2A	3133	1/1	0.95	0.09	46,46,46,46	0
56	MG	2a	3113	1/1	0.95	0.08	49,49,49,49	0
56	MG	1B	219	1/1	0.95	0.21	34,34,34,34	0
56	MG	1A	3690	1/1	0.95	0.13	7,7,7,7	0
56	MG	1a	1814	1/1	0.95	0.08	32,32,32,32	0
56	MG	2A	3791	1/1	0.95	0.13	35,35,35,35	0
56	MG	2a	3119	1/1	0.95	0.07	44,44,44,44	0
56	MG	1a	1638	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3106	1/1	0.95	0.26	17,17,17,17	0
56	MG	1A	3789	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3520	1/1	0.95	0.47	37,37,37,37	0
56	MG	2a	3125	1/1	0.95	0.04	58,58,58,58	0
56	MG	1a	1819	1/1	0.95	0.08	53,53,53,53	0
56	MG	1a	1643	1/1	0.95	0.16	54,54,54,54	0
56	MG	2A	3554	1/1	0.95	0.13	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	2A	3323	1/1	0.95	0.11	41,41,41,41	0
56	MG	1a	1644	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	4018	1/1	0.95	0.11	21,21,21,21	0
56	MG	1A	3262	1/1	0.95	0.82	33,33,33,33	0
56	MG	1a	1824	1/1	0.95	0.06	47,47,47,47	0
56	MG	2A	3328	1/1	0.95	0.28	33,33,33,33	0
56	MG	1B	228	1/1	0.95	0.17	46,46,46,46	0
56	MG	2A	3563	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	3695	1/1	0.95	0.16	25,25,25,25	0
56	MG	2A	3814	1/1	0.95	0.12	22,22,22,22	0
56	MG	2A	3565	1/1	0.95	0.10	34,34,34,34	0
56	MG	2A	3816	1/1	0.95	0.08	44,44,44,44	0
56	MG	2A	3566	1/1	0.95	0.09	60,60,60,60	0
56	MG	1A	3798	1/1	0.95	0.32	31,31,31,31	0
56	MG	1a	1828	1/1	0.95	0.18	49,49,49,49	0
56	MG	1A	3093	1/1	0.95	0.17	53,53,53,53	0
56	MG	1A	3604	1/1	0.95	0.17	25,25,25,25	0
56	MG	1A	3698	1/1	0.95	0.08	34,34,34,34	0
56	MG	1A	3608	1/1	0.95	0.14	26,26,26,26	0
56	MG	1A	3108	1/1	0.95	0.37	29,29,29,29	0
56	MG	2a	3152	1/1	0.95	0.14	61,61,61,61	0
56	MG	1D	306	1/1	0.95	0.16	31,31,31,31	0
56	MG	1A	3610	1/1	0.95	0.14	25,25,25,25	0
56	MG	1D	312	1/1	0.95	0.20	21,21,21,21	0
56	MG	2A	3161	1/1	0.95	0.67	47,47,47,47	0
56	MG	1A	3808	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3175	1/1	0.95	0.30	20,20,20,20	0
56	MG	1A	3928	1/1	0.95	0.12	15,15,15,15	0
56	MG	1A	3419	1/1	0.95	0.16	27,27,27,27	0
56	MG	2A	3590	1/1	0.95	0.13	52,52,52,52	0
56	MG	1A	3369	1/1	0.95	0.16	36,36,36,36	0
56	MG	2A	3592	1/1	0.95	0.13	64,64,64,64	0
56	MG	1A	3614	1/1	0.95	0.07	39,39,39,39	0
56	MG	1E	307	1/1	0.95	0.22	35,35,35,35	0
56	MG	1A	3027	1/1	0.95	0.26	17,17,17,17	0
56	MG	1A	3933	1/1	0.95	0.12	42,42,42,42	0
56	MG	1F	303	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3375	1/1	0.95	0.15	32,32,32,32	0
56	MG	1A	3935	1/1	0.95	0.11	31,31,31,31	0
56	MG	1a	1680	1/1	0.95	0.16	38,38,38,38	0
56	MG	2A	3602	1/1	0.95	0.13	20,20,20,20	0
56	MG	1A	3818	1/1	0.95	0.11	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	3179	1/1	0.95	0.14	59,59,59,59	0
56	MG	1x	106	1/1	0.95	0.05	59,59,59,59	0
56	MG	1A	3268	1/1	0.95	0.33	15,15,15,15	0
56	MG	1A	3536	1/1	0.95	0.18	30,30,30,30	0
56	MG	2A	3858	1/1	0.95	0.43	60,60,60,60	0
56	MG	1x	110	1/1	0.95	0.09	59,59,59,59	0
56	MG	2a	3184	1/1	0.95	0.13	34,34,34,34	0
56	MG	2a	3185	1/1	0.95	0.07	55,55,55,55	0
56	MG	2A	3183	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	3149	1/1	0.95	0.12	25,25,25,25	0
56	MG	1G	204	1/1	0.95	0.14	55,55,55,55	0
56	MG	2a	3189	1/1	0.95	0.48	61,61,61,61	0
56	MG	2a	3192	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3076	1/1	0.95	0.26	33,33,33,33	0
56	MG	1A	3828	1/1	0.95	0.12	37,37,37,37	0
56	MG	2A	3619	1/1	0.95	0.10	44,44,44,44	0
56	MG	1A	3832	1/1	0.95	0.09	38,38,38,38	0
56	MG	1N	203	1/1	0.95	0.21	42,42,42,42	0
56	MG	2a	3200	1/1	0.95	0.14	56,56,56,56	0
56	MG	2A	3190	1/1	0.95	0.11	54,54,54,54	0
56	MG	2a	3202	1/1	0.95	0.17	64,64,64,64	0
56	MG	1A	3540	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3428	1/1	0.95	0.09	28,28,28,28	0
56	MG	1A	3214	1/1	0.95	0.39	32,32,32,32	0
56	MG	2A	3001	1/1	0.95	0.23	34,34,34,34	0
56	MG	2a	3210	1/1	0.95	0.09	64,64,64,64	0
56	MG	2A	3629	1/1	0.95	0.12	53,53,53,53	0
56	MG	2a	3213	1/1	0.95	0.23	57,57,57,57	0
56	MG	1N	207	1/1	0.95	0.17	31,31,31,31	0
56	MG	2A	3391	1/1	0.95	0.15	45,45,45,45	0
56	MG	2A	3392	1/1	0.95	0.25	35,35,35,35	0
56	MG	1A	3273	1/1	0.95	0.28	16,16,16,16	0
56	MG	1O	202	1/1	0.95	0.27	37,37,37,37	0
56	MG	1A	3335	1/1	0.95	0.27	48,48,48,48	0
56	MG	2a	3221	1/1	0.95	0.12	61,61,61,61	0
56	MG	2a	3222	1/1	0.95	0.13	59,59,59,59	0
56	MG	2a	3223	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3545	1/1	0.95	0.13	27,27,27,27	0
56	MG	1A	3242	1/1	0.95	0.09	46,46,46,46	0
56	MG	2a	3227	1/1	0.95	0.12	65,65,65,65	0
56	MG	2A	3399	1/1	0.95	0.22	45,45,45,45	0
56	MG	1A	3276	1/1	0.95	0.46	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3435	1/1	0.95	0.43	34,34,34,34	0
56	MG	1A	3845	1/1	0.95	0.17	16,16,16,16	0
56	MG	2F	304	1/1	0.95	0.16	46,46,46,46	0
56	MG	1a	1710	1/1	0.95	0.12	36,36,36,36	0
56	MG	1R	201	1/1	0.95	0.12	29,29,29,29	0
56	MG	1A	3732	1/1	0.95	0.17	15,15,15,15	0
56	MG	2O	201	1/1	0.95	0.06	50,50,50,50	0
56	MG	1R	203	1/1	0.95	0.12	32,32,32,32	0
56	MG	1A	3641	1/1	0.95	0.06	44,44,44,44	0
56	MG	1A	3550	1/1	0.95	0.64	26,26,26,26	0
56	MG	2A	3213	1/1	0.95	0.35	40,40,40,40	0
56	MG	2q	202	1/1	0.95	0.09	52,52,52,52	0
56	MG	2q	203	1/1	0.95	0.07	70,70,70,70	0
56	MG	1a	1717	1/1	0.95	0.16	53,53,53,53	0
56	MG	2t	201	1/1	0.95	0.15	56,56,56,56	0
56	MG	2Q	203	1/1	0.95	0.25	45,45,45,45	0
56	MG	2A	3658	1/1	0.95	0.26	64,64,64,64	0
56	MG	1A	3243	1/1	0.95	0.10	32,32,32,32	0
56	MG	1A	3015	1/1	0.95	0.18	25,25,25,25	0
56	MG	1A	3851	1/1	0.95	0.09	43,43,43,43	0
56	MG	2A	3033	1/1	0.95	0.13	19,19,19,19	0
56	MG	1U	202	1/1	0.95	0.59	29,29,29,29	0
56	MG	1U	204	1/1	0.95	0.52	31,31,31,31	0
56	MG	1A	3246	1/1	0.95	0.17	22,22,22,22	0
56	MG	2A	3420	1/1	0.95	0.14	40,40,40,40	0
56	MG	2A	3224	1/1	0.95	0.22	56,56,56,56	0
56	MG	1A	3186	1/1	0.95	0.30	18,18,18,18	0
56	MG	2A	3423	1/1	0.95	0.12	59,59,59,59	0
56	MG	1A	3966	1/1	0.95	0.07	38,38,38,38	0
56	MG	1A	3248	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	4072	1/1	0.95	0.12	41,41,41,41	0
56	MG	1W	202	1/1	0.95	0.23	23,23,23,23	0
56	MG	29	101	1/1	0.95	0.18	37,37,37,37	0
56	MG	2A	3234	1/1	0.95	0.13	53,53,53,53	0
56	MG	1W	204	1/1	0.95	0.15	28,28,28,28	0
59	ZN	2Y	202	1/1	0.95	0.11	88,88,88,88	0
56	MG	1A	3557	1/1	0.95	0.12	34,34,34,34	0
56	MG	2A	3237	1/1	0.95	0.29	41,41,41,41	0
56	MG	1X	101	1/1	0.95	0.10	26,26,26,26	0
56	MG	2a	3023	1/1	0.96	0.14	44,44,44,44	0
56	MG	1A	3077	1/1	0.96	0.17	18,18,18,18	0
56	MG	1A	3812	1/1	0.96	0.10	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3026	1/1	0.96	0.09	34,34,34,34	0
56	MG	2A	3088	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3279	1/1	0.96	0.35	39,39,39,39	0
56	MG	2A	3484	1/1	0.96	0.15	40,40,40,40	0
56	MG	1A	3925	1/1	0.96	0.13	12,12,12,12	0
56	MG	2a	3031	1/1	0.96	0.09	40,40,40,40	0
56	MG	1a	1785	1/1	0.96	0.14	40,40,40,40	0
56	MG	2A	3093	1/1	0.96	0.08	37,37,37,37	0
56	MG	1A	3280	1/1	0.96	0.16	34,34,34,34	0
56	MG	1A	3325	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3159	1/1	0.96	0.19	36,36,36,36	0
56	MG	2A	3492	1/1	0.96	0.11	39,39,39,39	0
56	MG	2A	3493	1/1	0.96	0.21	36,36,36,36	0
56	MG	1A	3283	1/1	0.96	0.15	30,30,30,30	0
56	MG	1A	3511	1/1	0.96	0.14	32,32,32,32	0
56	MG	1D	302	1/1	0.96	0.36	26,26,26,26	0
56	MG	2a	3044	1/1	0.96	0.09	50,50,50,50	0
56	MG	1D	304	1/1	0.96	0.60	35,35,35,35	0
56	MG	1A	3067	1/1	0.96	0.15	13,13,13,13	0
56	MG	2A	3102	1/1	0.96	0.17	39,39,39,39	0
56	MG	1D	308	1/1	0.96	0.16	25,25,25,25	0
56	MG	1D	309	1/1	0.96	0.28	34,34,34,34	0
56	MG	1A	3822	1/1	0.96	0.26	62,62,62,62	0
56	MG	1A	3371	1/1	0.96	0.61	41,41,41,41	0
56	MG	2A	3740	1/1	0.96	0.10	42,42,42,42	0
56	MG	2A	3292	1/1	0.96	0.12	37,37,37,37	0
56	MG	1A	3826	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	3372	1/1	0.96	0.21	24,24,24,24	0
56	MG	2A	3509	1/1	0.96	0.12	25,25,25,25	0
56	MG	1A	3374	1/1	0.96	0.12	28,28,28,28	0
56	MG	2A	3746	1/1	0.96	0.09	62,62,62,62	0
56	MG	1A	3829	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3831	1/1	0.96	0.12	36,36,36,36	0
56	MG	2a	3063	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3572	1/1	0.96	0.48	33,33,33,33	0
56	MG	1A	3331	1/1	0.96	0.15	36,36,36,36	0
56	MG	1a	1646	1/1	0.96	0.18	41,41,41,41	0
56	MG	1A	3574	1/1	0.96	0.15	25,25,25,25	0
56	MG	1A	3656	1/1	0.96	0.12	9,9,9,9	0
56	MG	1a	1811	1/1	0.96	0.14	40,40,40,40	0
56	MG	1A	3020	1/1	0.96	0.15	26,26,26,26	0
56	MG	2A	3122	1/1	0.96	0.13	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3287	1/1	0.96	0.19	20,20,20,20	0
56	MG	1A	3578	1/1	0.96	0.10	32,32,32,32	0
56	MG	2A	3125	1/1	0.96	0.14	41,41,41,41	0
56	MG	1A	3839	1/1	0.96	0.22	14,14,14,14	0
56	MG	1F	307	1/1	0.96	0.25	15,15,15,15	0
56	MG	2A	3764	1/1	0.96	0.05	62,62,62,62	0
56	MG	2A	3132	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3840	1/1	0.96	0.14	12,12,12,12	0
56	MG	2A	3135	1/1	0.96	0.23	43,43,43,43	0
56	MG	2a	3082	1/1	0.96	0.11	72,72,72,72	0
56	MG	1A	3118	1/1	0.96	0.69	31,31,31,31	0
56	MG	2a	3084	1/1	0.96	0.12	57,57,57,57	0
56	MG	1A	3236	1/1	0.96	0.21	26,26,26,26	0
56	MG	1A	3189	1/1	0.96	0.29	23,23,23,23	0
56	MG	2a	3087	1/1	0.96	0.11	44,44,44,44	0
56	MG	1a	1663	1/1	0.96	0.11	57,57,57,57	0
56	MG	1A	3010	1/1	0.96	0.14	20,20,20,20	0
56	MG	2A	3773	1/1	0.96	0.34	65,65,65,65	0
56	MG	1A	3022	1/1	0.96	0.13	11,11,11,11	0
56	MG	1A	3666	1/1	0.96	0.15	20,20,20,20	0
56	MG	1A	3293	1/1	0.96	0.13	21,21,21,21	0
56	MG	1A	3668	1/1	0.96	0.13	36,36,36,36	0
56	MG	1a	1669	1/1	0.96	0.19	52,52,52,52	0
56	MG	1A	3431	1/1	0.96	0.14	37,37,37,37	0
56	MG	1A	3957	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	4065	1/1	0.96	0.07	29,29,29,29	0
56	MG	1A	3589	1/1	0.96	0.14	21,21,21,21	0
56	MG	1A	3959	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3590	1/1	0.96	0.13	15,15,15,15	0
56	MG	1a	1676	1/1	0.96	0.17	46,46,46,46	0
56	MG	2a	3105	1/1	0.96	0.06	66,66,66,66	0
56	MG	1e	202	1/1	0.96	0.06	64,64,64,64	0
56	MG	1O	203	1/1	0.96	0.42	56,56,56,56	0
56	MG	2a	3108	1/1	0.96	0.24	40,40,40,40	0
56	MG	1A	3527	1/1	0.96	0.21	27,27,27,27	0
56	MG	1A	3963	1/1	0.96	0.16	44,44,44,44	0
56	MG	1t	201	1/1	0.96	0.14	44,44,44,44	0
56	MG	1A	3854	1/1	0.96	0.43	54,54,54,54	0
56	MG	1Q	202	1/1	0.96	0.21	25,25,25,25	0
56	MG	1A	3673	1/1	0.96	0.12	12,12,12,12	0
56	MG	2a	3115	1/1	0.96	0.20	49,49,49,49	0
56	MG	1a	1684	1/1	0.96	0.19	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3796	1/1	0.96	0.16	29,29,29,29	0
56	MG	2A	3344	1/1	0.96	0.16	46,46,46,46	0
56	MG	1A	3195	1/1	0.96	0.12	17,17,17,17	0
56	MG	2a	3120	1/1	0.96	0.17	59,59,59,59	0
56	MG	1A	3529	1/1	0.96	0.20	22,22,22,22	0
56	MG	1A	3758	1/1	0.96	0.12	19,19,19,19	0
56	MG	1A	3530	1/1	0.96	0.25	26,26,26,26	0
56	MG	1A	3169	1/1	0.96	0.28	19,19,19,19	0
56	MG	1A	4078	1/1	0.96	0.17	6,6,6,6	0
56	MG	1A	3762	1/1	0.96	0.17	13,13,13,13	0
56	MG	2A	3576	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	4080	1/1	0.96	0.10	11,11,11,11	0
56	MG	2A	3580	1/1	0.96	0.20	45,45,45,45	0
56	MG	2a	3131	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	4082	1/1	0.96	0.20	31,31,31,31	0
56	MG	2A	3813	1/1	0.96	0.10	41,41,41,41	0
56	MG	1a	1694	1/1	0.96	0.20	39,39,39,39	0
56	MG	1A	3596	1/1	0.96	0.14	23,23,23,23	0
56	MG	1A	3033	1/1	0.96	0.55	28,28,28,28	0
56	MG	2A	3361	1/1	0.96	0.06	57,57,57,57	0
56	MG	1a	1698	1/1	0.96	0.18	41,41,41,41	0
56	MG	1A	3221	1/1	0.96	0.20	12,12,12,12	0
56	MG	1A	3244	1/1	0.96	0.12	49,49,49,49	0
56	MG	2A	3365	1/1	0.96	0.25	57,57,57,57	0
56	MG	1A	3303	1/1	0.96	0.15	28,28,28,28	0
56	MG	1A	3396	1/1	0.96	0.38	24,24,24,24	0
56	MG	1a	1704	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3605	1/1	0.96	0.20	29,29,29,29	0
56	MG	1A	3687	1/1	0.96	0.21	25,25,25,25	0
56	MG	2A	3371	1/1	0.96	0.16	44,44,44,44	0
56	MG	1a	1707	1/1	0.96	0.19	45,45,45,45	0
56	MG	1A	3775	1/1	0.96	0.06	28,28,28,28	0
56	MG	2a	3150	1/1	0.96	0.18	51,51,51,51	0
56	MG	1W	203	1/1	0.96	0.22	40,40,40,40	0
56	MG	1A	3875	1/1	0.96	0.16	34,34,34,34	0
56	MG	1A	3776	1/1	0.96	0.07	22,22,22,22	0
56	MG	2A	3605	1/1	0.96	0.10	38,38,38,38	0
56	MG	1W	207	1/1	0.96	0.24	15,15,15,15	0
56	MG	1A	3877	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3606	1/1	0.96	0.17	38,38,38,38	0
56	MG	2A	3192	1/1	0.96	0.19	41,41,41,41	0
56	MG	2A	3611	1/1	0.96	0.10	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	1715	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3607	1/1	0.96	0.18	21,21,21,21	0
56	MG	2A	3846	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3538	1/1	0.96	0.16	47,47,47,47	0
56	MG	2A	3013	1/1	0.96	0.23	27,27,27,27	0
56	MG	1A	3780	1/1	0.96	0.21	36,36,36,36	0
56	MG	1A	3882	1/1	0.96	0.10	15,15,15,15	0
56	MG	1A	4104	1/1	0.96	0.43	24,24,24,24	0
56	MG	2A	3621	1/1	0.96	0.07	38,38,38,38	0
56	MG	2A	3395	1/1	0.96	0.13	24,24,24,24	0
56	MG	2A	3017	1/1	0.96	0.14	29,29,29,29	0
56	MG	1Y	205	1/1	0.96	0.50	48,48,48,48	0
56	MG	1Z	301	1/1	0.96	0.36	34,34,34,34	0
56	MG	2A	3626	1/1	0.96	0.22	33,33,33,33	0
56	MG	2A	3203	1/1	0.96	0.26	55,55,55,55	0
56	MG	1A	3304	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3884	1/1	0.96	0.25	54,54,54,54	0
56	MG	2A	3023	1/1	0.96	0.58	43,43,43,43	0
56	MG	1A	3351	1/1	0.96	0.18	36,36,36,36	0
56	MG	2a	3182	1/1	0.96	0.06	62,62,62,62	0
56	MG	1A	3222	1/1	0.96	0.10	20,20,20,20	0
56	MG	2B	203	1/1	0.96	0.18	34,34,34,34	0
56	MG	1A	4112	1/1	0.96	0.09	43,43,43,43	0
56	MG	2A	3029	1/1	0.96	0.20	38,38,38,38	0
56	MG	1A	3784	1/1	0.96	0.18	11,11,11,11	0
56	MG	10	104	1/1	0.96	0.16	29,29,29,29	0
56	MG	2A	3032	1/1	0.96	0.10	45,45,45,45	0
56	MG	2a	3191	1/1	0.96	0.30	66,66,66,66	0
56	MG	1A	3443	1/1	0.96	0.23	27,27,27,27	0
56	MG	2A	3216	1/1	0.96	0.12	52,52,52,52	0
56	MG	2A	3644	1/1	0.96	0.19	47,47,47,47	0
56	MG	1A	3306	1/1	0.96	0.15	24,24,24,24	0
56	MG	1a	1733	1/1	0.96	0.20	57,57,57,57	0
56	MG	1A	3223	1/1	0.96	0.81	27,27,27,27	0
56	MG	1A	3172	1/1	0.96	0.10	23,23,23,23	0
56	MG	1a	1736	1/1	0.96	0.15	62,62,62,62	0
56	MG	2E	303	1/1	0.96	0.25	40,40,40,40	0
56	MG	1A	4119	1/1	0.96	0.21	21,21,21,21	0
56	MG	2A	3042	1/1	0.96	0.13	24,24,24,24	0
56	MG	2A	3652	1/1	0.96	0.21	35,35,35,35	0
56	MG	2a	3206	1/1	0.96	0.09	56,56,56,56	0
56	MG	2A	3226	1/1	0.96	0.15	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	2A	3655	1/1	0.96	0.12	31,31,31,31	0
56	MG	1A	3104	1/1	0.96	0.17	25,25,25,25	0
56	MG	2a	3212	1/1	0.96	0.21	38,38,38,38	0
56	MG	2A	3228	1/1	0.96	0.54	44,44,44,44	0
56	MG	1A	4121	1/1	0.96	0.66	27,27,27,27	0
56	MG	1a	1740	1/1	0.96	0.13	61,61,61,61	0
56	MG	2A	3231	1/1	0.96	0.27	46,46,46,46	0
56	MG	1A	3493	1/1	0.96	0.29	22,22,22,22	0
56	MG	15	102	1/1	0.96	0.32	28,28,28,28	0
56	MG	2A	3664	1/1	0.96	0.14	47,47,47,47	0
56	MG	2A	3430	1/1	0.96	0.11	56,56,56,56	0
56	MG	1a	1744	1/1	0.96	0.20	50,50,50,50	0
56	MG	1a	1745	1/1	0.96	0.08	32,32,32,32	0
56	MG	1A	4000	1/1	0.96	0.12	15,15,15,15	0
56	MG	1A	4127	1/1	0.96	0.74	27,27,27,27	0
56	MG	17	101	1/1	0.96	0.12	29,29,29,29	0
56	MG	2Q	205	1/1	0.96	0.12	43,43,43,43	0
56	MG	2R	3003	1/1	0.96	0.10	40,40,40,40	0
56	MG	2a	3230	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3357	1/1	0.96	0.24	31,31,31,31	0
56	MG	1A	3792	1/1	0.96	0.13	22,22,22,22	0
56	MG	1A	3793	1/1	0.96	0.19	23,23,23,23	0
56	MG	1A	3056	1/1	0.96	0.17	28,28,28,28	0
56	MG	1a	1753	1/1	0.96	0.24	45,45,45,45	0
56	MG	1A	3796	1/1	0.96	0.57	20,20,20,20	0
56	MG	2j	201	1/1	0.96	0.09	74,74,74,74	0
56	MG	1A	3797	1/1	0.96	0.12	43,43,43,43	0
56	MG	1A	3274	1/1	0.96	0.27	19,19,19,19	0
56	MG	1A	3909	1/1	0.96	0.14	33,33,33,33	0
56	MG	1A	3622	1/1	0.96	0.16	9,9,9,9	0
56	MG	2A	3683	1/1	0.96	0.13	16,16,16,16	0
56	MG	1A	3706	1/1	0.96	0.09	40,40,40,40	0
56	MG	1A	3178	1/1	0.96	0.19	41,41,41,41	0
56	MG	1A	3804	1/1	0.96	0.13	19,19,19,19	0
56	MG	27	101	1/1	0.96	0.80	41,41,41,41	0
56	MG	2v	101	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3624	1/1	0.96	0.13	37,37,37,37	0
56	MG	1B	213	1/1	0.96	0.13	41,41,41,41	0
56	MG	1a	1610	1/1	0.96	0.12	19,19,19,19	0
56	MG	2A	3693	1/1	0.96	0.07	40,40,40,40	0
56	MG	2A	3694	1/1	0.96	0.20	34,34,34,34	0
56	MG	1a	1611	1/1	0.96	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3460	1/1	0.96	0.21	31,31,31,31	0
56	MG	1A	3127	1/1	0.96	0.17	49,49,49,49	0
56	MG	1a	1768	1/1	0.96	0.14	46,46,46,46	0
56	MG	2A	3072	1/1	0.96	0.11	52,52,52,52	0
56	MG	1a	1770	1/1	0.96	0.08	34,34,34,34	0
56	MG	1A	4019	1/1	0.96	0.07	47,47,47,47	0
56	MG	2A	3075	1/1	0.96	0.47	42,42,42,42	0
56	MG	2A	3468	1/1	0.96	0.18	38,38,38,38	0
57	LUJ	1a	1832	44/44	0.96	0.26	29,39,44,48	0
56	MG	1A	3317	1/1	0.96	0.31	30,30,30,30	0
56	MG	2A	3472	1/1	0.96	0.17	30,30,30,30	0
56	MG	2A	3706	1/1	0.96	0.07	62,62,62,62	0
56	MG	2A	3077	1/1	0.96	0.28	41,41,41,41	0
56	MG	1A	3555	1/1	0.96	0.23	38,38,38,38	0
56	MG	1A	3717	1/1	0.96	0.13	27,27,27,27	0
56	MG	1A	3920	1/1	0.96	0.15	25,25,25,25	0
56	MG	1a	1778	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3156	1/1	0.96	0.32	18,18,18,18	0
56	MG	1B	226	1/1	0.96	0.12	26,26,26,26	0
56	MG	1y	102	1/1	0.97	0.09	40,40,40,40	0
56	MG	2A	3529	1/1	0.97	0.13	43,43,43,43	0
56	MG	2A	3530	1/1	0.97	0.16	29,29,29,29	0
56	MG	1B	203	1/1	0.97	0.25	33,33,33,33	0
56	MG	2a	3048	1/1	0.97	0.09	51,51,51,51	0
56	MG	2A	3532	1/1	0.97	0.10	45,45,45,45	0
56	MG	2A	3533	1/1	0.97	0.13	40,40,40,40	0
56	MG	2A	3332	1/1	0.97	0.12	33,33,33,33	0
56	MG	2A	3163	1/1	0.97	0.19	29,29,29,29	0
56	MG	2A	3751	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3635	1/1	0.97	0.12	29,29,29,29	0
56	MG	2A	3537	1/1	0.97	0.08	47,47,47,47	0
56	MG	1A	3228	1/1	0.97	0.20	55,55,55,55	0
56	MG	2A	3166	1/1	0.97	0.23	35,35,35,35	0
56	MG	1A	3816	1/1	0.97	0.13	28,28,28,28	0
56	MG	2a	3059	1/1	0.97	0.13	48,48,48,48	0
56	MG	1A	3638	1/1	0.97	0.17	27,27,27,27	0
56	MG	1a	1725	1/1	0.97	0.16	32,32,32,32	0
56	MG	2A	3003	1/1	0.97	0.24	36,36,36,36	0
56	MG	1A	3639	1/1	0.97	0.15	32,32,32,32	0
56	MG	1A	3181	1/1	0.97	0.17	24,24,24,24	0
56	MG	1B	211	1/1	0.97	0.34	46,46,46,46	0
56	MG	2A	3007	1/1	0.97	0.21	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	16	101	1/1	0.97	0.16	32,32,32,32	0
56	MG	2A	3551	1/1	0.97	0.08	58,58,58,58	0
56	MG	2A	3552	1/1	0.97	0.12	23,23,23,23	0
56	MG	1A	3182	1/1	0.97	0.28	36,36,36,36	0
56	MG	1A	3644	1/1	0.97	0.15	24,24,24,24	0
56	MG	2A	3555	1/1	0.97	0.18	38,38,38,38	0
56	MG	1B	214	1/1	0.97	0.20	29,29,29,29	0
56	MG	2A	3350	1/1	0.97	0.28	42,42,42,42	0
56	MG	17	103	1/1	0.97	0.23	21,21,21,21	0
56	MG	1B	217	1/1	0.97	0.10	18,18,18,18	0
56	MG	1A	3029	1/1	0.97	0.42	21,21,21,21	0
56	MG	18	102	1/1	0.97	0.11	38,38,38,38	0
56	MG	18	103	1/1	0.97	0.18	26,26,26,26	0
56	MG	1A	3086	1/1	0.97	0.16	30,30,30,30	0
56	MG	1A	3825	1/1	0.97	0.24	58,58,58,58	0
56	MG	2A	3360	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3647	1/1	0.97	0.16	21,21,21,21	0
56	MG	1a	1741	1/1	0.97	0.19	36,36,36,36	0
56	MG	2A	3783	1/1	0.97	0.09	59,59,59,59	0
56	MG	1B	222	1/1	0.97	0.12	44,44,44,44	0
56	MG	2A	3025	1/1	0.97	0.12	33,33,33,33	0
56	MG	1A	3185	1/1	0.97	0.38	18,18,18,18	0
56	MG	1A	3649	1/1	0.97	0.16	11,11,11,11	0
56	MG	2a	3092	1/1	0.97	0.22	45,45,45,45	0
56	MG	1A	3650	1/1	0.97	0.13	10,10,10,10	0
56	MG	1A	3571	1/1	0.97	0.28	25,25,25,25	0
56	MG	2A	3574	1/1	0.97	0.09	40,40,40,40	0
56	MG	1A	3087	1/1	0.97	0.19	17,17,17,17	0
56	MG	1A	3030	1/1	0.97	0.20	9,9,9,9	0
56	MG	1A	4038	1/1	0.97	0.12	13,13,13,13	0
56	MG	2A	3579	1/1	0.97	0.12	28,28,28,28	0
56	MG	1A	3031	1/1	0.97	0.37	17,17,17,17	0
56	MG	2A	3581	1/1	0.97	0.11	51,51,51,51	0
56	MG	1A	3003	1/1	0.97	0.12	17,17,17,17	0
56	MG	2A	3583	1/1	0.97	0.20	41,41,41,41	0
56	MG	1A	3742	1/1	0.97	0.10	22,22,22,22	0
56	MG	2A	3800	1/1	0.97	0.10	35,35,35,35	0
56	MG	1A	3282	1/1	0.97	0.36	34,34,34,34	0
56	MG	2A	3802	1/1	0.97	0.12	34,34,34,34	0
56	MG	2A	3038	1/1	0.97	0.16	40,40,40,40	0
56	MG	1A	3744	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3052	1/1	0.97	0.17	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	3041	1/1	0.97	0.19	41,41,41,41	0
56	MG	1A	3116	1/1	0.97	0.15	24,24,24,24	0
56	MG	2A	3206	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3841	1/1	0.97	0.19	31,31,31,31	0
56	MG	2A	3387	1/1	0.97	0.17	46,46,46,46	0
56	MG	2A	3388	1/1	0.97	0.30	38,38,38,38	0
56	MG	1D	305	1/1	0.97	0.09	10,10,10,10	0
56	MG	1A	3659	1/1	0.97	0.09	21,21,21,21	0
56	MG	1D	307	1/1	0.97	0.74	28,28,28,28	0
56	MG	1A	3580	1/1	0.97	0.22	15,15,15,15	0
56	MG	1A	3581	1/1	0.97	0.15	38,38,38,38	0
56	MG	2A	3601	1/1	0.97	0.08	49,49,49,49	0
56	MG	1a	1623	1/1	0.97	0.19	42,42,42,42	0
56	MG	1D	310	1/1	0.97	0.20	29,29,29,29	0
56	MG	1A	3151	1/1	0.97	0.15	45,45,45,45	0
56	MG	1A	3008	1/1	0.97	0.12	12,12,12,12	0
56	MG	2A	3606	1/1	0.97	0.08	31,31,31,31	0
56	MG	2a	3128	1/1	0.97	0.15	40,40,40,40	0
56	MG	1D	313	1/1	0.97	0.30	23,23,23,23	0
56	MG	1a	1769	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3070	1/1	0.97	0.32	20,20,20,20	0
56	MG	1A	3094	1/1	0.97	0.23	22,22,22,22	0
56	MG	1a	1772	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3016	1/1	0.97	0.16	38,38,38,38	0
56	MG	1A	3096	1/1	0.97	0.17	17,17,17,17	0
56	MG	2A	3225	1/1	0.97	0.11	48,48,48,48	0
56	MG	1a	1632	1/1	0.97	0.11	25,25,25,25	0
56	MG	2A	3617	1/1	0.97	0.30	47,47,47,47	0
56	MG	1A	3588	1/1	0.97	0.24	24,24,24,24	0
56	MG	1A	3202	1/1	0.97	0.14	41,41,41,41	0
56	MG	1A	3122	1/1	0.97	0.41	23,23,23,23	0
56	MG	1A	3035	1/1	0.97	0.11	13,13,13,13	0
56	MG	1A	3855	1/1	0.97	0.09	23,23,23,23	0
56	MG	1A	3098	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	4063	1/1	0.97	0.12	37,37,37,37	0
56	MG	1A	3075	1/1	0.97	0.27	22,22,22,22	0
56	MG	1A	3300	1/1	0.97	0.10	17,17,17,17	0
56	MG	1A	3961	1/1	0.97	0.19	26,26,26,26	0
56	MG	1A	3162	1/1	0.97	0.44	25,25,25,25	0
56	MG	1F	309	1/1	0.97	0.09	36,36,36,36	0
56	MG	1A	3163	1/1	0.97	0.15	22,22,22,22	0
56	MG	2A	3631	1/1	0.97	0.43	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	3768	1/1	0.97	0.09	21,21,21,21	0
56	MG	2A	3633	1/1	0.97	0.10	53,53,53,53	0
56	MG	1a	1791	1/1	0.97	0.12	62,62,62,62	0
56	MG	1a	1649	1/1	0.97	0.21	53,53,53,53	0
56	MG	2A	3426	1/1	0.97	0.23	33,33,33,33	0
56	MG	2A	3637	1/1	0.97	0.15	54,54,54,54	0
56	MG	2a	3159	1/1	0.97	0.08	64,64,64,64	0
56	MG	1A	3253	1/1	0.97	0.17	46,46,46,46	0
56	MG	1G	203	1/1	0.97	0.06	61,61,61,61	0
56	MG	1A	3864	1/1	0.97	0.50	23,23,23,23	0
56	MG	2a	3163	1/1	0.97	0.09	62,62,62,62	0
56	MG	1G	205	1/1	0.97	0.14	40,40,40,40	0
56	MG	1a	1655	1/1	0.97	0.14	45,45,45,45	0
56	MG	1a	1798	1/1	0.97	0.08	48,48,48,48	0
56	MG	2B	205	1/1	0.97	0.11	52,52,52,52	0
56	MG	1a	1656	1/1	0.97	0.17	48,48,48,48	0
56	MG	2B	207	1/1	0.97	0.17	60,60,60,60	0
56	MG	2A	3435	1/1	0.97	0.13	19,19,19,19	0
56	MG	1A	3164	1/1	0.97	0.26	26,26,26,26	0
56	MG	1A	3600	1/1	0.97	0.16	33,33,33,33	0
56	MG	2A	3438	1/1	0.97	0.12	33,33,33,33	0
56	MG	2A	3087	1/1	0.97	0.18	59,59,59,59	0
56	MG	1A	3212	1/1	0.97	0.11	36,36,36,36	0
56	MG	2A	3089	1/1	0.97	0.12	34,34,34,34	0
56	MG	1A	3773	1/1	0.97	0.13	37,37,37,37	0
56	MG	2B	218	1/1	0.97	0.21	40,40,40,40	0
56	MG	2A	3654	1/1	0.97	0.27	57,57,57,57	0
56	MG	1A	3774	1/1	0.97	0.06	16,16,16,16	0
56	MG	2a	3181	1/1	0.97	0.14	53,53,53,53	0
56	MG	1a	1805	1/1	0.97	0.24	49,49,49,49	0
56	MG	1A	3473	1/1	0.97	0.23	38,38,38,38	0
56	MG	1A	3603	1/1	0.97	0.12	8,8,8,8	0
56	MG	1A	3036	1/1	0.97	0.67	26,26,26,26	0
56	MG	2E	306	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3037	1/1	0.97	0.26	24,24,24,24	0
56	MG	1A	3039	1/1	0.97	0.12	18,18,18,18	0
56	MG	1A	3132	1/1	0.97	0.09	40,40,40,40	0
56	MG	2a	3190	1/1	0.97	0.15	56,56,56,56	0
56	MG	1A	3217	1/1	0.97	0.17	26,26,26,26	0
56	MG	2A	3454	1/1	0.97	0.19	52,52,52,52	0
56	MG	1P	201	1/1	0.97	0.32	19,19,19,19	0
56	MG	1A	3311	1/1	0.97	0.08	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	3040	1/1	0.97	0.44	21,21,21,21	0
56	MG	2a	3196	1/1	0.97	0.14	63,63,63,63	0
56	MG	1A	3171	1/1	0.97	0.18	17,17,17,17	0
56	MG	2A	3459	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3004	1/1	0.97	0.19	17,17,17,17	0
56	MG	1A	3173	1/1	0.97	0.16	10,10,10,10	0
56	MG	1A	3373	1/1	0.97	0.17	20,20,20,20	0
56	MG	1A	3318	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3005	1/1	0.97	0.17	29,29,29,29	0
56	MG	2A	3676	1/1	0.97	0.26	36,36,36,36	0
56	MG	2A	3274	1/1	0.97	0.09	39,39,39,39	0
56	MG	2a	3207	1/1	0.97	0.16	44,44,44,44	0
56	MG	1A	3617	1/1	0.97	0.10	14,14,14,14	0
56	MG	2a	3209	1/1	0.97	0.10	46,46,46,46	0
56	MG	2R	3002	1/1	0.97	0.13	46,46,46,46	0
56	MG	2A	3110	1/1	0.97	0.15	30,30,30,30	0
56	MG	2A	3111	1/1	0.97	0.16	36,36,36,36	0
56	MG	2A	3470	1/1	0.97	0.21	21,21,21,21	0
56	MG	1a	1679	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3320	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3176	1/1	0.97	0.21	31,31,31,31	0
56	MG	1A	3889	1/1	0.97	0.09	43,43,43,43	0
56	MG	1T	201	1/1	0.97	0.10	34,34,34,34	0
56	MG	2A	3117	1/1	0.97	0.40	54,54,54,54	0
56	MG	2W	201	1/1	0.97	0.09	25,25,25,25	0
56	MG	1A	3011	1/1	0.97	0.14	28,28,28,28	0
56	MG	1A	3891	1/1	0.97	0.28	18,18,18,18	0
56	MG	1A	4102	1/1	0.97	0.41	26,26,26,26	0
56	MG	1a	1833	1/1	0.97	0.16	39,39,39,39	0
56	MG	1A	3794	1/1	0.97	0.08	18,18,18,18	0
56	MG	2A	3289	1/1	0.97	0.10	57,57,57,57	0
56	MG	1A	3491	1/1	0.97	0.37	17,17,17,17	0
56	MG	1A	3139	1/1	0.97	0.16	30,30,30,30	0
56	MG	1A	4106	1/1	0.97	0.29	28,28,28,28	0
56	MG	1A	3002	1/1	0.97	0.28	33,33,33,33	0
56	MG	2A	3127	1/1	0.97	0.33	40,40,40,40	0
56	MG	2A	3128	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	4108	1/1	0.97	0.21	16,16,16,16	0
56	MG	2A	3130	1/1	0.97	0.14	40,40,40,40	0
56	MG	2A	3131	1/1	0.97	0.13	39,39,39,39	0
56	MG	2A	3494	1/1	0.97	0.21	31,31,31,31	0
56	MG	1A	3707	1/1	0.97	0.20	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	3300	1/1	0.97	0.18	32,32,32,32	0
56	MG	2A	3711	1/1	0.97	0.07	40,40,40,40	0
56	MG	1l	201	1/1	0.97	0.13	30,30,30,30	0
56	MG	2A	3498	1/1	0.97	0.13	44,44,44,44	0
56	MG	2A	3134	1/1	0.97	0.13	38,38,38,38	0
56	MG	1A	3898	1/1	0.97	0.11	28,28,28,28	0
56	MG	1A	3899	1/1	0.97	0.08	45,45,45,45	0
56	MG	1W	205	1/1	0.97	0.28	21,21,21,21	0
56	MG	1A	3799	1/1	0.97	0.12	27,27,27,27	0
56	MG	1A	4114	1/1	0.97	0.37	20,20,20,20	0
56	MG	1a	1700	1/1	0.97	0.16	34,34,34,34	0
56	MG	1A	3709	1/1	0.97	0.17	27,27,27,27	0
56	MG	1A	4002	1/1	0.97	0.15	11,11,11,11	0
56	MG	1A	3710	1/1	0.97	0.14	13,13,13,13	0
56	MG	1A	3802	1/1	0.97	0.18	52,52,52,52	0
56	MG	1Y	201	1/1	0.97	0.40	47,47,47,47	0
56	MG	1A	3381	1/1	0.97	0.12	29,29,29,29	0
56	MG	1A	3326	1/1	0.97	0.10	18,18,18,18	0
56	MG	1A	3908	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	4122	1/1	0.97	0.24	21,21,21,21	0
56	MG	1A	3558	1/1	0.97	0.23	22,22,22,22	0
56	MG	1A	3384	1/1	0.97	0.45	22,22,22,22	0
56	MG	2A	3732	1/1	0.97	0.11	35,35,35,35	0
56	MG	2A	3517	1/1	0.97	0.20	45,45,45,45	0
56	MG	1A	3715	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3498	1/1	0.97	0.26	34,34,34,34	0
56	MG	1A	3630	1/1	0.97	0.09	60,60,60,60	0
56	MG	1x	111	1/1	0.97	0.10	43,43,43,43	0
59	ZN	1Y	206	1/1	0.97	0.18	61,61,61,61	0
56	MG	1A	4013	1/1	0.97	0.07	26,26,26,26	0
56	MG	1A	4133	1/1	0.97	0.75	24,24,24,24	0
56	MG	1A	3441	1/1	0.97	0.20	23,23,23,23	0
59	ZN	26	501	1/1	0.97	0.16	53,53,53,53	0
56	MG	1A	3141	1/1	0.97	0.45	25,25,25,25	0
56	MG	1A	3564	1/1	0.97	0.35	21,21,21,21	0
56	MG	1A	3902	1/1	0.98	0.13	18,18,18,18	0
56	MG	1A	3903	1/1	0.98	0.11	16,16,16,16	0
56	MG	1A	3296	1/1	0.98	0.33	15,15,15,15	0
56	MG	1A	3642	1/1	0.98	0.15	29,29,29,29	0
56	MG	1a	1642	1/1	0.98	0.08	49,49,49,49	0
56	MG	1A	3643	1/1	0.98	0.08	26,26,26,26	0
56	MG	2A	3383	1/1	0.98	0.17	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	3297	1/1	0.98	0.26	27,27,27,27	0
56	MG	2A	3386	1/1	0.98	0.16	40,40,40,40	0
56	MG	2A	3822	1/1	0.98	0.13	37,37,37,37	0
56	MG	1A	3740	1/1	0.98	0.11	30,30,30,30	0
56	MG	2A	3027	1/1	0.98	0.10	38,38,38,38	0
56	MG	2A	3491	1/1	0.98	0.21	48,48,48,48	0
56	MG	2A	3709	1/1	0.98	0.08	42,42,42,42	0
56	MG	2A	3389	1/1	0.98	0.25	30,30,30,30	0
56	MG	1A	3131	1/1	0.98	0.14	11,11,11,11	0
56	MG	1a	1647	1/1	0.98	0.17	28,28,28,28	0
56	MG	1A	3691	1/1	0.98	0.09	9,9,9,9	0
56	MG	1A	3204	1/1	0.98	0.16	24,24,24,24	0
56	MG	1A	3387	1/1	0.98	0.24	22,22,22,22	0
56	MG	2A	3833	1/1	0.98	0.13	40,40,40,40	0
56	MG	2A	3834	1/1	0.98	0.09	53,53,53,53	0
56	MG	1A	3388	1/1	0.98	0.19	18,18,18,18	0
56	MG	1A	3142	1/1	0.98	0.20	17,17,17,17	0
56	MG	1A	3124	1/1	0.98	0.36	28,28,28,28	0
56	MG	2A	3838	1/1	0.98	0.06	51,51,51,51	0
56	MG	2A	3301	1/1	0.98	0.07	49,49,49,49	0
56	MG	1A	3084	1/1	0.98	0.19	26,26,26,26	0
56	MG	2a	3038	1/1	0.98	0.18	57,57,57,57	0
56	MG	1Z	305	1/1	0.98	0.11	32,32,32,32	0
56	MG	1A	4109	1/1	0.98	0.43	31,31,31,31	0
56	MG	1A	3208	1/1	0.98	0.14	39,39,39,39	0
56	MG	2a	3042	1/1	0.98	0.29	63,63,63,63	0
56	MG	1A	3858	1/1	0.98	0.09	30,30,30,30	0
56	MG	1A	3393	1/1	0.98	0.47	29,29,29,29	0
56	MG	1A	3330	1/1	0.98	0.09	42,42,42,42	0
56	MG	1A	3191	1/1	0.98	0.12	29,29,29,29	0
56	MG	1A	3046	1/1	0.98	0.16	16,16,16,16	0
56	MG	1A	3703	1/1	0.98	0.12	10,10,10,10	0
56	MG	1a	1829	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3333	1/1	0.98	0.10	28,28,28,28	0
56	MG	1A	3193	1/1	0.98	0.19	23,23,23,23	0
56	MG	1A	3866	1/1	0.98	0.31	25,25,25,25	0
56	MG	1A	4051	1/1	0.98	0.23	13,13,13,13	0
56	MG	1A	3576	1/1	0.98	0.05	31,31,31,31	0
56	MG	2A	3415	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	3502	1/1	0.98	0.12	33,33,33,33	0
56	MG	1A	4123	1/1	0.98	0.26	32,32,32,32	0
56	MG	2A	3418	1/1	0.98	0.17	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4124	1/1	0.98	0.13	27,27,27,27	0
56	MG	1A	3760	1/1	0.98	0.11	29,29,29,29	0
56	MG	1A	3708	1/1	0.98	0.15	33,33,33,33	0
56	MG	1A	3194	1/1	0.98	0.15	11,11,11,11	0
56	MG	2A	3526	1/1	0.98	0.13	30,30,30,30	0
56	MG	1A	3815	1/1	0.98	0.10	48,48,48,48	0
56	MG	1A	3763	1/1	0.98	0.09	21,21,21,21	0
56	MG	1A	4131	1/1	0.98	0.27	20,20,20,20	0
56	MG	2a	3198	1/1	0.98	0.10	52,52,52,52	0
56	MG	1A	3286	1/1	0.98	0.13	33,33,33,33	0
56	MG	1A	3047	1/1	0.98	0.09	30,30,30,30	0
56	MG	1A	3102	1/1	0.98	0.32	23,23,23,23	0
56	MG	2A	3639	1/1	0.98	0.16	44,44,44,44	0
56	MG	2B	211	1/1	0.98	0.21	45,45,45,45	0
56	MG	1A	4135	1/1	0.98	0.14	15,15,15,15	0
56	MG	1A	4136	1/1	0.98	0.24	29,29,29,29	0
56	MG	2a	3074	1/1	0.98	0.11	58,58,58,58	0
56	MG	1a	1765	1/1	0.98	0.18	52,52,52,52	0
56	MG	2B	215	1/1	0.98	0.17	48,48,48,48	0
56	MG	1A	3158	1/1	0.98	0.96	24,24,24,24	0
56	MG	1A	3137	1/1	0.98	0.19	16,16,16,16	0
56	MG	2A	3757	1/1	0.98	0.09	32,32,32,32	0
56	MG	1A	3546	1/1	0.98	0.46	27,27,27,27	0
56	MG	2D	302	1/1	0.98	0.59	39,39,39,39	0
56	MG	1A	3823	1/1	0.98	0.17	18,18,18,18	0
56	MG	1A	3341	1/1	0.98	0.30	38,38,38,38	0
56	MG	2E	302	1/1	0.98	0.18	30,30,30,30	0
56	MG	2a	3217	1/1	0.98	0.10	57,57,57,57	0
56	MG	1A	3314	1/1	0.98	0.29	20,20,20,20	0
56	MG	1B	207	1/1	0.98	0.13	35,35,35,35	0
56	MG	1A	3315	1/1	0.98	0.30	14,14,14,14	0
56	MG	2A	3544	1/1	0.98	0.08	50,50,50,50	0
56	MG	2a	3089	1/1	0.98	0.10	46,46,46,46	0
56	MG	1Q	201	1/1	0.98	0.14	22,22,22,22	0
56	MG	2A	3342	1/1	0.98	0.13	42,42,42,42	0
56	MG	2A	3547	1/1	0.98	0.17	31,31,31,31	0
56	MG	1a	1775	1/1	0.98	0.12	26,26,26,26	0
56	MG	1A	3719	1/1	0.98	0.14	13,13,13,13	0
56	MG	1A	3199	1/1	0.98	0.10	12,12,12,12	0
56	MG	1A	3628	1/1	0.98	0.08	8,8,8,8	0
56	MG	1a	1696	1/1	0.98	0.24	37,37,37,37	0
56	MG	1A	3830	1/1	0.98	0.13	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	1A	3345	1/1	0.98	0.59	20,20,20,20	0
56	MG	1A	3272	1/1	0.98	0.17	13,13,13,13	0
56	MG	2A	3663	1/1	0.98	0.06	39,39,39,39	0
56	MG	2A	3084	1/1	0.98	0.07	46,46,46,46	0
56	MG	2A	3452	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3631	1/1	0.98	0.20	29,29,29,29	0
56	MG	2A	3353	1/1	0.98	0.17	35,35,35,35	0
56	MG	1A	3676	1/1	0.98	0.15	14,14,14,14	0
56	MG	1A	3677	1/1	0.98	0.13	20,20,20,20	0
56	MG	2l	203	1/1	0.98	0.25	50,50,50,50	0
56	MG	2l	204	1/1	0.98	0.12	36,36,36,36	0
56	MG	2R	3001	1/1	0.98	0.26	46,46,46,46	0
56	MG	2A	3356	1/1	0.98	0.20	39,39,39,39	0
56	MG	1A	3893	1/1	0.98	0.32	18,18,18,18	0
56	MG	1A	4015	1/1	0.98	0.08	23,23,23,23	0
56	MG	1A	4016	1/1	0.98	0.18	22,22,22,22	0
56	MG	2A	3462	1/1	0.98	0.10	26,26,26,26	0
56	MG	1A	4081	1/1	0.98	0.16	31,31,31,31	0
56	MG	1A	3023	1/1	0.98	0.24	21,21,21,21	0
56	MG	1U	203	1/1	0.98	0.40	22,22,22,22	0
56	MG	1A	3479	1/1	0.98	0.13	26,26,26,26	0
56	MG	2U	204	1/1	0.98	0.06	37,37,37,37	0
56	MG	2V	201	1/1	0.98	0.70	56,56,56,56	0
56	MG	2x	105	1/1	0.98	0.09	43,43,43,43	0
56	MG	1U	205	1/1	0.98	0.20	13,13,13,13	0
56	MG	1A	4084	1/1	0.98	0.20	32,32,32,32	0
56	MG	2A	3681	1/1	0.98	0.07	44,44,44,44	0
56	MG	2Y	201	1/1	0.98	0.16	25,25,25,25	0
56	MG	2A	3008	1/1	0.98	0.11	30,30,30,30	0
56	MG	1A	3348	1/1	0.98	0.17	30,30,30,30	0
56	MG	1A	3038	1/1	0.98	0.07	47,47,47,47	0
56	MG	2A	3685	1/1	0.98	0.13	28,28,28,28	0
56	MG	1B	229	1/1	0.98	0.17	42,42,42,42	0
56	MG	2A	3687	1/1	0.98	0.10	46,46,46,46	0
56	MG	2A	3688	1/1	0.98	0.39	45,45,45,45	0
56	MG	2A	3577	1/1	0.98	0.13	43,43,43,43	0
56	MG	2A	3803	1/1	0.98	0.10	65,65,65,65	0
56	MG	2A	3012	1/1	0.98	0.26	38,38,38,38	0
56	MG	1A	3174	1/1	0.98	0.09	13,13,13,13	0
56	MG	2A	3806	1/1	0.98	0.09	40,40,40,40	0
56	MG	1A	3321	1/1	0.98	0.22	39,39,39,39	0
56	MG	1A	3597	1/1	0.98	0.14	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	1A	3559	1/1	0.98	0.47	22,22,22,22	0
56	MG	1A	4025	1/1	0.98	0.17	40,40,40,40	0
56	MG	2A	3584	1/1	0.98	0.16	31,31,31,31	0
60	SF4	1d	501	8/8	0.98	0.17	38,50,55,61	0
60	SF4	2d	303	8/8	0.98	0.17	55,66,68,68	0
56	MG	1a	1650	1/1	0.99	0.09	42,42,42,42	0
56	MG	1A	3637	1/1	0.99	0.15	21,21,21,21	0
56	MG	1A	3533	1/1	0.99	0.19	12,12,12,12	0
56	MG	1A	3499	1/1	0.99	0.16	35,35,35,35	0
56	MG	1A	3012	1/1	0.99	0.08	16,16,16,16	0
56	MG	2A	3471	1/1	0.99	0.12	25,25,25,25	0
56	MG	1A	3167	1/1	0.99	0.25	29,29,29,29	0
56	MG	2A	3819	1/1	0.99	0.10	47,47,47,47	0
56	MG	1A	3918	1/1	0.99	0.12	46,46,46,46	0
56	MG	1A	3524	1/1	0.99	0.22	32,32,32,32	0
56	MG	1x	107	1/1	0.99	0.19	74,74,74,74	0
56	MG	1A	3074	1/1	0.99	0.14	15,15,15,15	0
56	MG	2A	3378	1/1	0.99	0.08	43,43,43,43	0
56	MG	1X	102	1/1	0.99	0.21	17,17,17,17	0
56	MG	2A	3018	1/1	0.99	0.13	53,53,53,53	0
56	MG	2A	3616	1/1	0.99	0.19	50,50,50,50	0
56	MG	1A	3383	1/1	0.99	0.23	20,20,20,20	0
56	MG	1A	4128	1/1	0.99	0.11	18,18,18,18	0
56	MG	1S	202	1/1	0.99	0.14	35,35,35,35	0
56	MG	1A	3138	1/1	0.99	0.18	9,9,9,9	0
56	MG	2a	3226	1/1	0.99	0.12	44,44,44,44	0
56	MG	2A	3385	1/1	0.99	0.15	36,36,36,36	0
56	MG	1A	3746	1/1	0.99	0.14	23,23,23,23	0
56	MG	1A	3123	1/1	0.99	0.16	34,34,34,34	0
56	MG	2A	3453	1/1	0.99	0.28	33,33,33,33	0
56	MG	1A	3071	1/1	0.99	0.16	20,20,20,20	0
56	MG	1l	203	1/1	0.99	0.21	48,48,48,48	0
56	MG	1n	101	1/1	0.99	0.11	26,26,26,26	0
56	MG	1q	201	1/1	0.99	0.06	39,39,39,39	0
56	MG	1B	235	1/1	0.99	0.04	37,37,37,37	0
59	ZN	15	104	1/1	0.99	0.23	38,38,38,38	0
59	ZN	16	103	1/1	0.99	0.22	35,35,35,35	0
59	ZN	19	102	1/1	0.99	0.18	33,33,33,33	0
59	ZN	1n	102	1/1	0.99	0.15	47,47,47,47	0
56	MG	1B	215	1/1	0.99	0.07	37,37,37,37	0
56	MG	1B	216	1/1	0.99	0.20	22,22,22,22	0
59	ZN	25	103	1/1	0.99	0.20	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3041	1/1	0.99	0.20	20,20,20,20	0
56	MG	1D	303	1/1	0.99	0.49	34,34,34,34	0
56	MG	1A	3497	1/1	0.99	0.10	44,44,44,44	0
56	MG	1A	3720	1/1	0.99	0.14	9,9,9,9	0
56	MG	1A	3299	1/1	0.99	0.15	15,15,15,15	0
56	MG	1A	3423	1/1	1.00	0.20	45,45,45,45	0
56	MG	2A	3221	1/1	1.00	0.21	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.