wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2026 – 12:12 PM EDT

PDB ID	:	8UD6 / pdb_00008ud6
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with cresomycin, mRNA, deacylated A-site tRNAphe, aminoacylated P-site fMet-tRNAmet, and deacylated E-site tRNAphe at 2.70A resolution
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Deposited on	:	2023-09-28
Resolution	:	2.70 Å(reported)

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

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

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

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

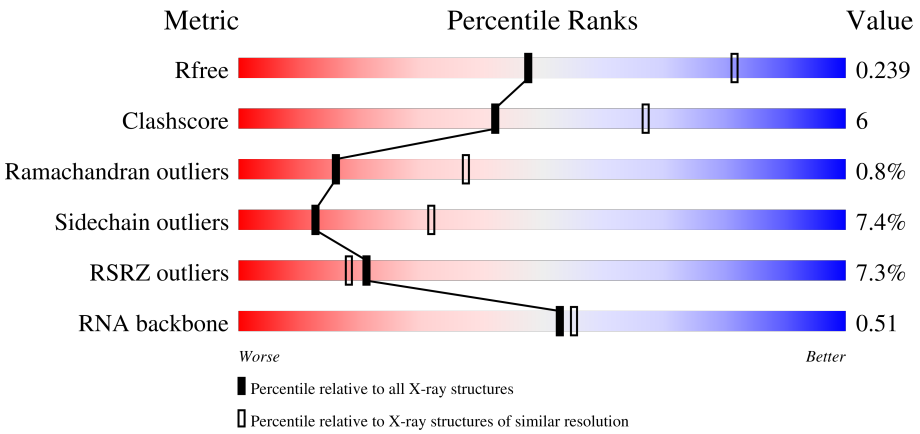
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	4% 70% 23% 5% •
1	2A	2915	4% 64% 27% 5% •

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
2	1B	121	82% 15%
2	2B	121	3% 60% 33% 7%
3	1D	276	% 82% 17%
3	2D	276	% 84% 15%
4	1E	206	84% 13%
4	2E	206	% 78% 18%
5	1F	210	76% 18%
5	2F	210	% 73% 21%
6	1G	182	6% 77% 20%
6	2G	182	22% 61% 30% 8%
7	1H	180	% 72% 23%
7	2H	180	17% 68% 24%
8	1I	148	5% 73% 20% 6%
8	2I	148	5% 78% 20%
9	1N	140	83% 15%
9	2N	140	4% 76% 23%
10	1O	122	93% 7%
10	2O	122	84% 15%
11	1P	150	% 85% 11%
11	2P	150	3% 77% 21%
12	1Q	141	% 81% 18%
12	2Q	141	13% 82% 18%
13	1R	118	86% 13%
13	2R	118	81% 18%
14	1S	112	2% 79% 14%

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Mol	Chain	Length	Quality of chain
14	2S	112	12% 62% 32%
15	1T	146	3% 80% 10% 10%
15	2T	146	3% 75% 14% 10%
16	1U	118	% 76% 21%
16	2U	118	% 81% 17%
17	1V	101	87% 11%
17	2V	101	% 85% 13%
18	1W	113	2% 89% 8%
18	2W	113	2% 81% 15%
19	1X	96	2% 85% 12%
19	2X	96	5% 79% 19%
20	1Y	110	2% 81% 15%
20	2Y	110	15% 79% 14% 5%
21	1Z	206	9% 51% 19% 25%
21	2Z	206	19% 51% 21% 5% 22%
22	10	85	8% 89% 7%
22	20	85	13% 74% 21%
23	11	98	% 93%
23	21	98	% 86% 10%
24	12	72	% 86% 10%
24	22	72	78% 18%
25	13	60	2% 88% 10%
25	23	60	7% 75% 22%
26	14	71	11% 58% 35%
26	24	71	31% 52% 38% 7%

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Mol	Chain	Length	Quality of chain
27	15	60	2% 82% 15%
27	25	60	2% 85% 13%
28	16	54	76% 20%
28	26	54	2% 85% 13%
29	17	49	4% 84% 12%
29	27	49	4% 82% 12%
30	18	65	71% 28%
30	28	65	2% 75% 23%
31	19	37	86% 14%
31	29	37	8% 86% 14%
32	1a	1521	4% 63% 31% 5%
32	2a	1521	11% 57% 35% 7%
33	1b	256	12% 58% 28% 10%
33	2b	256	28% 52% 31% 8% 10%
34	1c	239	5% 69% 16% 14%
34	2c	239	38% 56% 26% 14%
35	1d	209	7% 67% 28%
35	2d	209	5% 71% 24%
36	1e	162	% 68% 20% 9%
36	2e	162	12% 55% 32% 9%
37	1f	101	3% 79% 18%
37	2f	101	3% 77% 19%
38	1g	156	6% 84% 13%
38	2g	156	11% 72% 24%
39	1h	138	% 70% 25%

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Mol	Chain	Length	Quality of chain
39	2h	138	9% 71% 25%
40	1i	128	15% 66% 30%
40	2i	128	34% 60% 38%
41	1j	105	13% 64% 26% 8%
41	2j	105	52% 45% 42% 5% 9%
42	1k	129	3% 71% 16% 12%
42	2k	129	6% 70% 19% 12%
43	1l	132	4% 81% 10% 8%
43	2l	132	9% 69% 20% 8%
44	1m	126	6% 67% 27%
44	2m	126	37% 58% 36%
45	1n	61	5% 70% 26%
45	2n	61	77% 70% 26%
46	1o	89	4% 78% 19%
46	2o	89	3% 80% 17%
47	1p	88	11% 66% 22% 6% 7%
47	2p	88	8% 70% 22% 7%
48	1q	105	% 81% 11% 6%
48	2q	105	6% 77% 16% 6%
49	1r	88	% 60% 15% 23%
49	2r	88	% 55% 18% 5% 23%
50	1s	93	3% 67% 22% 11%
50	2s	93	40% 54% 31% 11%
51	1t	106	5% 61% 26% 9%
51	2t	106	8% 72% 16% 9%

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Mol	Chain	Length	Quality of chain
52	1u	27	11% 56% 26% • 15%
52	2u	27	59% 56% 26% • 15%
53	1v	24	4% 50% • 46%
53	2v	24	21% 38% 17% 46%
54	1w	76	12% 42% 42% 8% • 5%
54	1y	76	14% 39% 30% 26% • •
54	2w	76	16% 51% 33% 8% 8%
54	2y	76	21% 37% 39% 18% • •
55	1x	77	4% 75% 22% ••
55	2x	77	3% 64% 30% 5% •

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	PSU	2y	55	-	-	X	-
56	MG	1a	1716	-	-	-	X
56	MG	2A	3155	-	-	-	X
56	MG	2A	3276	-	-	-	X
56	MG	2A	3340	-	-	-	X
56	MG	2A	3582	-	-	-	X
56	MG	2a	1630	-	-	-	X
56	MG	2a	1709	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 298872 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
			Total	C	N	O	P			
1	1A	2871	61852	27531	11572	19878	2871	0	0	0
1	2A	2800	60322	26848	11284	19390	2800	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MF-mRNA.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
54	1w	72	1550	694	277	505	72	2	0	0	0
54	1y	74	1585	707	285	518	74	1	0	0	0
54	2w	70	1502	671	270	489	70	2	0	0	0
54	2y	73	1565	698	283	510	73	1	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
55	1x	76	1635	731	296	530	76	2	0	0	0
55	2x	76	1635	731	296	530	76	2	0	0	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1A	1059	1059	1059	0	0
56	1B	34	34	34	0	0
56	1D	12	12	12	0	0
56	1E	17	17	17	0	0
56	1F	12	12	12	0	0
56	1G	5	5	5	0	0
56	1I	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1N	5	5	5	0	0
56	1O	6	6	6	0	0
56	1P	6	6	6	0	0
56	1Q	6	6	6	0	0
56	1R	6	6	6	0	0
56	1S	2	2	2	0	0
56	1T	3	3	3	0	0
56	1U	10	10	10	0	0
56	1V	6	6	6	0	0
56	1W	7	7	7	0	0
56	1X	6	6	6	0	0
56	1Y	2	2	2	0	0
56	1Z	2	2	2	0	0
56	10	9	9	9	0	0
56	11	5	5	5	0	0
56	12	2	2	2	0	0
56	13	4	4	4	0	0
56	14	1	1	1	0	0
56	15	7	7	7	0	0
56	16	1	1	1	0	0
56	17	5	5	5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	18	6	6	6	0	0
56	19	1	1	1	0	0
56	1a	208	208	208	0	0
56	1b	1	1	1	0	0
56	1d	1	1	1	0	0
56	1e	2	2	2	0	0
56	1f	1	1	1	0	0
56	1k	1	1	1	0	0
56	1l	2	2	2	0	0
56	1m	2	2	2	0	0
56	1n	1	1	1	0	0
56	1p	1	1	1	0	0
56	1r	1	1	1	0	0
56	1t	1	1	1	0	0
56	1w	3	3	3	0	0
56	1x	14	14	14	0	0
56	2A	771	771	771	0	0
56	2B	20	20	20	0	0
56	2D	8	8	8	0	0
56	2E	10	10	10	0	0
56	2F	5	5	5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	2G	1	1	1	0	0
56	2N	1	1	1	0	0
56	2O	1	1	1	0	0
56	2P	2	2	2	0	0
56	2Q	3	3	3	0	0
56	2R	2	2	2	0	0
56	2T	2	2	2	0	0
56	2U	1	1	1	0	0
56	2V	2	2	2	0	0
56	2W	2	2	2	0	0
56	2X	2	2	2	0	0
56	20	2	2	2	0	0
56	21	3	3	3	0	0
56	23	2	2	2	0	0
56	25	1	1	1	0	0
56	27	1	1	1	0	0
56	28	2	2	2	0	0
56	2a	214	214	214	0	0
56	2d	1	1	1	0	0
56	2e	1	1	1	0	0
56	2f	1	1	1	0	0

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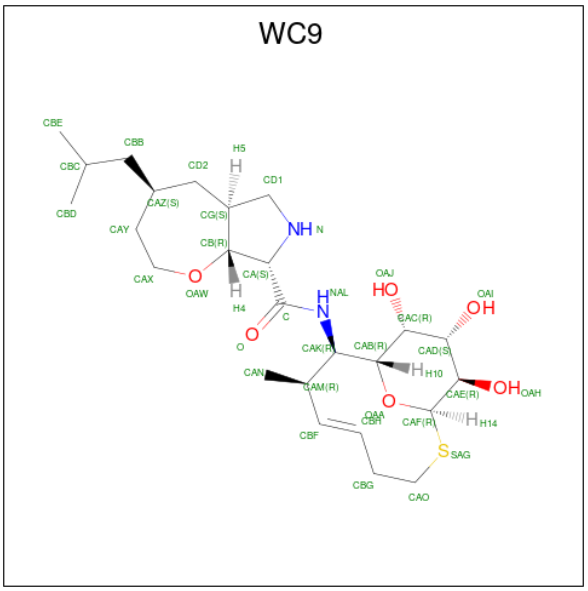
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2g	1	Total Mg 1 1	0	0
56	2i	2	Total Mg 2 2	0	0
56	2j	1	Total Mg 1 1	0	0
56	2k	1	Total Mg 1 1	0	0
56	2l	3	Total Mg 3 3	0	0
56	2q	3	Total Mg 3 3	0	0
56	2r	2	Total Mg 2 2	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	1	Total Mg 1 1	0	0
56	2w	1	Total Mg 1 1	0	0
56	2x	5	Total Mg 5 5	0	0
56	2y	2	Total Mg 2 2	0	0

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total K 1 1	0	0
57	2x	1	Total K 1 1	0	0

- Molecule 58 is (4S,5aS,8S,8aR)-4-(2-methylpropyl)-N-[(1R,5Z,7R,8R,9R,10R,11S,12R)-10,11,12-trihydroxy-7-methyl-13-oxa-2-thiabicyclo[7.3.1]tridec-5-en-8-yl]octahydro-2H-oxepino[2,3-c]pyrrole-8-carboxamide (non-preferred name) (CCD ID: WC9) (formula: $C_{25}H_{42}N_2O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
58	1A	1	34	25	2	6	1	0	0
			Total	C	N	O	S		
58	2A	1	34	25	2	6	1	0	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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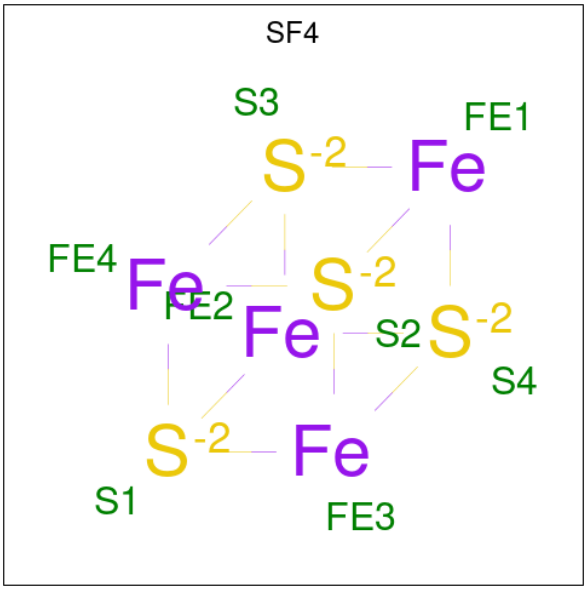
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: 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	1685	Total O 1685 1685	0	0
61	1B	54	Total O 54 54	0	0
61	1D	26	Total O 26 26	0	0
61	1E	25	Total O 25 25	0	0
61	1F	15	Total O 15 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	3	Total O 3 3	0	0
61	1H	1	Total O 1 1	0	0
61	1N	3	Total O 3 3	0	0
61	1O	5	Total O 5 5	0	0
61	1P	17	Total O 17 17	0	0
61	1Q	6	Total O 6 6	0	0
61	1R	9	Total O 9 9	0	0
61	1S	2	Total O 2 2	0	0
61	1T	7	Total O 7 7	0	0
61	1U	11	Total O 11 11	0	0
61	1V	5	Total O 5 5	0	0
61	1W	7	Total O 7 7	0	0
61	1X	3	Total O 3 3	0	0
61	1Y	1	Total O 1 1	0	0
61	10	12	Total O 12 12	0	0
61	11	8	Total O 8 8	0	0
61	12	2	Total O 2 2	0	0
61	13	3	Total O 3 3	0	0
61	14	1	Total O 1 1	0	0
61	15	6	Total O 6 6	0	0
61	16	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	17	8	Total O 8 8	0	0
61	18	11	Total O 11 11	0	0
61	1a	213	Total O 213 213	0	0
61	1b	1	Total O 1 1	0	0
61	1f	2	Total O 2 2	0	0
61	1g	1	Total O 1 1	0	0
61	1i	1	Total O 1 1	0	0
61	1j	1	Total O 1 1	0	0
61	1l	2	Total O 2 2	0	0
61	1q	1	Total O 1 1	0	0
61	1v	2	Total O 2 2	0	0
61	1w	4	Total O 4 4	0	0
61	1x	9	Total O 9 9	0	0
61	2A	848	Total O 848 848	0	0
61	2B	16	Total O 16 16	0	0
61	2D	16	Total O 16 16	0	0
61	2E	10	Total O 10 10	0	0
61	2F	11	Total O 11 11	0	0
61	2I	1	Total O 1 1	0	0
61	2O	3	Total O 3 3	0	0
61	2P	6	Total O 6 6	0	0

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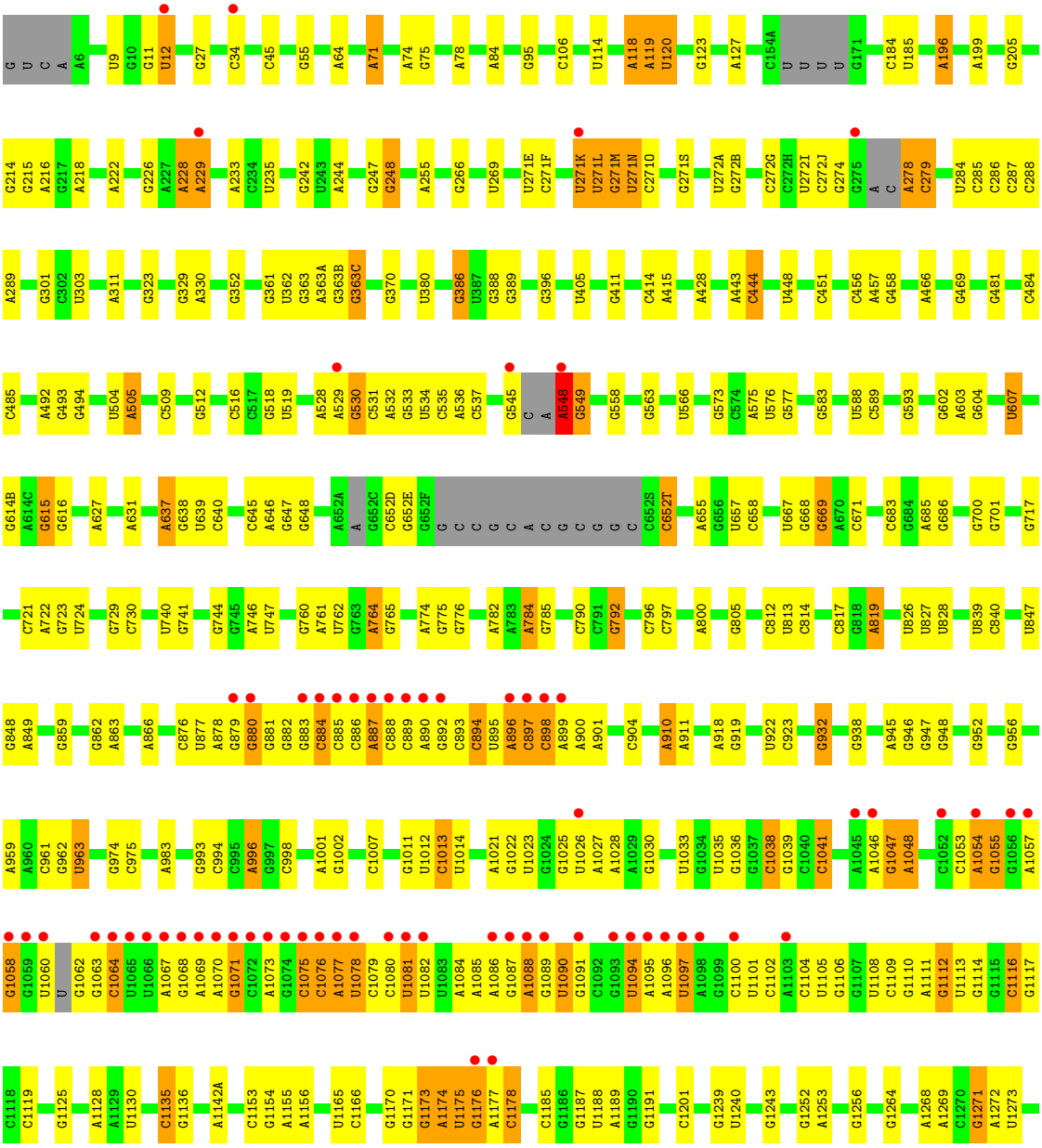
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2Q	1	Total O 1 1	0	0
61	2R	2	Total O 2 2	0	0
61	2T	4	Total O 4 4	0	0
61	2U	3	Total O 3 3	0	0
61	2V	1	Total O 1 1	0	0
61	2W	2	Total O 2 2	0	0
61	2X	1	Total O 1 1	0	0
61	2Y	1	Total O 1 1	0	0
61	20	1	Total O 1 1	0	0
61	21	7	Total O 7 7	0	0
61	27	4	Total O 4 4	0	0
61	28	5	Total O 5 5	0	0
61	29	1	Total O 1 1	0	0
61	2a	145	Total O 145 145	0	0
61	2d	3	Total O 3 3	0	0
61	2j	3	Total O 3 3	0	0
61	2l	3	Total O 3 3	0	0
61	2r	1	Total O 1 1	0	0
61	2t	1	Total O 1 1	0	0
61	2x	4	Total O 4 4	0	0
61	2y	4	Total O 4 4	0	0

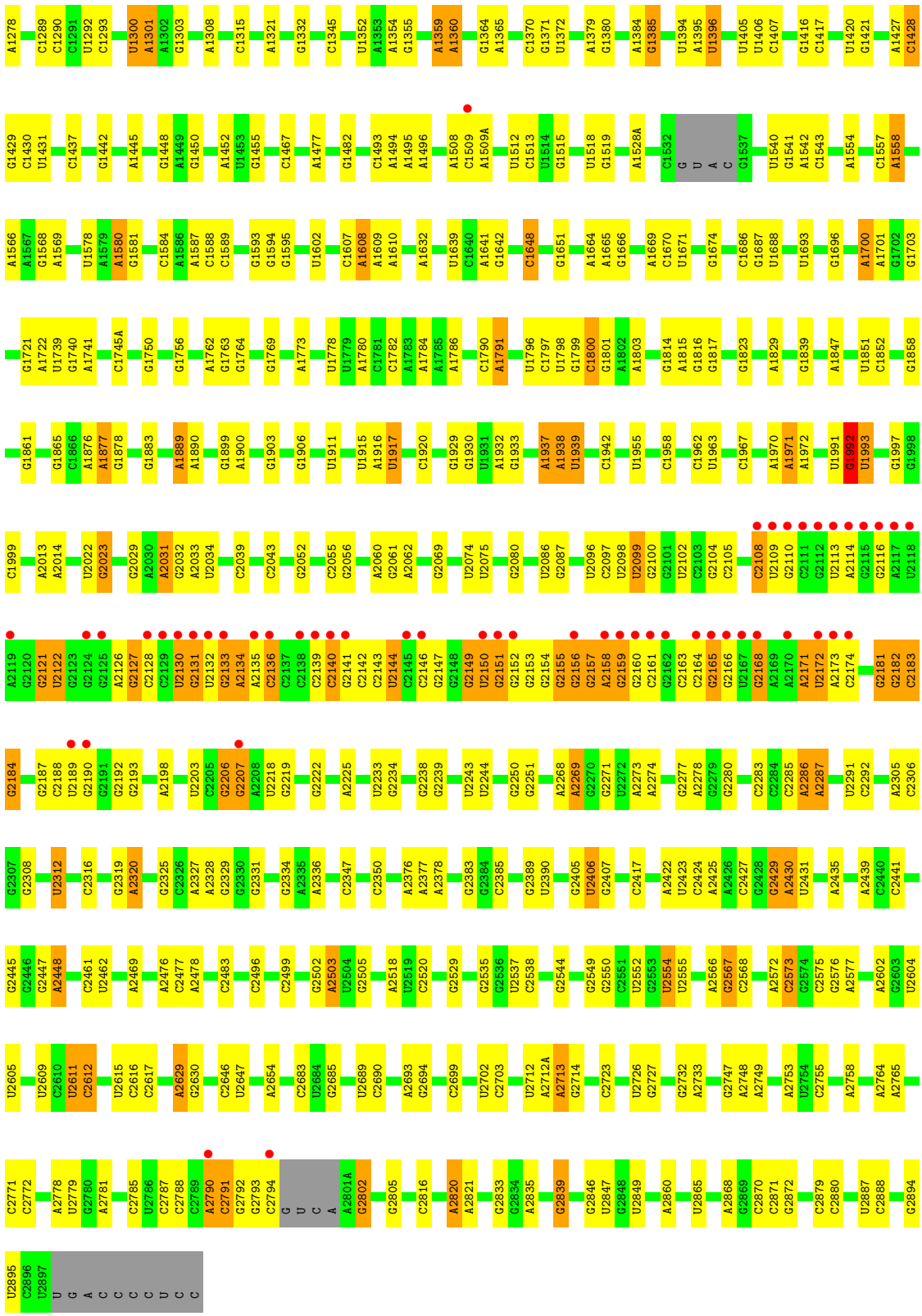
3 Residue-property plots (i)

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

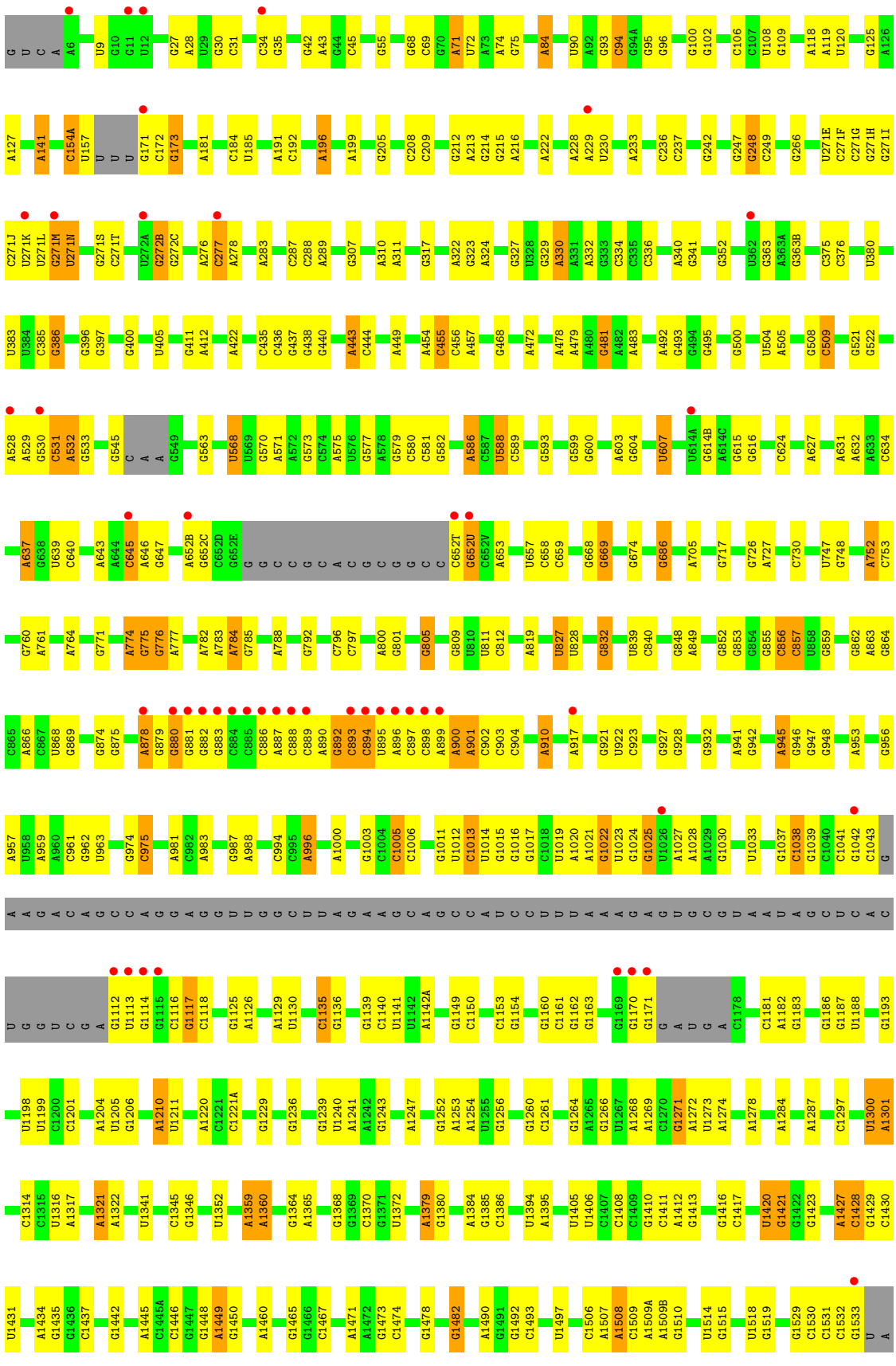
Chain 1A:

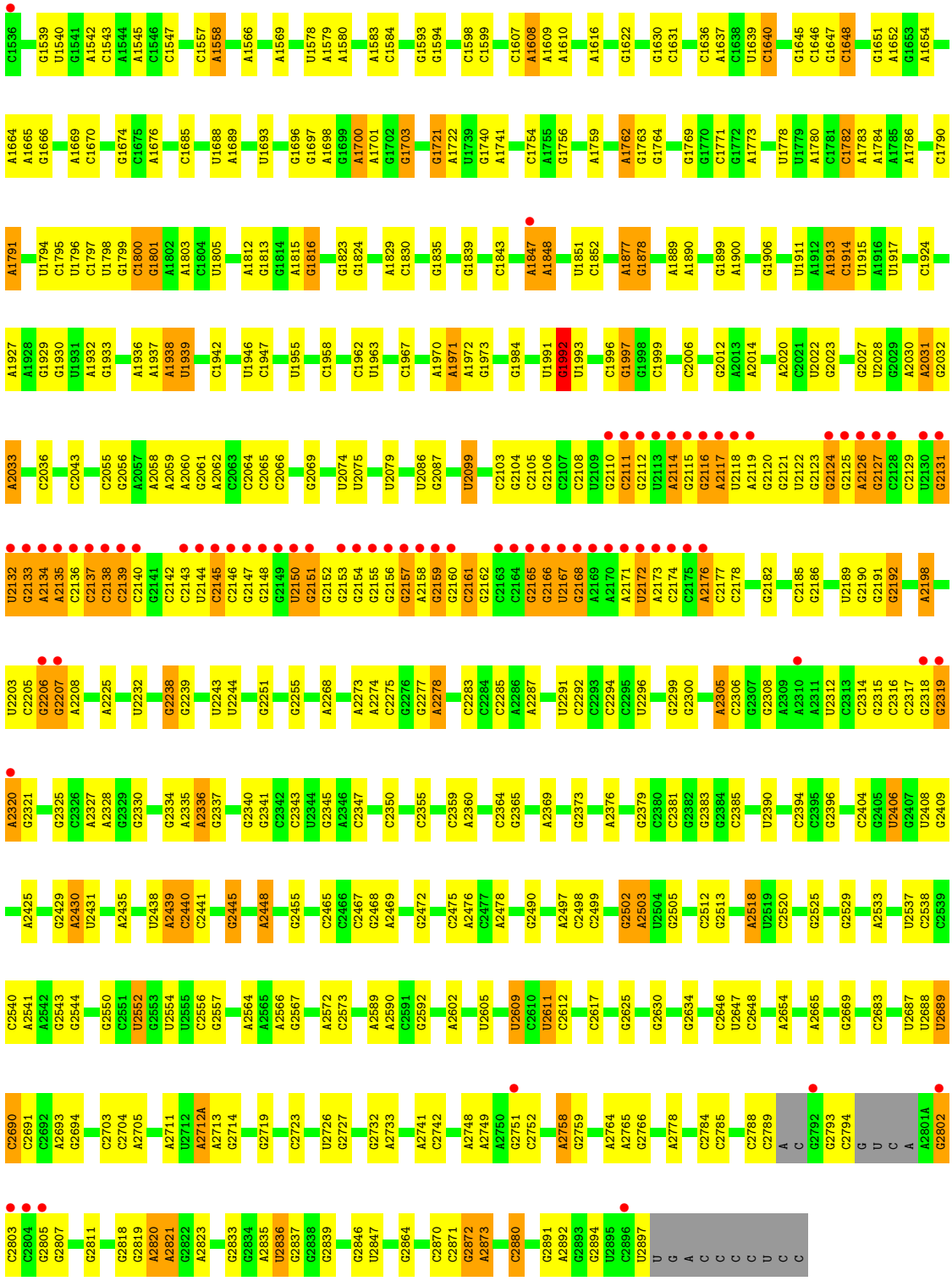




- Molecule 1: 23S Ribosomal RNA

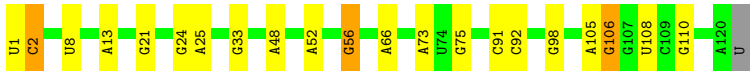
Chain 2A:


G U C A A6 U9 G10 G11 U12 G27 A28 U29 G30 C31 C34 G35 G42 A43 G44 C45 G55 G68 C69 G70 A71 U72 A73 A74 G75 A84 U90 A92 G93 C94 G94A G95 G96 G100 G102 C106 C107 U108 G109 A118 A119 U120 G125 A126
A127 A141 C154A U157 U U U G171 C172 G173 A181 C184 U185 A191 C192 A196 A199 G205 C208 C209 G212 A213 G214 G215 A216 A222 A228 A229 U230 A233 C236 C237 G242 G247 G248 C249 G266 U271E C271F C271G G271H G271I
C271J U271K U271L G271M U271N G271S C271T U272A G272B G272C A276 C277 A278 A283 C287 C288 A289 G307 A310 A311 G317 A322 G323 A324 G327 U328 G329 A330 A331 A332 G333 C334 C335 C336 A340 G341 G352 U362 G363 A363A G363B C375 C376 U380
U383 U384 C385 G386 G396 G397 G400 U405 G411 A412 A422 C435 C436 G437 G438 G440 A443 C444 A449 A454 C455 C456 A457 G468 A472 A478 A479 A480 G481 A482 A483 A492 G493 G494 G495 G500 U504 A505 G508 C509 G521 G522
A528 A529 G530 C531 A532 G533 G545 C A A G549 G563 U568 U569 G570 A571 A572 G573 C574 A575 U576 G577 A578 G579 C580 C581 G582 A586 C587 U588 C589 G593 G599 G600 A603 G604 U607 U614A G614B A614C G615 G616 C624 A627 A631 A632 A633 C634
A637 G638 U639 C640 A643 A644 C645 A646 G647 A652B G652C G652D G652E G G G C C G C A C G G C G C C C652T G652U G652V A653 U657 C658 C659 G668 G669 G674 G686 A705 G717 G726 A727 C730 U747 G748 A752 C753
G760 A761 A764 G771 A774 G775 G776 A777 A782 A783 A784 G785 A788 G792 C796 C797 A800 G801 G805 G809 U810 U811 C812 A819 U827 U828 G832 U839 C840 G848 A849 G852 G853 G854 G855 C856 C857 U858 G859 G862 A863 G864
C865 A866 C867 U868 G869 G874 G875 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 G893 C894 U895 A896 C897 C898 A899 A900 A901 C902 C903 C904 A910 A917 G921 U922 C923 G927 G928 G932 A941 G942 A945 G946 G947 G948 A953 G956
A957 U958 A959 A960 C961 G962 U963 G974 C975 A981 C982 A983 G987 A988 C994 C995 A996 A1000 G1003 C1004 C1005 C1006 G1011 U1012 C1013 U1014 G1015 G1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 U1033 G1037 C1038 G1039 C1040 C1041 G1042 C1043 G
A A G A C A G C C A G G A G G U U G G C U U A G A A G C C A U C C U U U A A A G A G A G C U C A C
U G G U C G A G1112 U1113 G1114 G1115 G1116 G1117 C1118 G1125 A1126 A1129 U1130 C1135 G1136 G1139 C1140 U1141 U1142 A1142A G1149 C1150 C1153 G1154 G1160 C1161 G1162 G1163 G1169 G1170 G1171 G A U G A C1178 C1181 A1182 G1183 G1186 G1187 U1188 G1193
U1198 U1199 C1200 C1201 A1204 U1205 G1206 A1210 U1211 A1220 C1221 C1221A G1229 G1236 G1239 U1240 A1241 A1242 G1243 A1247 G1252 A1253 A1254 U1255 G1256 G1260 C1261 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1278 A1284 A1287 C1297 U1300 A1301
C1314 C1315 U1316 A1317 A1321 A1322 U1341 C1345 G1346 U1352 A1359 A1360 G1364 A1365 G1368 G1369 C1370 G1371 U1372 A1379 G1380 A1384 G1385 C1386 U1394 A1395 U1405 U1406 C1407 C1408 C1409 G1410 C1411 A1412 G1413 G1416 C1417 U1420 G1421 G1422 G1423 A1427 C1428 G1429 C1430
U1431 A1434 G1435 G1436 C1437 G1442 A1445 C1445A C1446 G1447 G1448 A1449 G1450 A1460 G1465 G1466 C1467 A1471 A1472 G1473 C1474 G1478 G1482 A1490 G1491 G1492 C1493 U1497 C1506 A1507 A1508 C1509 A1509A A1509B G1510 U1514 G1515 U1518 G1519 G1529 C1530 C1531 C1532 G1533 U A



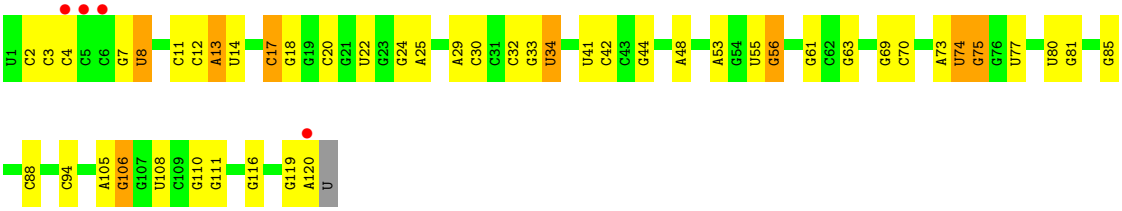
- Molecule 2: 5S Ribosomal RNA

Chain 1B:



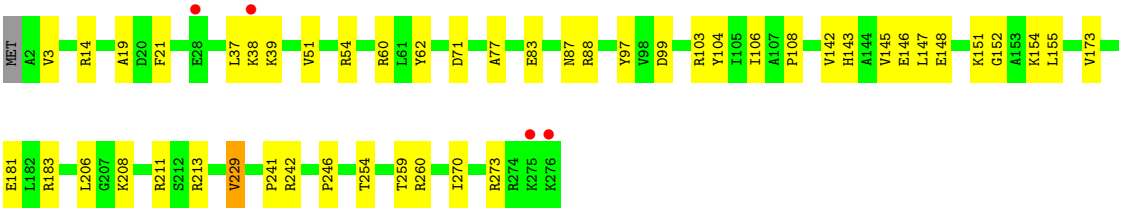
- Molecule 2: 5S Ribosomal RNA

Chain 2B:



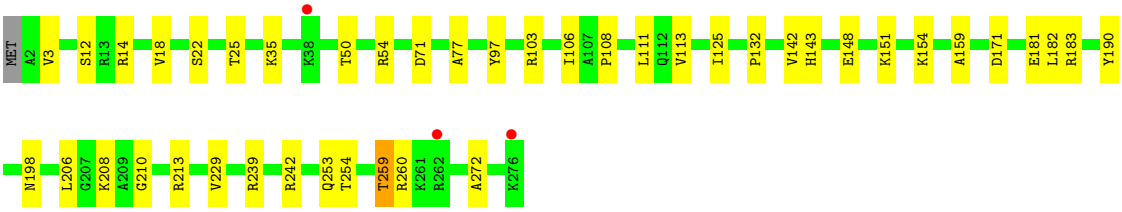
- Molecule 3: 50S ribosomal protein L2

Chain 1D:



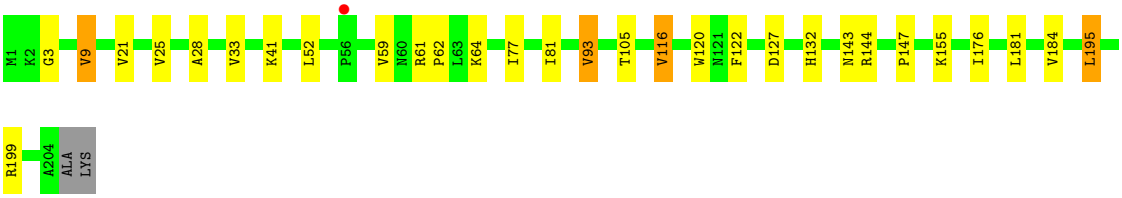
- Molecule 3: 50S ribosomal protein L2

Chain 2D:



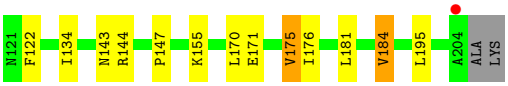
- Molecule 4: 50S ribosomal protein L3

Chain 1E:



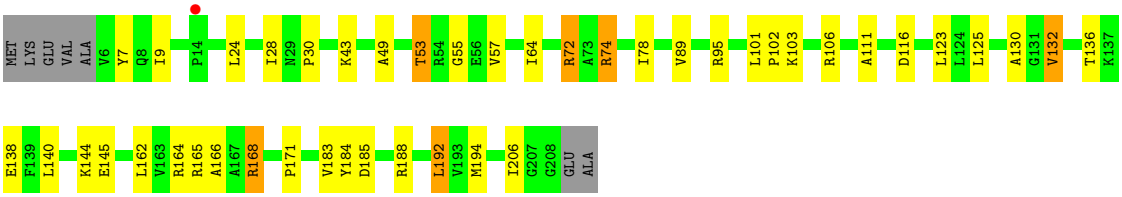
- Molecule 4: 50S ribosomal protein L3

Chain 2E:



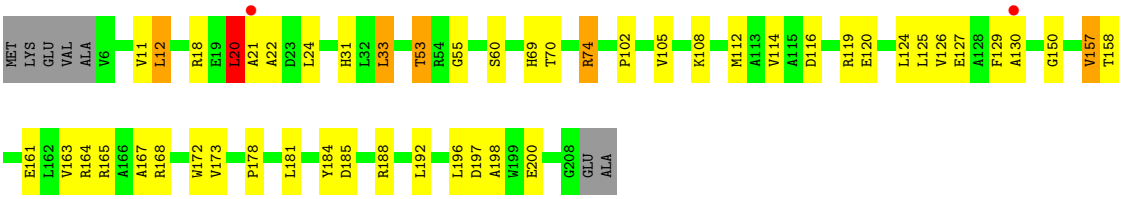
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



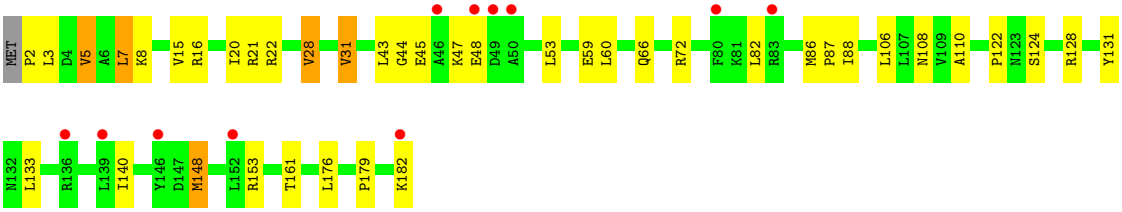
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



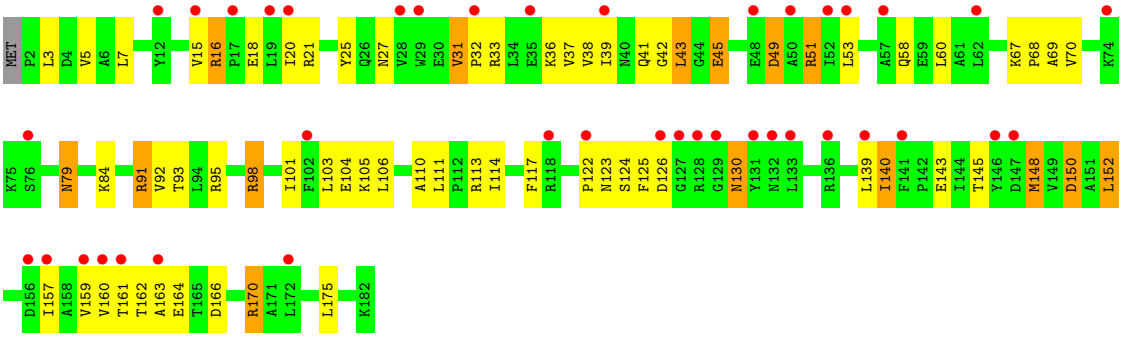
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



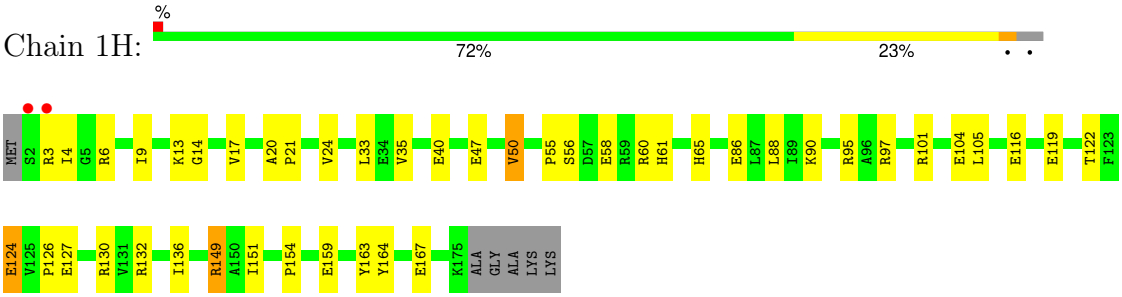
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



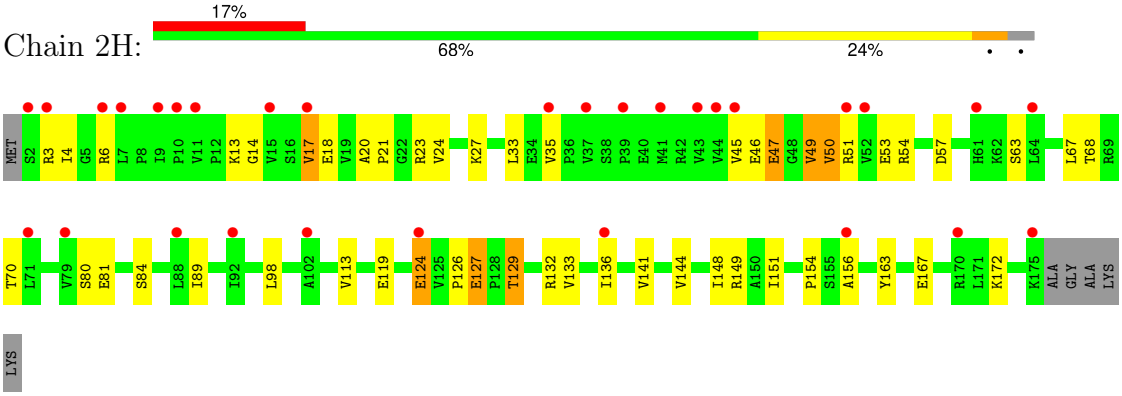
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



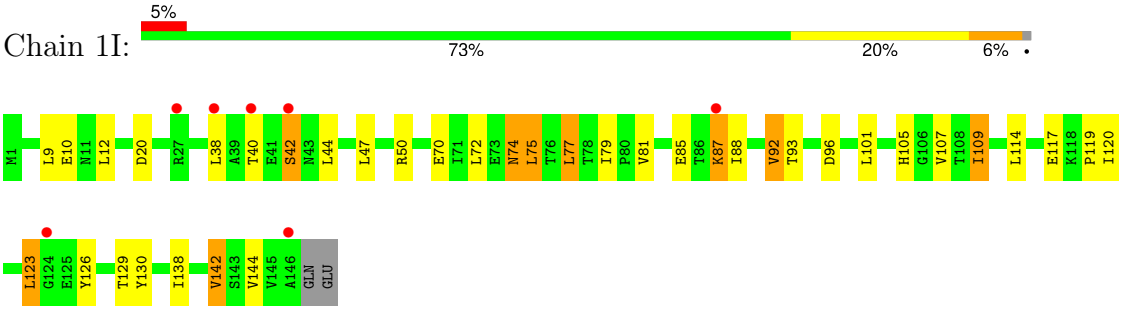
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



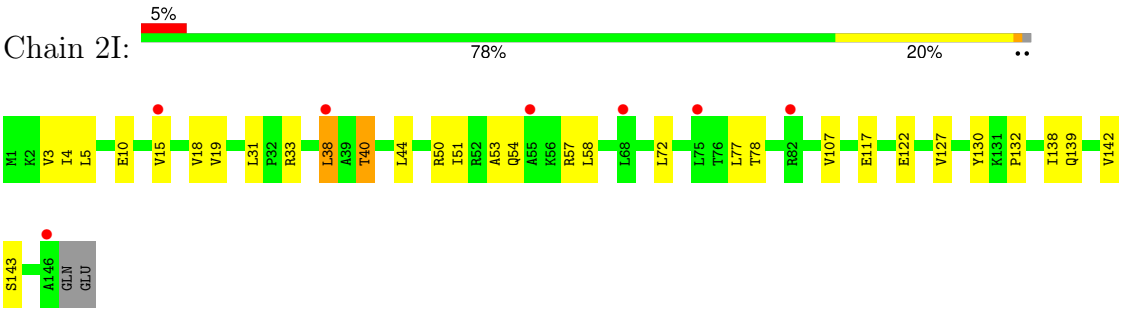
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



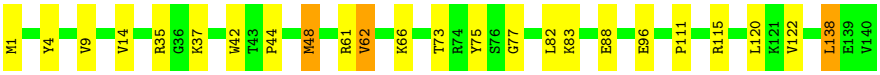
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



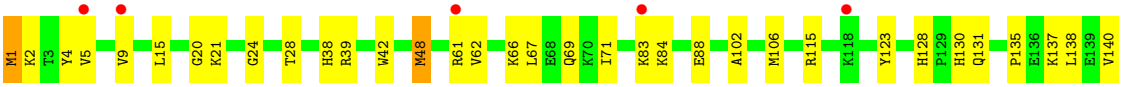
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



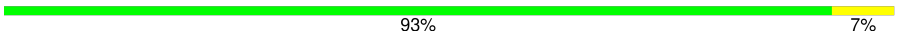
• Molecule 9: 50S ribosomal protein L13

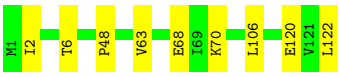
Chain 2N:



• Molecule 10: 50S ribosomal protein L14

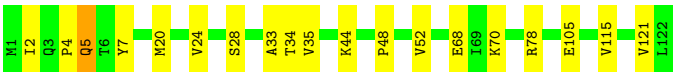
Chain 1O:





• Molecule 10: 50S ribosomal protein L14

Chain 2O:

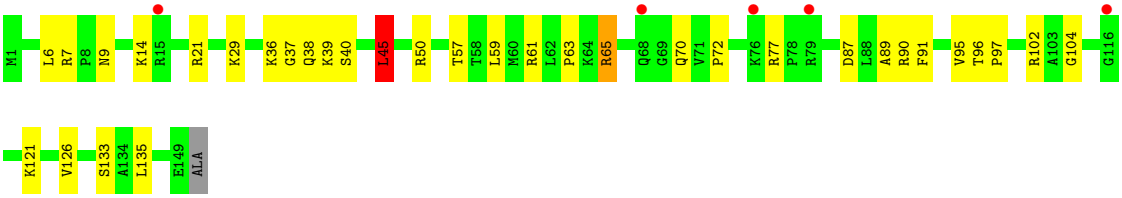


• Molecule 11: 50S ribosomal protein L15

Chain 1P:

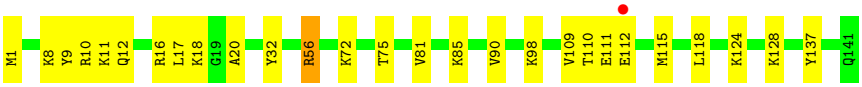
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



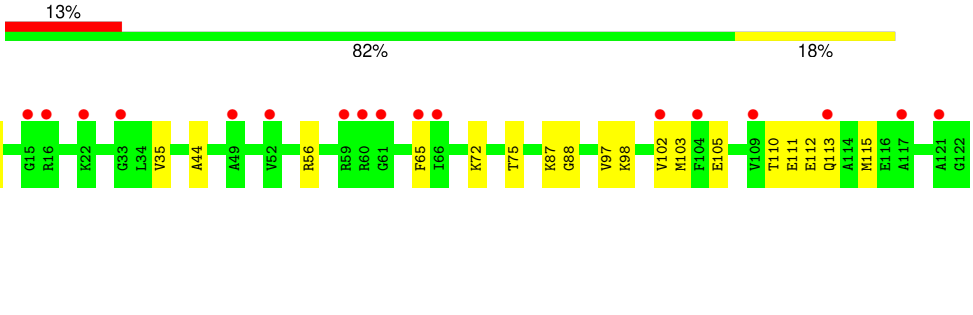
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



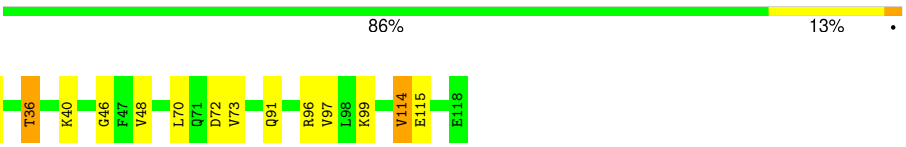
- Molecule 12: 50S ribosomal protein L16

Chain 2Q:



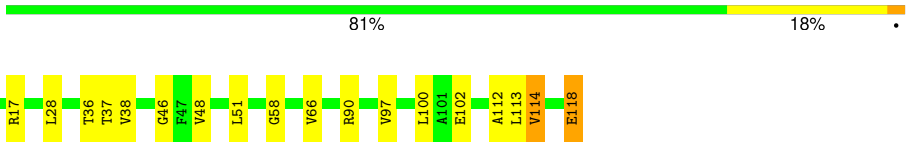
- Molecule 13: 50S ribosomal protein L17

Chain 1R:



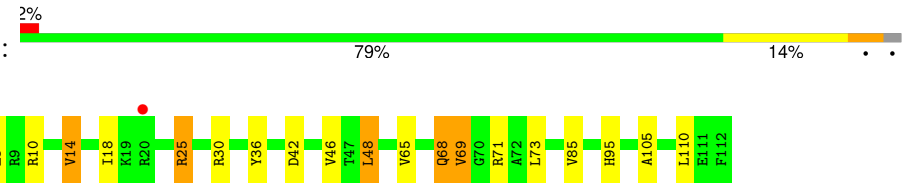
- Molecule 13: 50S ribosomal protein L17

Chain 2R:



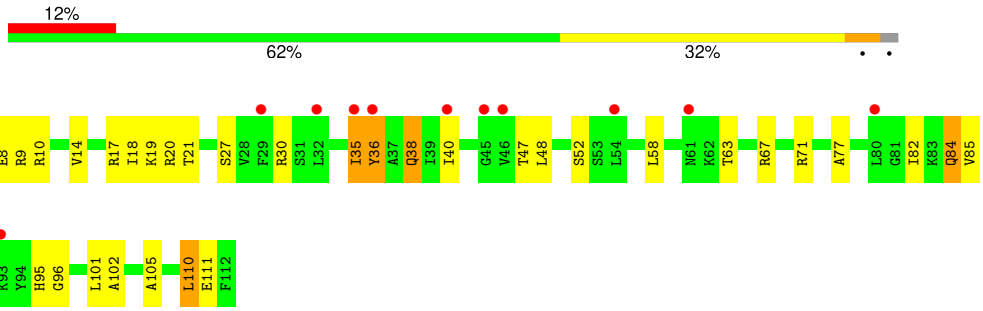
- Molecule 14: 50S ribosomal protein L18

Chain 1S:



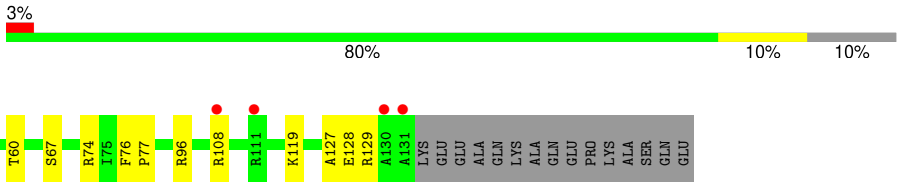
- Molecule 14: 50S ribosomal protein L18

Chain 2S:



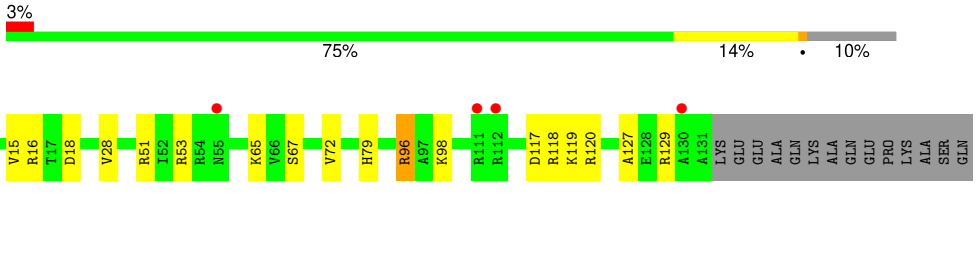
- Molecule 15: 50S ribosomal protein L19

Chain 1T:



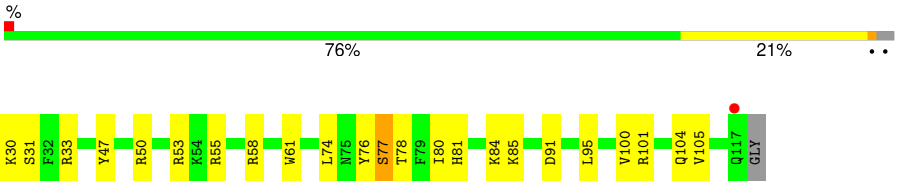
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



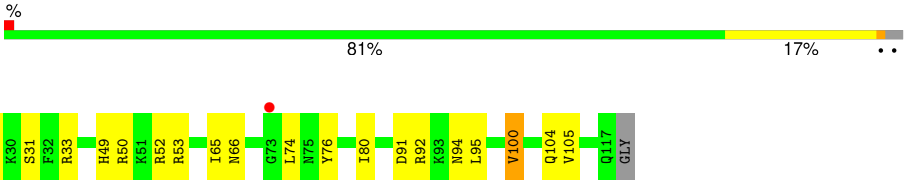
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



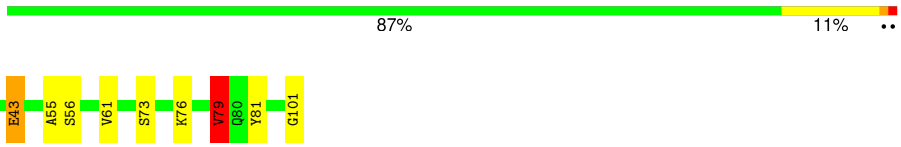
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



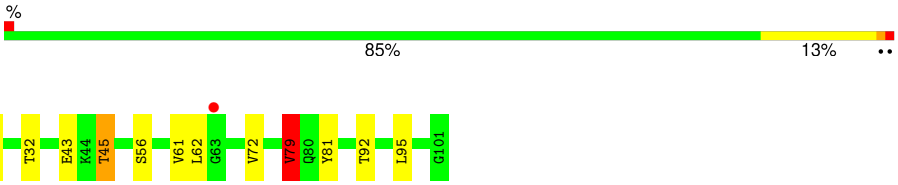
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



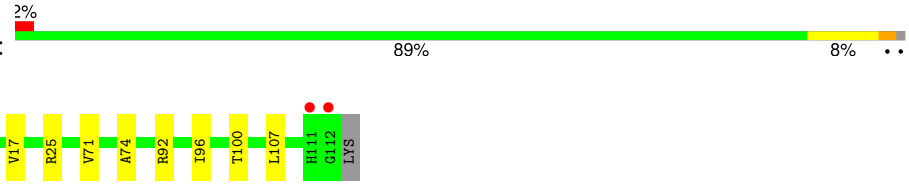
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



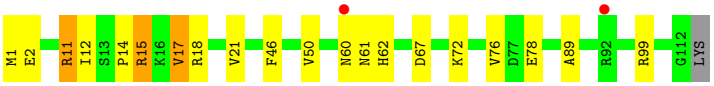
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



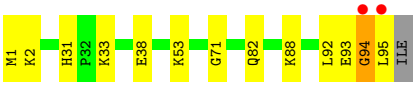
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



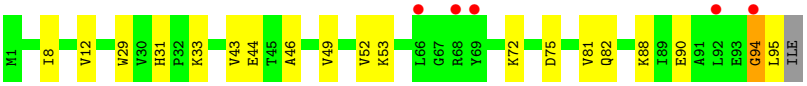
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



• Molecule 19: 50S ribosomal protein L23

Chain 2X:

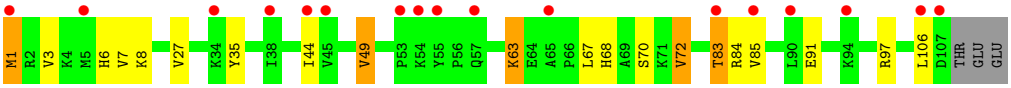


• Molecule 20: 50S ribosomal protein L24

Chain 1Y:

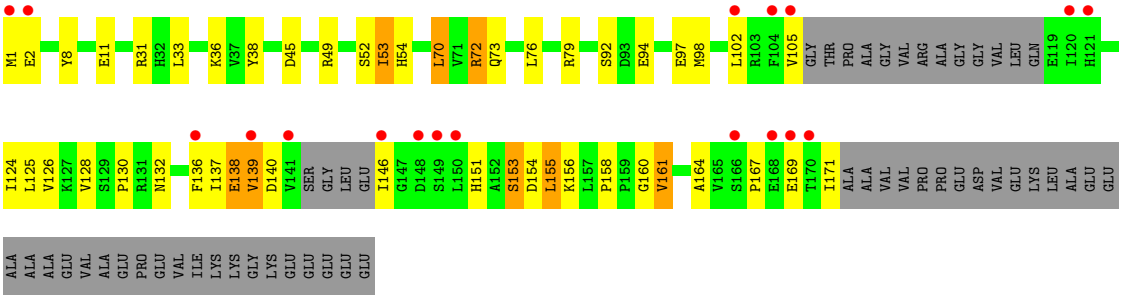
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



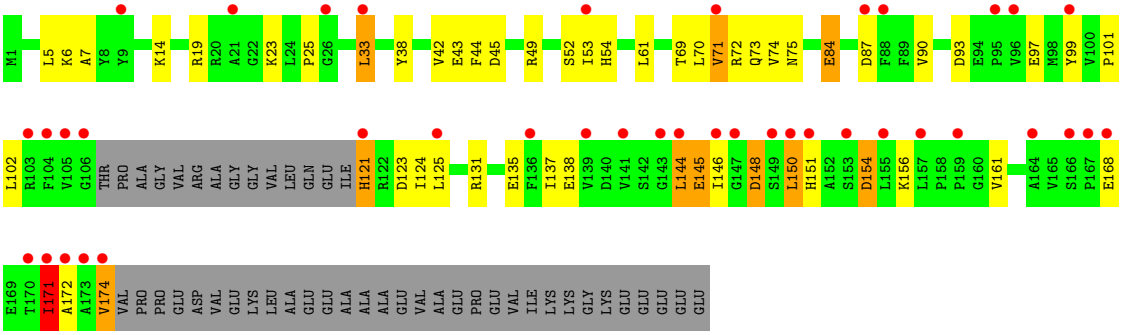
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



• Molecule 21: 50S ribosomal protein L25

Chain 2Z:

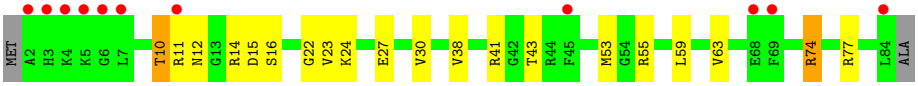


- Molecule 22: 50S ribosomal protein L27

Chain 10:

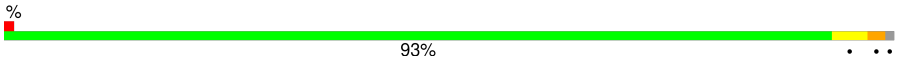
- Molecule 22: 50S ribosomal protein L27

Chain 20:



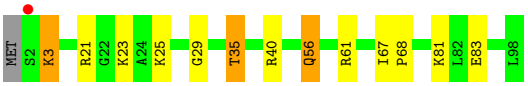
- Molecule 23: 50S ribosomal protein L28

Chain 11:



- Molecule 23: 50S ribosomal protein L28

Chain 21:



- Molecule 24: 50S ribosomal protein L29

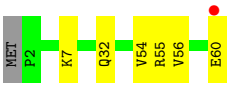
Chain 12:

- Molecule 24: 50S ribosomal protein L29

Chain 22:

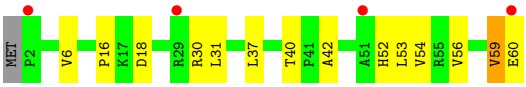
• Molecule 25: 50S ribosomal protein L30

Chain 13:



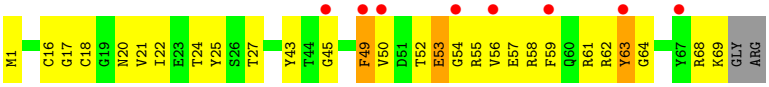
• Molecule 25: 50S ribosomal protein L30

Chain 23:



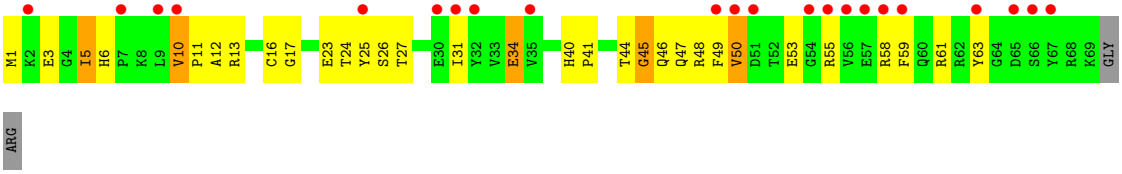
• Molecule 26: 50S ribosomal protein L31

Chain 14:



• Molecule 26: 50S ribosomal protein L31

Chain 24:

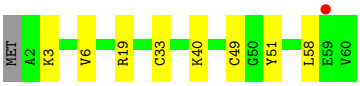


• Molecule 27: 50S ribosomal protein L32

Chain 15:

• Molecule 27: 50S ribosomal protein L32

Chain 25:

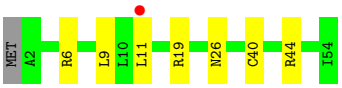


• Molecule 28: 50S ribosomal protein L33

Chain 16:

• Molecule 28: 50S ribosomal protein L33

Chain 26:

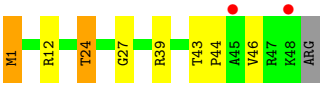


• Molecule 29: 50S ribosomal protein L34

Chain 17:

• Molecule 29: 50S ribosomal protein L34

Chain 27:

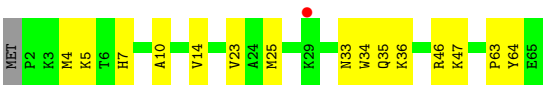


• Molecule 30: 50S ribosomal protein L35

Chain 18:

• Molecule 30: 50S ribosomal protein L35

Chain 28:



• Molecule 31: 50S ribosomal protein L36

Chain 19: 86% 14%

M1 V7 K13 C14 K15 E28 Q34 G37

• Molecule 31: 50S ribosomal protein L36

Chain 29: 8% 86% 14%

M1 K2 S6 D12 V16 V25 Q34 G37

• Molecule 32: 16S Ribosomal RNA

Chain 1a: 4% 63% 31% 5% •

U U G U4 U5 G6 G7 A8 G9 U17 C18 G22 A32 G39 U45 G46 C47 C48 A51 U56 G57 G61 G66 C67 G68 G78 G79 G U U U U A C U90 C91 C92 G93 U96 G97 G98 A101 G105 C106 G107 G108 A109 C110

G115 A116 C121 A130 C131 C136 G142 A143 G144 G147 G148 A149 A152 G159 A160 A161 A162 C163 U164 C165 G166 A171 A172 U173 C174 C175 C176 C177 U180 G181 U182 G183 G184 A185 C186 C187 C188 G189 U189K G189L C193 C194 A195 A196 A197 G200 C201

U202 U203 U204 G216 C217 G220 C221 U222 U223 G236 A243 A246 G247 A250 G251 U256 G257 G258 A262 A263 G266 C267 C268 C269 A270 C271 C272 G276 C277 G289 U294 G299 A300 G306 A313 G316 A321 C328 A329 G332 G333

C342 U343 A344 C345 G346 G347 G348 G351 C352 A353 G354 U367 C372 A373 A374 U375 G376 G377 C381 A382 A383 G384 G388 G392 A393 A397 C398 G399 C400 U405 G406 G407 A408 G409 A412 G413 U421 C422 G423 G424 U429 A430 A431 A432 G438 A439 A441 C442

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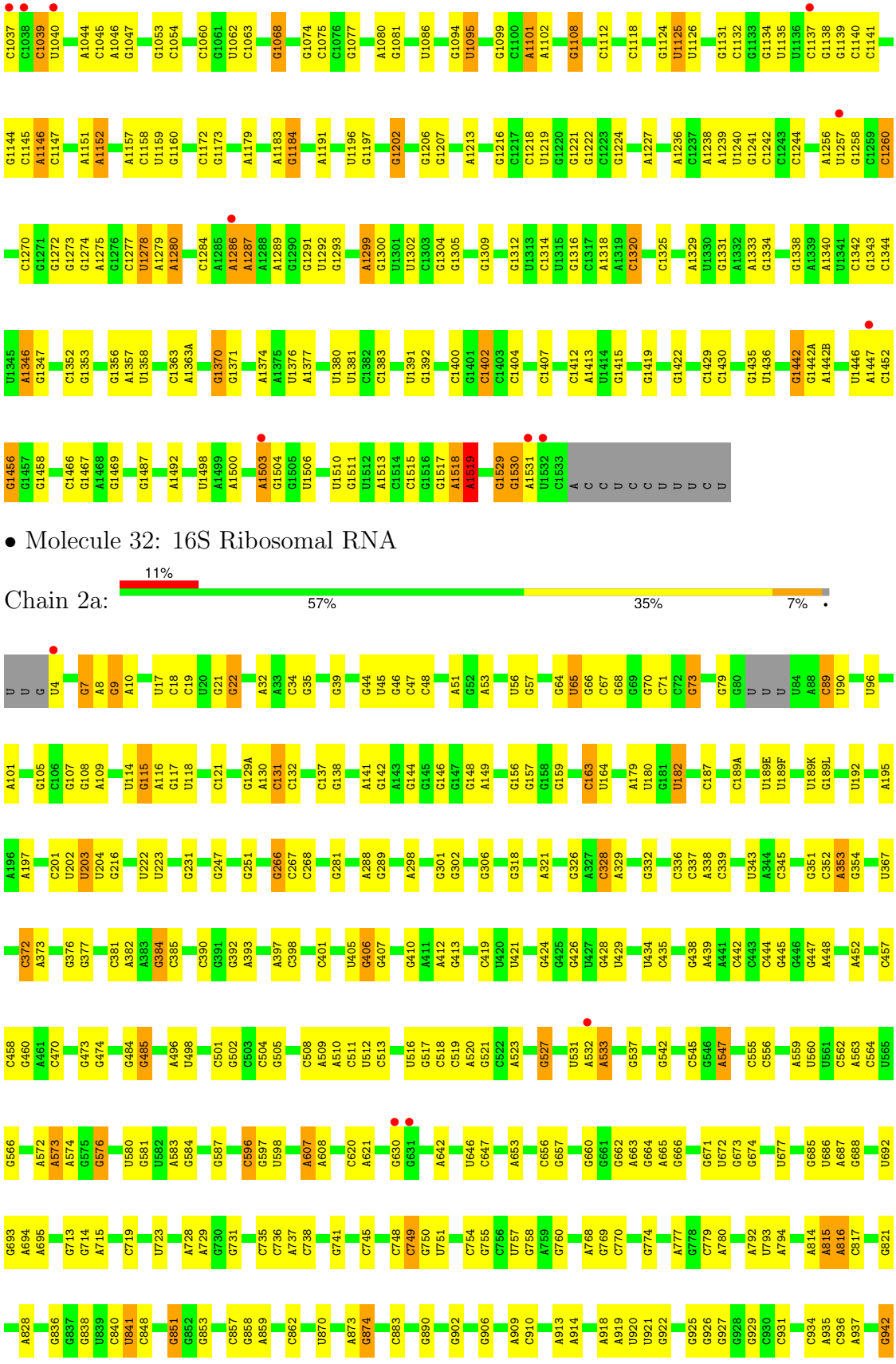
G575 G576 G577 U580 G581 C596 C600 C601 G610 U619 C620 A621 A622 G625 U626 G627 G628 G629 G630 G631 A653 G661 G662 A663 G664 A665 G666 G667 G673 G674 U677 U678 C679 C680 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 G711 A712 G713

G714 A715 A716 C719 C720 G721 A722 U723 G724 G725 G731 G734 A737 C738 G741 G742 C748 C749 G750 G755 C756 U757 G758 A766 A767 A768 G769 A777 C783 A792 U793 A794 G800 C812 U813 A814 A815 A816 C817 G821 A828 G829 G837 G838

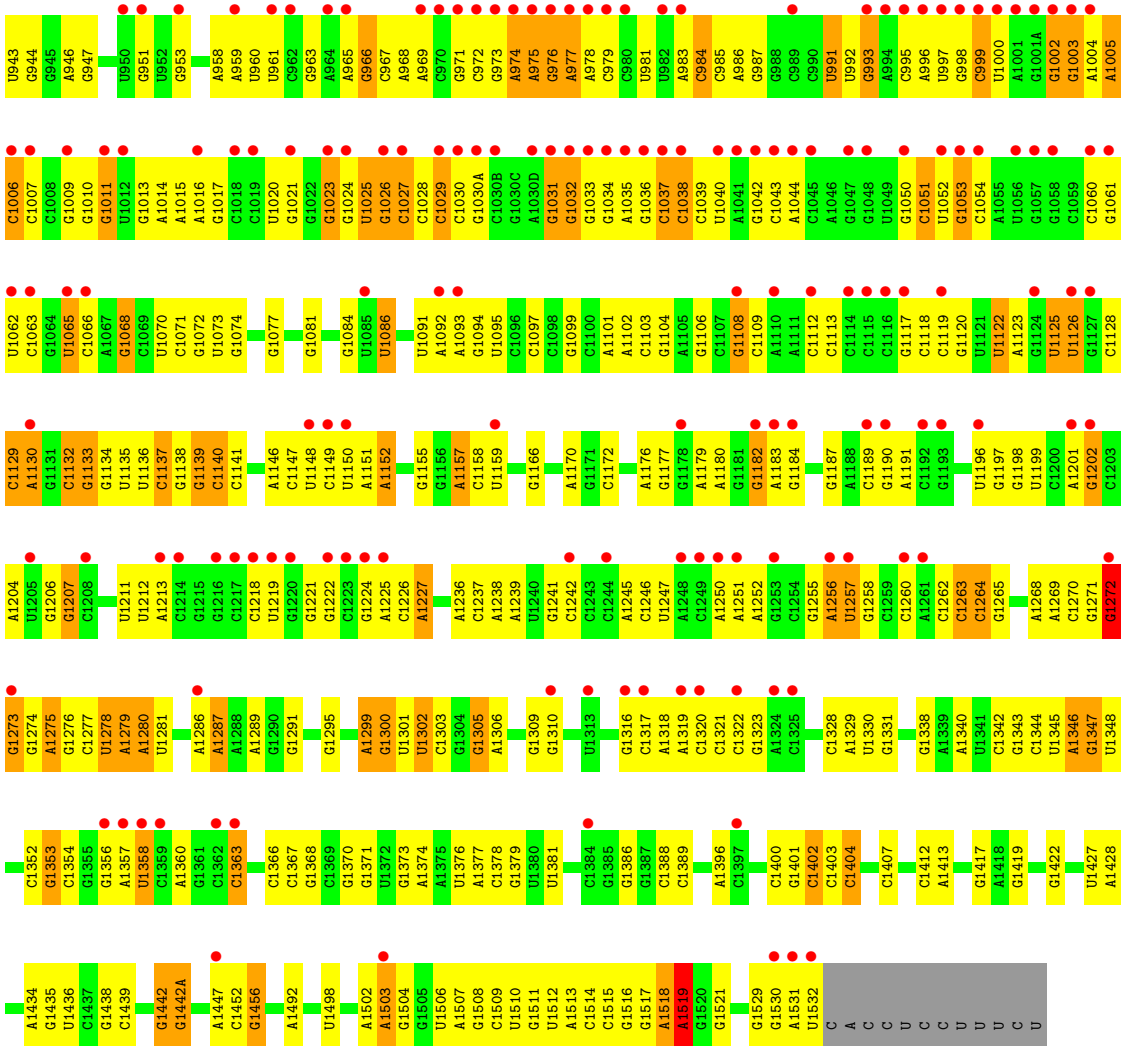
U839 C840 U841 C848 C849 U850 G851 A865 C875 C880 G881 G885 G890 U891 A892 G902 G906 A909 C910 A913 A914 A918 A919 U920 U921 G922 A923 G926 G927 G933 C934 A935 A938 G939 G942 U943 G944 G945 A946 G947 G953 G954 U955 U960

U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 C985 A986 U992 G993 A996 U997 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B G1030C A1030D G1031 G1032 G1033 G1034 A1035 G1036



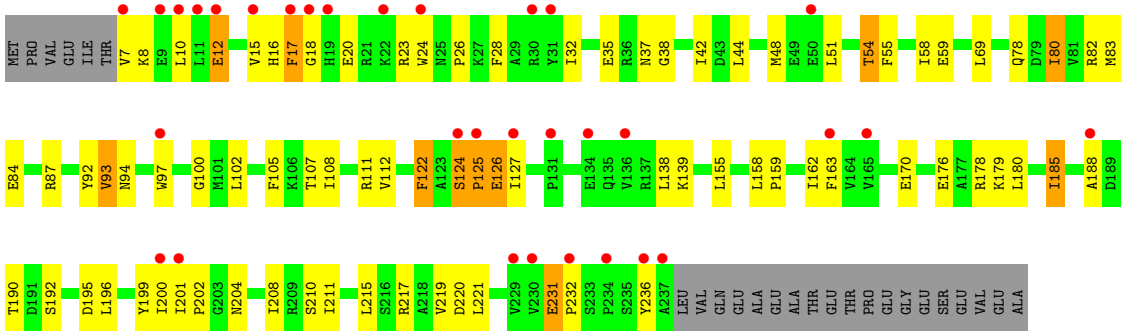
• Molecule 32: 16S Ribosomal RNA

Chain 2a:



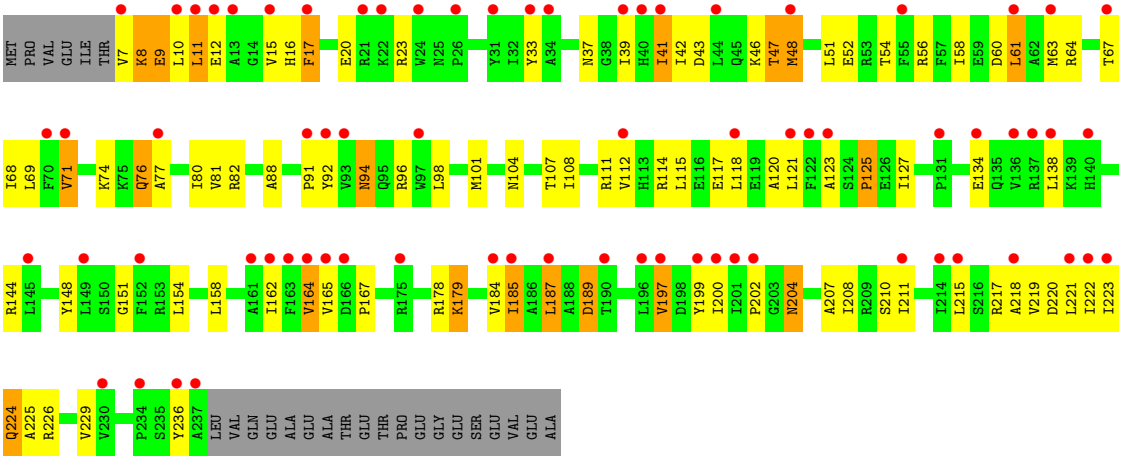
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



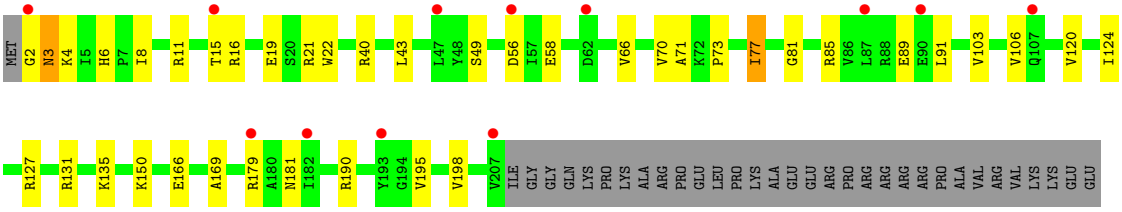
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



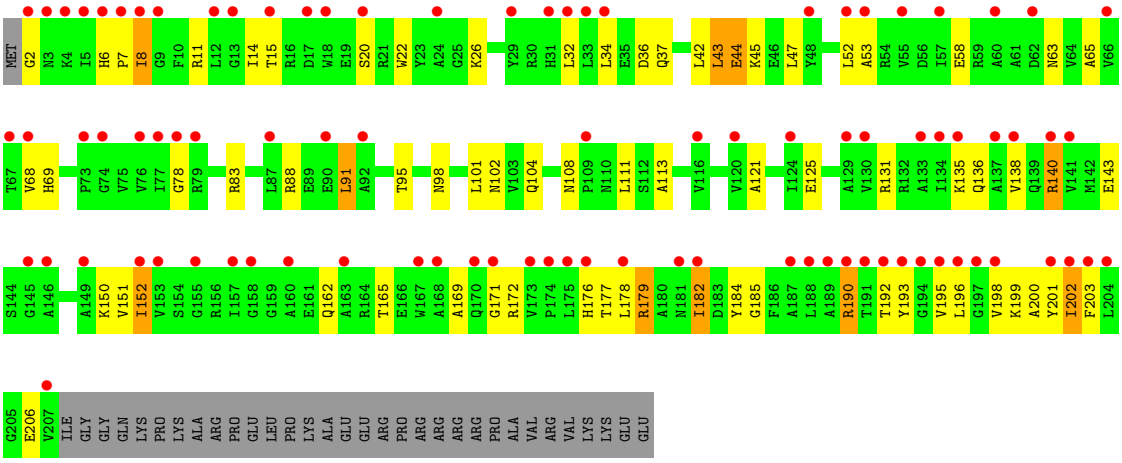
- Molecule 34: 30S ribosomal protein S3

Chain 1c:



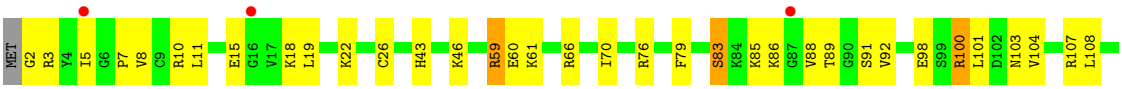
- Molecule 34: 30S ribosomal protein S3

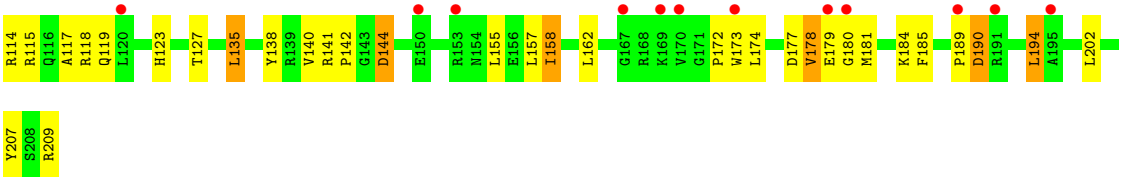
Chain 2c:



- Molecule 35: 30S ribosomal protein S4

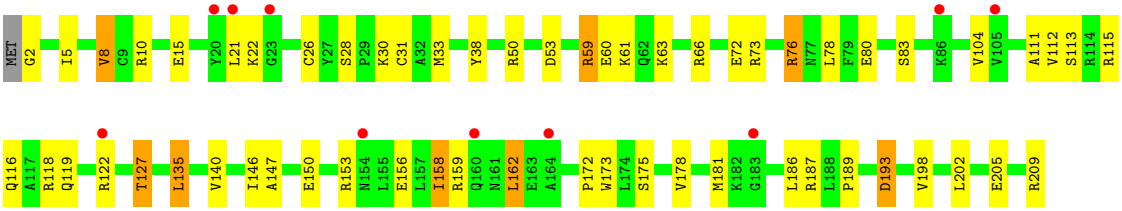
Chain 1d:





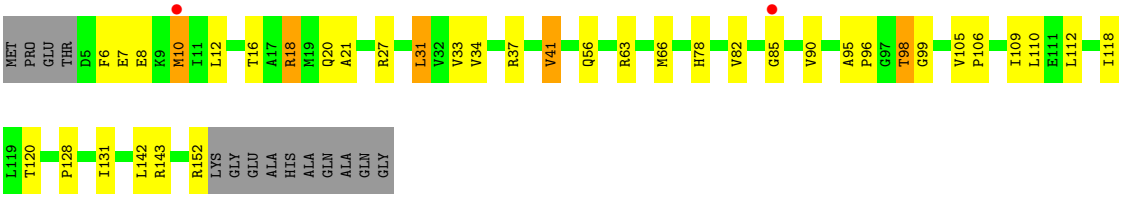
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



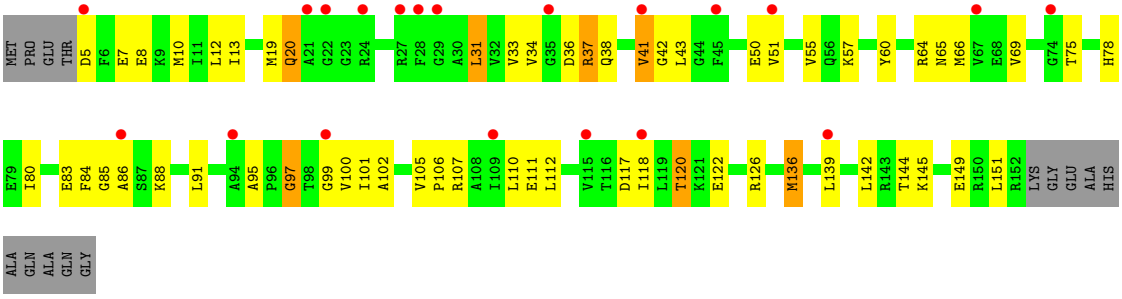
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



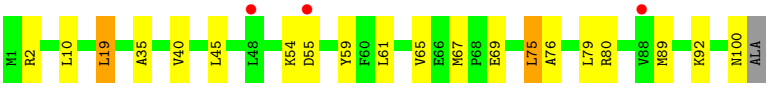
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



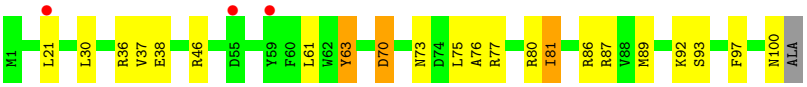
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



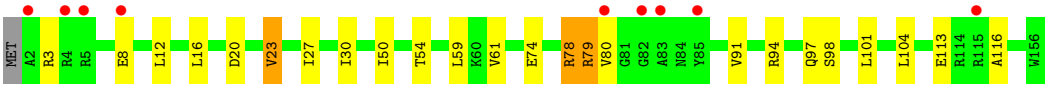
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



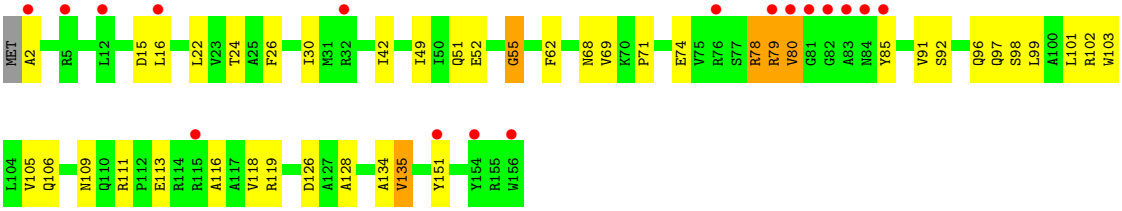
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



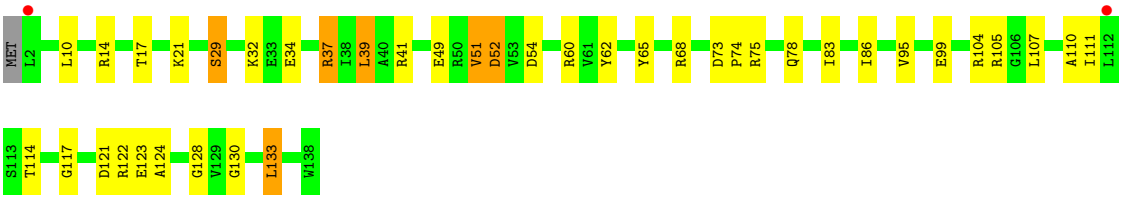
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



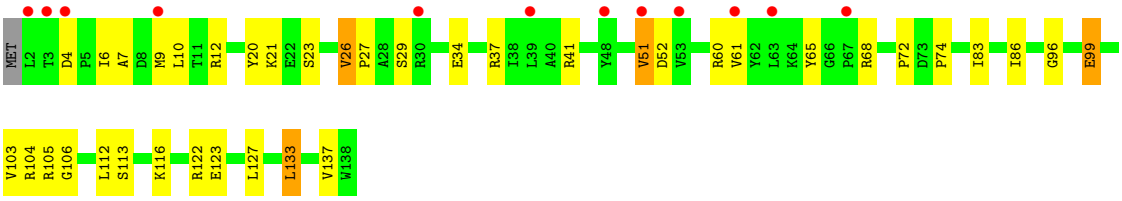
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



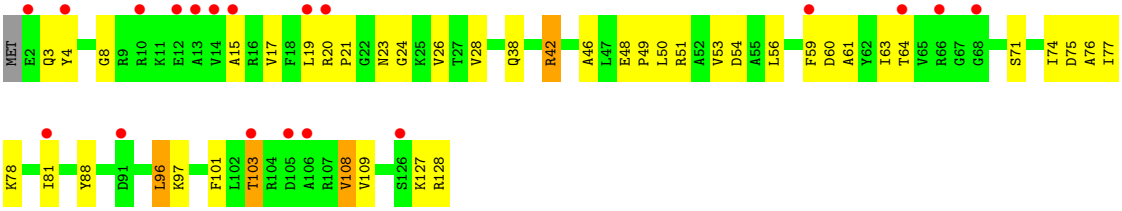
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



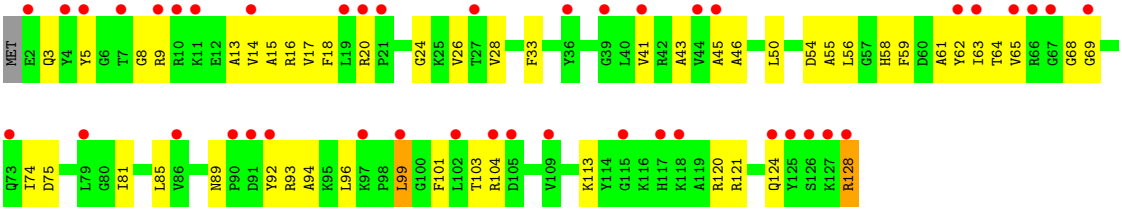
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



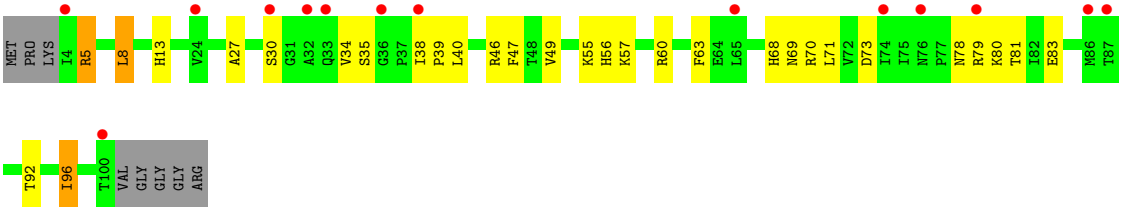
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



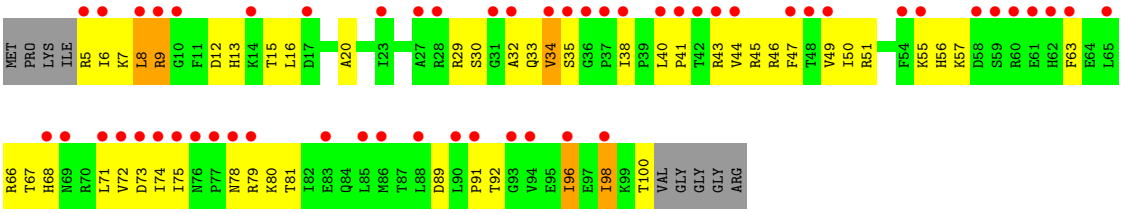
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



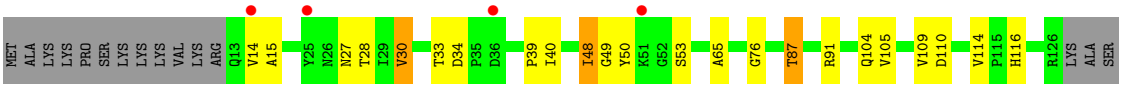
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



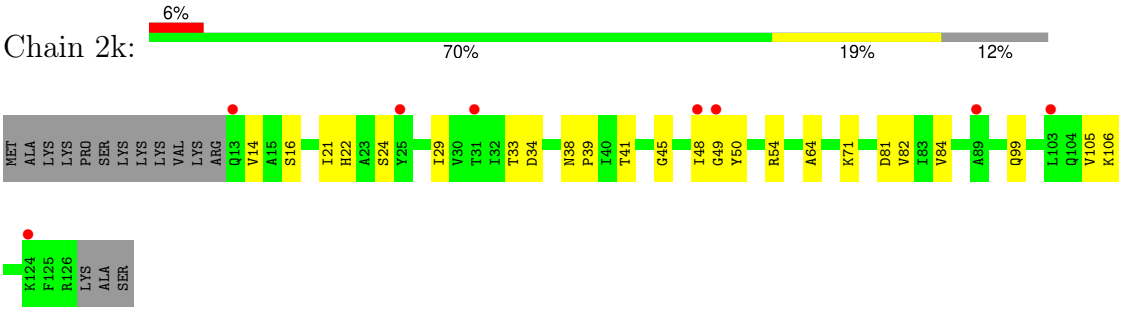
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



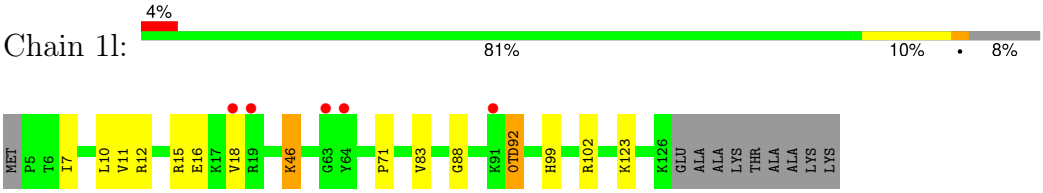
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



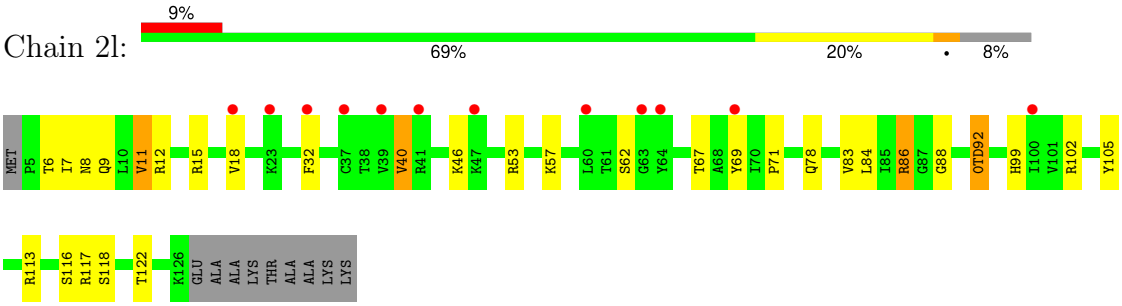
- Molecule 43: 30S ribosomal protein S12

Chain 1l:



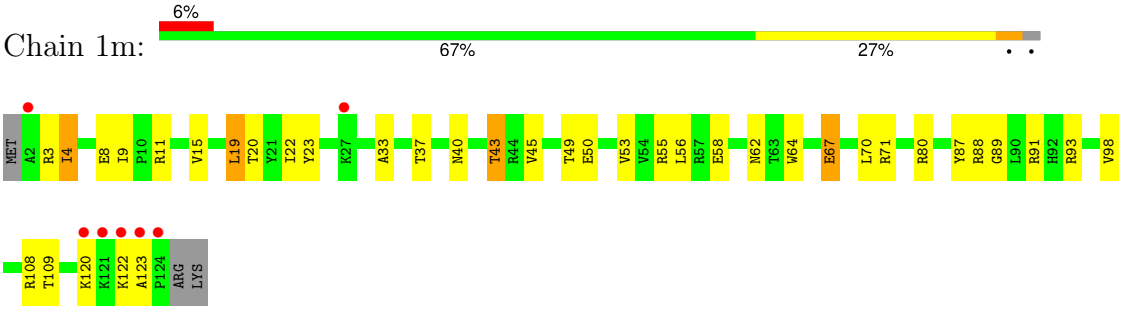
- Molecule 43: 30S ribosomal protein S12

Chain 2l:



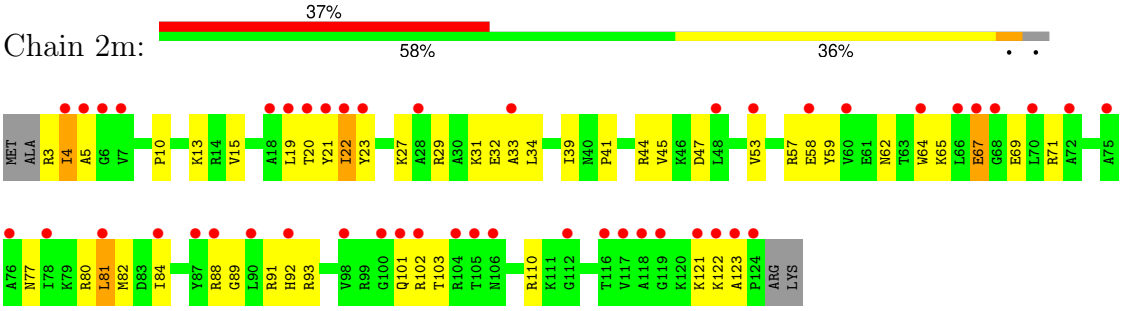
- Molecule 44: 30S ribosomal protein S13

Chain 1m:



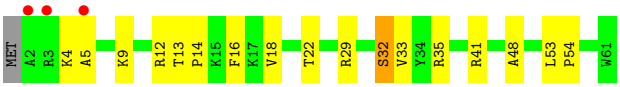
- Molecule 44: 30S ribosomal protein S13

Chain 2m:



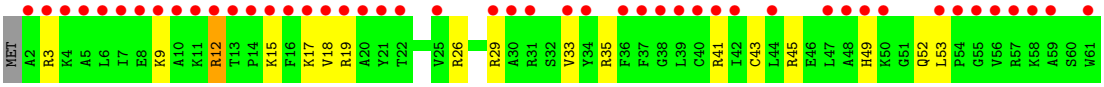
- Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:

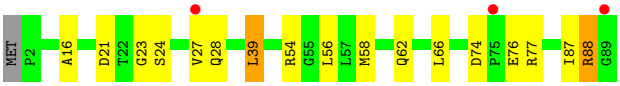


• Molecule 46: 30S ribosomal protein S15

Chain 1o:

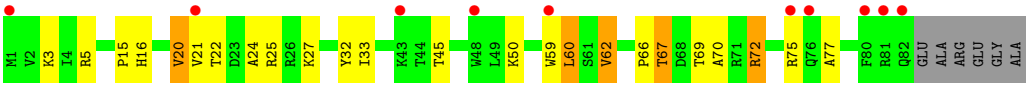
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



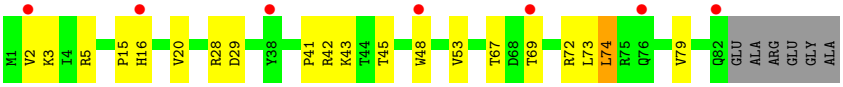
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



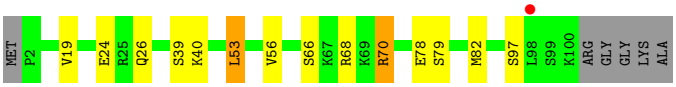
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



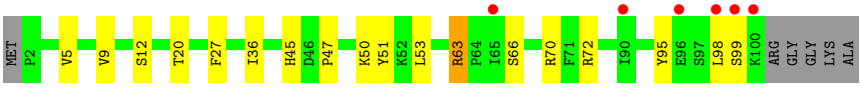
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



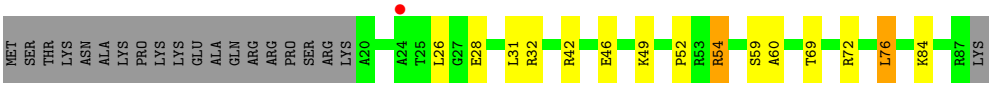
- Molecule 48: 30S ribosomal protein S17

Chain 2q:



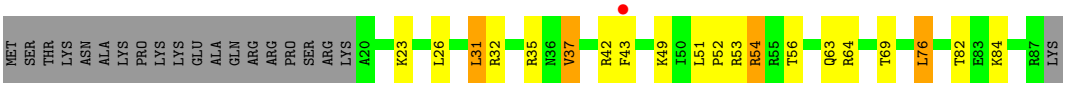
- Molecule 49: 30S ribosomal protein S18

Chain 1r:



- Molecule 49: 30S ribosomal protein S18

Chain 2r:

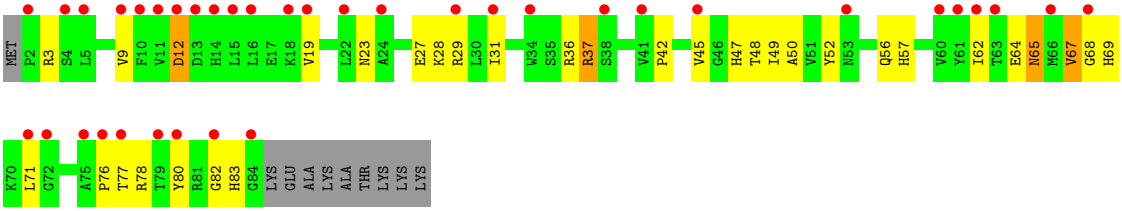


- Molecule 50: 30S ribosomal protein S19

Chain 1s:

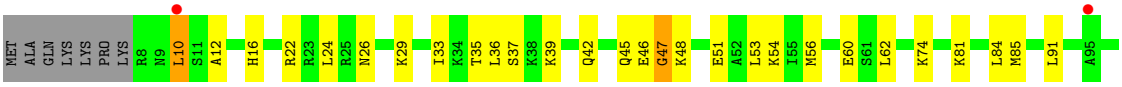
- Molecule 50: 30S ribosomal protein S19

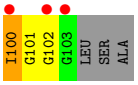
Chain 2s:



- Molecule 51: 30S ribosomal protein S20

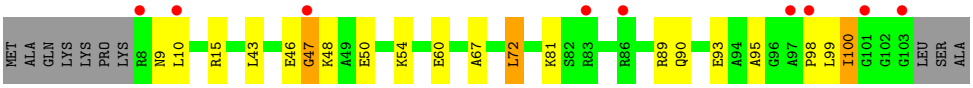
Chain 1t:





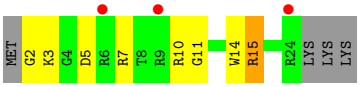
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



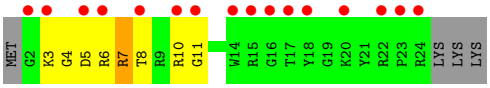
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



• Molecule 52: 30S ribosomal protein Thx

Chain 2u:

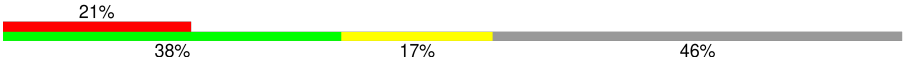


• Molecule 53: MF-mRNA

Chain 1v:

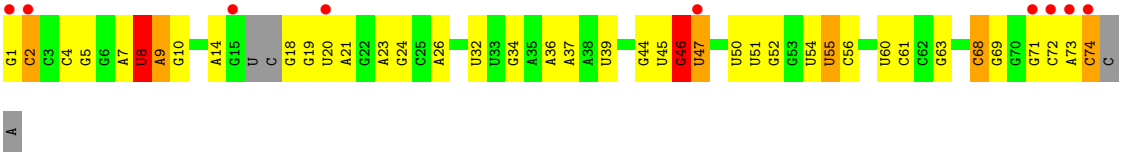
• Molecule 53: MF-mRNA

Chain 2v:



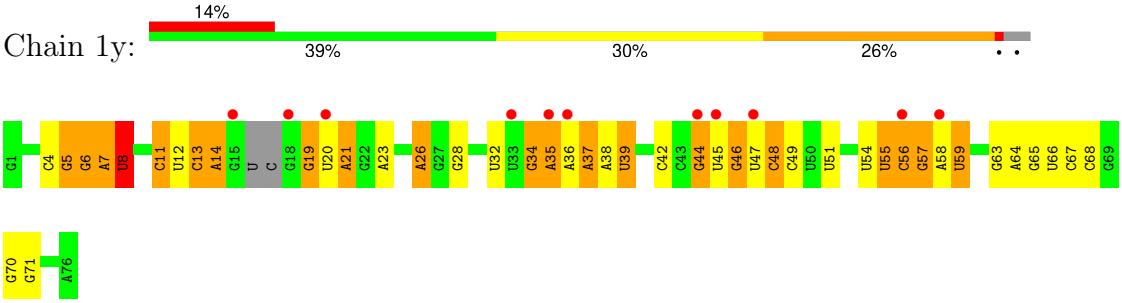
• Molecule 54: A- and E-site Deacylated tRNAphe

Chain 1w:



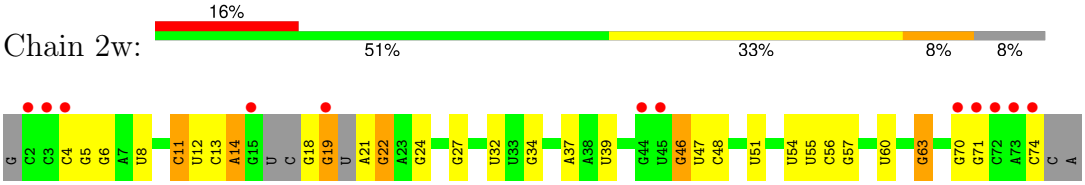
- Molecule 54: A- and E-site Deacylated tRNAphe

Chain 1y:



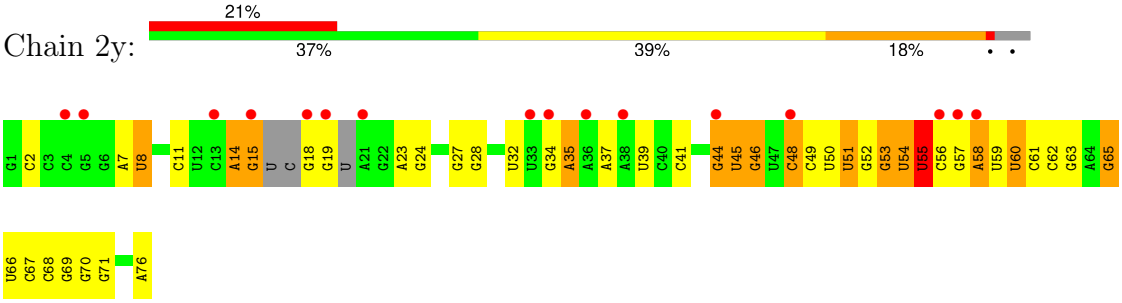
- Molecule 54: A- and E-site Deacylated tRNAphe

Chain 2w:



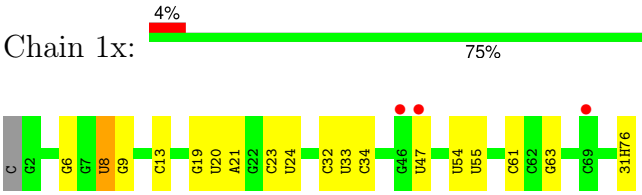
- Molecule 54: A- and E-site Deacylated tRNAphe

Chain 2y:



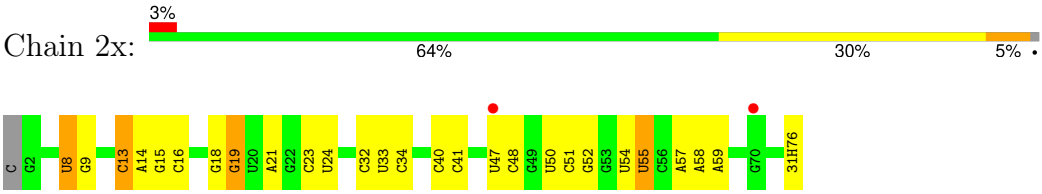
- Molecule 55: P-site Aminoacyl-tRNA fMet-tRNAmet

Chain 1x:



- Molecule 55: P-site Aminoacyl-tRNA fMet-tRNAmet

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	210.00Å 449.39Å 623.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	182.26 – 2.70 182.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (182.26-2.70) 99.4 (182.26-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.201 , 0.241 0.200 , 0.239	Depositor DCC
R_{free} test set	79417 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	60.0	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 73.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	298872	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 31H, 0TD, MIA, OMU, PSU, SF4, WC9, OMC, K, MG, 5MC, 2MG, 4OC, 4SU, UR3, 2MA, ZN, M2G, G7M, OMG, 5MU

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	0.27	0/69011	0.45	3/107720 (0.0%)
1	2A	0.21	0/67295	0.39	1/105042 (0.0%)
2	1B	0.20	0/2882	0.37	0/4494
2	2B	0.18	0/2879	0.35	0/4487
3	1D	0.27	0/2186	0.50	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.26	0/1592	0.50	0/2149
4	2E	0.21	0/1592	0.45	0/2149
5	1F	0.25	0/1619	0.49	0/2193
5	2F	0.20	0/1615	0.45	0/2188
6	1G	0.21	0/1448	0.43	0/1957
6	2G	0.20	0/1453	0.41	0/1963
7	1H	0.21	0/1356	0.41	0/1834
7	2H	0.18	0/1356	0.35	0/1834
8	1I	0.20	0/1112	0.39	0/1514
8	2I	0.20	0/1079	0.41	0/1475
9	1N	0.24	0/1144	0.45	0/1543
9	2N	0.18	0/1144	0.38	0/1543
10	1O	0.24	0/943	0.43	0/1269
10	2O	0.20	0/943	0.43	0/1269
11	1P	0.25	0/1152	0.51	0/1533
11	2P	0.21	0/1152	0.51	0/1533
12	1Q	0.28	0/1143	0.46	0/1527
12	2Q	0.20	0/1143	0.42	0/1527
13	1R	0.26	0/982	0.49	0/1312
13	2R	0.19	0/982	0.43	0/1312
14	1S	0.21	0/883	0.47	0/1176
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.23	0/1105	0.45	0/1477
15	2T	0.21	0/1097	0.43	0/1468
16	1U	0.26	0/977	0.45	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.19	0/977	0.38	0/1301
17	1V	0.24	0/782	0.45	0/1049
17	2V	0.17	0/782	0.37	0/1049
18	1W	0.27	0/897	0.45	0/1205
18	2W	0.21	0/897	0.40	0/1205
19	1X	0.27	0/764	0.50	2/1025 (0.2%)
19	2X	0.21	0/764	0.51	2/1025 (0.2%)
20	1Y	0.23	0/819	0.47	0/1095
20	2Y	0.18	0/819	0.41	0/1095
21	1Z	0.21	0/1267	0.43	0/1717
21	2Z	0.22	0/1299	0.47	1/1763 (0.1%)
22	10	0.25	0/662	0.46	0/881
22	20	0.21	0/662	0.49	1/881 (0.1%)
23	11	0.25	0/762	0.44	0/1014
23	21	0.23	0/762	0.44	0/1014
24	12	0.24	0/590	0.41	0/781
24	22	0.21	0/590	0.37	0/781
25	13	0.24	0/474	0.45	0/635
25	23	0.18	0/469	0.38	0/630
26	14	0.25	0/565	0.60	0/761
26	24	0.25	0/545	0.46	0/737
27	15	0.26	0/469	0.50	0/635
27	25	0.21	0/469	0.39	0/635
28	16	0.25	0/460	0.44	0/613
28	26	0.21	0/456	0.42	0/608
29	17	0.27	0/426	0.48	0/561
29	27	0.24	0/426	0.48	0/561
30	18	0.27	0/525	0.46	0/691
30	28	0.19	0/525	0.48	0/691
31	19	0.26	0/310	0.48	0/407
31	29	0.20	0/310	0.43	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.19	0/35886	0.37	3/56005 (0.0%)
33	1b	0.24	0/1881	0.46	0/2542
33	2b	0.23	0/1860	0.50	0/2518
34	1c	0.19	0/1572	0.39	0/2126
34	2c	0.22	0/1566	0.45	1/2119 (0.0%)
35	1d	0.19	0/1685	0.43	0/2262
35	2d	0.20	0/1704	0.46	0/2284
36	1e	0.21	0/1145	0.49	0/1543
36	2e	0.21	0/1149	0.44	0/1548
37	1f	0.18	0/823	0.40	0/1115
37	2f	0.20	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.18	0/1250	0.39	0/1679
38	2g	0.19	0/1254	0.39	0/1683
39	1h	0.20	0/1108	0.40	0/1494
39	2h	0.19	0/1108	0.42	0/1494
40	1i	0.20	0/1002	0.46	0/1346
40	2i	0.21	0/997	0.47	1/1343 (0.1%)
41	1j	0.20	0/722	0.45	0/982
41	2j	0.22	0/727	0.47	0/988
42	1k	0.17	0/844	0.40	0/1145
42	2k	0.18	0/848	0.38	0/1149
43	1l	0.21	0/937	0.44	0/1260
43	2l	0.18	0/937	0.41	0/1260
44	1m	0.19	0/969	0.46	0/1302
44	2m	0.21	0/961	0.49	0/1291
45	1n	0.18	0/501	0.42	0/664
45	2n	0.21	0/501	0.43	0/664
46	1o	0.19	0/739	0.40	0/985
46	2o	0.17	0/739	0.40	0/985
47	1p	0.19	0/697	0.45	0/939
47	2p	0.18	0/693	0.45	0/935
48	1q	0.19	0/836	0.41	0/1117
48	2q	0.18	0/836	0.37	0/1117
49	1r	0.19	0/560	0.40	0/746
49	2r	0.18	0/560	0.40	0/746
50	1s	0.18	0/667	0.44	0/900
50	2s	0.29	0/661	0.57	0/893
51	1t	0.20	0/730	0.48	0/965
51	2t	0.20	0/729	0.46	0/965
52	1u	0.17	0/203	0.41	0/266
52	2u	0.18	0/203	0.42	0/266
53	1v	0.19	0/310	0.35	0/480
53	2v	0.18	0/310	0.31	0/480
54	1w	0.28	0/1559	0.37	0/2424
54	1y	0.28	2/1606 (0.1%)	0.38	0/2497
54	2w	0.30	2/1509 (0.1%)	0.37	0/2345
54	2y	0.29	2/1583 (0.1%)	0.40	0/2459
55	1x	0.27	0/1700	0.40	0/2650
55	2x	0.24	0/1700	0.37	0/2650
All	All	0.22	6/316546 (0.0%)	0.41	15/473905 (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
5	2F	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	46	G7M	O3'-P	5.51	1.61	1.56
54	1y	8	4SU	O3'-P	5.35	1.61	1.56
54	2y	46	G7M	O3'-P	5.27	1.61	1.56
54	1y	46	G7M	O3'-P	5.16	1.61	1.56
54	2w	8	4SU	O3'-P	5.09	1.61	1.56

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1992	G	C2'-C3'-O3'	7.42	120.63	109.50
19	2X	94	GLY	CA-C-N	6.56	133.50	121.70
19	2X	94	GLY	C-N-CA	6.56	133.50	121.70
1	2A	1992	G	C2'-C3'-O3'	6.53	119.30	109.50
21	2Z	135	GLU	N-CA-C	-5.87	107.93	114.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2F	20	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31197	432	0
1	2A	60322	0	30428	497	0
2	1B	2577	0	1305	14	0
2	2B	2575	0	1303	24	0
3	1D	2136	0	2218	37	0
3	2D	2136	0	2218	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1E	1559	0	1618	17	0
4	2E	1559	0	1618	25	0
5	1F	1584	0	1625	26	0
5	2F	1580	0	1619	40	0
6	1G	1423	0	1436	25	0
6	2G	1428	0	1438	42	0
7	1H	1330	0	1407	26	0
7	2H	1330	0	1407	28	0
8	1I	1097	0	1140	25	0
8	2I	1064	0	1082	14	0
9	1N	1117	0	1184	17	0
9	2N	1117	0	1184	17	0
10	1O	933	0	996	7	0
10	2O	933	0	996	12	0
11	1P	1135	0	1212	17	0
11	2P	1135	0	1212	24	0
12	1Q	1122	0	1179	20	0
12	2Q	1122	0	1179	15	0
13	1R	968	0	1033	11	0
13	2R	968	0	1033	16	0
14	1S	873	0	927	12	0
14	2S	870	0	923	29	0
15	1T	1091	0	1151	5	0
15	2T	1083	0	1136	14	0
16	1U	959	0	1019	18	0
16	2U	959	0	1019	14	0
17	1V	771	0	830	7	0
17	2V	771	0	830	9	0
18	1W	886	0	940	4	0
18	2W	886	0	940	10	0
19	1X	750	0	814	8	0
19	2X	750	0	814	14	0
20	1Y	806	0	881	8	0
20	2Y	806	0	881	10	0
21	1Z	1240	0	1240	31	0
21	2Z	1271	0	1273	42	0
22	10	653	0	674	9	0
22	20	653	0	674	15	0
23	11	755	0	826	6	0
23	21	755	0	826	13	0
24	12	588	0	643	5	0
24	22	588	0	643	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	13	469	0	518	1	0
25	23	464	0	514	6	0
26	14	552	0	533	21	0
26	24	532	0	503	24	0
27	15	455	0	465	7	0
27	25	455	0	465	4	0
28	16	453	0	473	6	0
28	26	449	0	469	4	0
29	17	418	0	467	1	0
29	27	418	0	467	4	0
30	18	517	0	582	13	0
30	28	517	0	582	11	0
31	19	307	0	335	3	0
31	29	307	0	335	3	0
32	1a	32246	0	16295	295	0
32	2a	32327	0	16338	397	0
33	1b	1846	0	1867	48	0
33	2b	1825	0	1828	63	0
34	1c	1548	0	1535	23	0
34	2c	1542	0	1517	51	0
35	1d	1655	0	1672	42	0
35	2d	1674	0	1714	43	0
36	1e	1129	0	1185	24	0
36	2e	1133	0	1191	36	0
37	1f	810	0	804	12	0
37	2f	816	0	808	14	0
38	1g	1231	0	1238	11	0
38	2g	1235	0	1249	27	0
39	1h	1088	0	1126	25	0
39	2h	1088	0	1126	23	0
40	1i	983	0	986	29	0
40	2i	978	0	966	39	0
41	1j	709	0	650	22	0
41	2j	714	0	672	36	0
42	1k	829	0	825	9	0
42	2k	833	0	836	13	0
43	1l	932	0	981	8	0
43	2l	932	0	981	17	0
44	1m	958	0	1002	25	0
44	2m	950	0	988	35	0
45	1n	492	0	529	12	0
45	2n	492	0	529	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1o	728	0	760	12	0
46	2o	728	0	760	10	0
47	1p	681	0	697	16	0
47	2p	677	0	686	11	0
48	1q	823	0	891	9	0
48	2q	823	0	891	8	0
49	1r	555	0	618	9	0
49	2r	555	0	618	12	0
50	1s	652	0	662	18	0
50	2s	646	0	644	28	0
51	1t	728	0	798	19	0
51	2t	727	0	796	13	0
52	1u	199	0	208	7	0
52	2u	199	0	208	5	0
53	1v	277	0	140	1	0
53	2v	277	0	140	3	0
54	1w	1550	0	796	20	0
54	1y	1585	0	803	18	0
54	2w	1502	0	762	13	0
54	2y	1565	0	794	27	0
55	1x	1635	0	839	5	0
55	2x	1635	0	839	13	0
56	10	9	0	0	0	0
56	11	5	0	0	0	0
56	12	2	0	0	0	0
56	13	4	0	0	0	0
56	14	1	0	0	0	0
56	15	7	0	0	0	0
56	16	1	0	0	0	0
56	17	5	0	0	0	0
56	18	6	0	0	0	0
56	19	1	0	0	0	0
56	1A	1059	0	0	0	0
56	1B	34	0	0	0	0
56	1D	12	0	0	0	0
56	1E	17	0	0	0	0
56	1F	12	0	0	0	0
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	5	0	0	0	0
56	1O	6	0	0	0	0
56	1P	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1Q	6	0	0	0	0
56	1R	6	0	0	0	0
56	1S	2	0	0	0	0
56	1T	3	0	0	0	0
56	1U	10	0	0	0	0
56	1V	6	0	0	0	0
56	1W	7	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	2	0	0	0	0
56	1Z	2	0	0	0	0
56	1a	208	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	1	0	0	0	0
56	1k	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	2	0	0	0	0
56	1n	1	0	0	0	0
56	1p	1	0	0	0	0
56	1r	1	0	0	0	0
56	1t	1	0	0	0	0
56	1w	3	0	0	0	0
56	1x	14	0	0	0	0
56	20	2	0	0	0	0
56	21	3	0	0	0	0
56	23	2	0	0	0	0
56	25	1	0	0	0	0
56	27	1	0	0	0	0
56	28	2	0	0	0	0
56	2A	771	0	0	0	0
56	2B	20	0	0	0	0
56	2D	8	0	0	0	0
56	2E	10	0	0	0	0
56	2F	5	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	2	0	0	0	0
56	2T	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2U	1	0	0	0	0
56	2V	2	0	0	0	0
56	2W	2	0	0	0	0
56	2X	2	0	0	0	0
56	2a	214	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2g	1	0	0	0	0
56	2i	2	0	0	0	0
56	2j	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	3	0	0	0	0
56	2q	3	0	0	0	0
56	2r	2	0	0	0	0
56	2t	1	0	0	0	0
56	2v	1	0	0	0	0
56	2w	1	0	0	0	0
56	2x	5	0	0	0	0
56	2y	2	0	0	0	0
57	1A	1	0	0	0	0
57	2x	1	0	0	0	0
58	1A	34	0	0	1	0
58	2A	34	0	0	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	1	0
61	10	12	0	0	1	0
61	11	8	0	0	0	0
61	12	2	0	0	0	0
61	13	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	14	1	0	0	0	0
61	15	6	0	0	0	0
61	16	1	0	0	0	0
61	17	8	0	0	0	0
61	18	11	0	0	1	0
61	1A	1685	0	0	48	0
61	1B	54	0	0	1	0
61	1D	26	0	0	0	0
61	1E	25	0	0	1	0
61	1F	15	0	0	1	0
61	1G	3	0	0	2	0
61	1H	1	0	0	0	0
61	1N	3	0	0	0	0
61	1O	5	0	0	0	0
61	1P	17	0	0	0	0
61	1Q	6	0	0	0	0
61	1R	9	0	0	0	0
61	1S	2	0	0	0	0
61	1T	7	0	0	0	0
61	1U	11	0	0	0	0
61	1V	5	0	0	0	0
61	1W	7	0	0	0	0
61	1X	3	0	0	0	0
61	1Y	1	0	0	1	0
61	1a	213	0	0	15	0
61	1b	1	0	0	0	0
61	1f	2	0	0	0	0
61	1g	1	0	0	0	0
61	1i	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	2	0	0	0	0
61	1q	1	0	0	0	0
61	1v	2	0	0	0	0
61	1w	4	0	0	0	0
61	1x	9	0	0	0	0
61	20	1	0	0	0	0
61	21	7	0	0	0	0
61	27	4	0	0	0	0
61	28	5	0	0	0	0
61	29	1	0	0	0	0
61	2A	848	0	0	56	0
61	2B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2D	16	0	0	1	0
61	2E	10	0	0	0	0
61	2F	11	0	0	0	0
61	2I	1	0	0	0	0
61	2O	3	0	0	0	0
61	2P	6	0	0	0	0
61	2Q	1	0	0	0	0
61	2R	2	0	0	0	0
61	2T	4	0	0	0	0
61	2U	3	0	0	0	0
61	2V	1	0	0	0	0
61	2W	2	0	0	0	0
61	2X	1	0	0	0	0
61	2Y	1	0	0	0	0
61	2a	145	0	0	18	0
61	2d	3	0	0	0	0
61	2j	3	0	0	2	0
61	2l	3	0	0	1	0
61	2r	1	0	0	0	0
61	2t	1	0	0	0	0
61	2x	4	0	0	0	0
61	2y	4	0	0	0	0
All	All	298872	0	196667	3034	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 3034 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.25	1.34
1:1A:1082:U:O4	1:1A:1086:A:N1	1.92	1.03
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.45	0.98
1:2A:784:A:OP2	61:2A:3801:HOH:O	1.84	0.95
54:2y:55:PSU:HN1	54:2y:57:G:H5"	1.29	0.94

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
3	2D	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24	48
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	48
5	1F	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24	48
5	2F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	48
6	1G	179/182 (98%)	165 (92%)	14 (8%)	0	100	100
6	2G	179/182 (98%)	154 (86%)	21 (12%)	4 (2%)	5	14
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21	44
7	2H	172/180 (96%)	156 (91%)	14 (8%)	2 (1%)	10	27
8	1I	144/148 (97%)	129 (90%)	15 (10%)	0	100	100
8	2I	144/148 (97%)	125 (87%)	18 (12%)	1 (1%)	18	41
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	18	41
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16	37
11	1P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	9	23
11	2P	147/150 (98%)	130 (88%)	13 (9%)	4 (3%)	4	10
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	4 (3%)	1 (1%)	14	35
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	97 (90%)	8 (7%)	3 (3%)	4	9
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	16
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	32
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%)	2 (2%)	2 (2%)	5	14
19	2X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	12	32
20	2Y	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
21	1Z	148/206 (72%)	137 (93%)	10 (7%)	1 (1%)	18	41
21	2Z	156/206 (76%)	125 (80%)	28 (18%)	3 (2%)	6	17
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	29
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	29
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	50 (75%)	13 (19%)	4 (6%)	1	2
26	24	67/71 (94%)	52 (78%)	13 (19%)	2 (3%)	3	8
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	198 (86%)	24 (10%)	7 (3%)	3	8
33	2b	229/256 (90%)	192 (84%)	29 (13%)	8 (4%)	3	6
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	169 (83%)	33 (16%)	2 (1%)	12	32
35	1d	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
35	2d	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
36	1e	146/162 (90%)	138 (94%)	7 (5%)	1 (1%)	18	41
36	2e	146/162 (90%)	129 (88%)	13 (9%)	4 (3%)	4	10
37	1f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	12	32
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	147 (96%)	5 (3%)	1 (1%)	18	41
38	2g	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	9	25
39	1h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100	100
40	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16	37
40	2i	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	16	37
41	1j	95/105 (90%)	79 (83%)	15 (16%)	1 (1%)	11	29
41	2j	94/105 (90%)	78 (83%)	14 (15%)	2 (2%)	5	15
42	1k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	6	18
42	2k	112/129 (87%)	103 (92%)	8 (7%)	1 (1%)	14	35
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
44	1m	121/126 (96%)	109 (90%)	11 (9%)	1 (1%)	16	37
44	2m	120/126 (95%)	103 (86%)	15 (12%)	2 (2%)	7	19
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	84 (98%)	1 (1%)	1 (1%)	10	27
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
48	2q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	10	27
50	2s	81/93 (87%)	70 (86%)	9 (11%)	2 (2%)	4	11
51	1t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	3	7
51	2t	94/106 (89%)	83 (88%)	9 (10%)	2 (2%)	5	15
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	3
All	All	11370/12128 (94%)	10547 (93%)	733 (6%)	90 (1%)	16	37

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
17	1V	79	VAL
21	1Z	53	ILE
33	1b	17	PHE
33	1b	126	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	206 (96%)	9 (4%)	26	55
3	2D	215/218 (99%)	206 (96%)	9 (4%)	26	55
4	1E	164/166 (99%)	156 (95%)	8 (5%)	22	49
4	2E	164/166 (99%)	153 (93%)	11 (7%)	15	36
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	150 (94%)	9 (6%)	18	43
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9	22
6	2G	143/156 (92%)	119 (83%)	24 (17%)	2	6
7	1H	144/148 (97%)	137 (95%)	7 (5%)	22	49
7	2H	144/148 (97%)	129 (90%)	15 (10%)	7	17
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3	7
8	2I	105/124 (85%)	93 (89%)	12 (11%)	5	14
9	1N	118/119 (99%)	111 (94%)	7 (6%)	18	42
9	2N	118/119 (99%)	111 (94%)	7 (6%)	18	42
10	1O	100/100 (100%)	100 (100%)	0	100	100
10	2O	100/100 (100%)	98 (98%)	2 (2%)	48	76
11	1P	115/116 (99%)	107 (93%)	8 (7%)	14	34
11	2P	115/116 (99%)	109 (95%)	6 (5%)	21	47
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	24	52
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	51	78
13	1R	101/101 (100%)	97 (96%)	4 (4%)	28	56
13	2R	101/101 (100%)	98 (97%)	3 (3%)	36	66
14	1S	86/88 (98%)	77 (90%)	9 (10%)	6	17
14	2S	85/88 (97%)	78 (92%)	7 (8%)	10	27
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21	47
15	2T	113/127 (89%)	110 (97%)	3 (3%)	39	69
16	1U	93/94 (99%)	86 (92%)	7 (8%)	12	31
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26	54
17	1V	80/82 (98%)	74 (92%)	6 (8%)	12	31
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9	23
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19	44
18	2W	90/92 (98%)	83 (92%)	7 (8%)	11	29
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	70
19	2X	77/78 (99%)	76 (99%)	1 (1%)	61	83
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	10	27
20	2Y	85/91 (93%)	74 (87%)	11 (13%)	4	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	135/179 (75%)	121 (90%)	14 (10%)	7	17
21	2Z	137/179 (76%)	124 (90%)	13 (10%)	8	20
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	65
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	39
23	11	80/83 (96%)	79 (99%)	1 (1%)	61	83
23	21	80/83 (96%)	77 (96%)	3 (4%)	29	58
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	65
24	22	65/67 (97%)	61 (94%)	4 (6%)	16	39
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	29
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	28
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	9
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	7
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	41
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	56
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	29
28	26	50/52 (96%)	48 (96%)	2 (4%)	28	56
29	17	41/42 (98%)	35 (85%)	6 (15%)	3	8
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	19
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	59
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	59
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	67
33	1b	192/220 (87%)	175 (91%)	17 (9%)	9	23
33	2b	187/220 (85%)	156 (83%)	31 (17%)	2	6
34	1c	142/188 (76%)	133 (94%)	9 (6%)	16	39
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7	19
35	1d	169/181 (93%)	149 (88%)	20 (12%)	5	13
35	2d	173/181 (96%)	158 (91%)	15 (9%)	9	24
36	1e	113/123 (92%)	104 (92%)	9 (8%)	11	28
36	2e	114/123 (93%)	101 (89%)	13 (11%)	5	14
37	1f	84/90 (93%)	78 (93%)	6 (7%)	13	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	78 (92%)	7 (8%)	10	27
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7	18
38	2g	120/127 (94%)	112 (93%)	8 (7%)	15	36
39	1h	114/119 (96%)	106 (93%)	8 (7%)	14	34
39	2h	114/119 (96%)	104 (91%)	10 (9%)	9	23
40	1i	90/99 (91%)	81 (90%)	9 (10%)	7	19
40	2i	89/99 (90%)	82 (92%)	7 (8%)	11	28
41	1j	66/92 (72%)	61 (92%)	5 (8%)	12	30
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	13
42	1k	82/99 (83%)	74 (90%)	8 (10%)	7	19
42	2k	83/99 (84%)	80 (96%)	3 (4%)	31	60
43	1l	96/108 (89%)	91 (95%)	5 (5%)	21	47
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	32
44	1m	93/101 (92%)	86 (92%)	7 (8%)	12	31
44	2m	92/101 (91%)	82 (89%)	10 (11%)	6	16
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	12
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	18
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21	48
46	2o	78/80 (98%)	75 (96%)	3 (4%)	29	58
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	13
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9	23
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20	46
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20	46
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14	35
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5	13
50	1s	69/80 (86%)	67 (97%)	2 (3%)	37	67
50	2s	67/80 (84%)	57 (85%)	10 (15%)	3	8
51	1t	70/82 (85%)	67 (96%)	3 (4%)	26	54
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18	43
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	44
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9303/10064 (92%)	8615 (93%)	688 (7%)	13 32

5 of 688 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	2Y	85	VAL
35	2d	193	ASP
21	2Z	154	ASP
20	2Y	83	THR
33	2b	39	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
42	2k	117	ASN
46	2o	13	GLN
41	1j	69	ASN
41	1j	56	HIS
49	2r	63	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	402 (14%)	26 (0%)
1	2A	2791/2915 (95%)	426 (15%)	25 (0%)
2	1B	119/121 (98%)	8 (6%)	0
2	2B	118/121 (97%)	24 (20%)	0
32	1a	1497/1521 (98%)	222 (14%)	0
32	2a	1501/1521 (98%)	278 (18%)	0
53	1v	12/24 (50%)	0	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	70/76 (92%)	21 (30%)	0
54	1y	72/76 (94%)	28 (38%)	0
54	2w	67/76 (88%)	15 (22%)	0
54	2y	70/76 (92%)	24 (34%)	0
55	1x	74/77 (96%)	8 (10%)	0
55	2x	74/77 (96%)	8 (10%)	0
All	All	9341/9620 (97%)	1465 (15%)	51 (0%)

5 of 1465 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A

5 of 51 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	249	C
1	2A	774	A
1	2A	2439	A
1	2A	266	G
1	2A	310	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	G7M	2y	46	54	23,26,27	1.59	3 (13%)	34,39,42	1.79	4 (11%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.03	4 (19%)
1	5MC	1A	1962	56,1	19,22,23	1.77	3 (15%)	26,32,35	1.22	3 (11%)
54	4SU	2y	8	54	18,21,22	1.79	5 (27%)	25,30,33	2.06	5 (20%)
1	PSU	2A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	2.01	3 (14%)
1	OMG	1A	2251	56,55,1	23,26,27	1.21	3 (13%)	32,38,41	2.02	6 (18%)
54	PSU	2y	39	54	18,21,22	1.41	2 (11%)	21,30,33	1.66	4 (19%)
32	G7M	1a	527	32,56	23,26,27	1.53	3 (13%)	34,39,42	1.71	5 (14%)
1	5MC	2A	1962	56,1	19,22,23	1.59	3 (15%)	26,32,35	1.16	2 (7%)
54	G7M	2w	46	54	23,26,27	1.46	4 (17%)	34,39,42	1.69	5 (14%)
54	G7M	1w	46	54	23,26,27	1.56	3 (13%)	34,39,42	1.64	4 (11%)
55	5MU	1x	54	55,56	19,22,23	1.43	6 (31%)	27,32,35	2.04	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	MIA	2w	37	53,54	24,27,32	2.20	5 (20%)	32,39,47	2.66	11 (34%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.93	3 (14%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	0.94	1 (4%)
54	PSU	1y	39	54	18,21,22	1.39	2 (11%)	21,30,33	1.87	3 (14%)
43	0TD	1l	92	43	8,9,10	4.47	1 (12%)	6,11,13	4.99	2 (33%)
55	4SU	1x	8	55	18,21,22	2.23	6 (33%)	25,30,33	1.68	6 (24%)
32	5MC	1a	1407	32	19,22,23	1.63	3 (15%)	26,32,35	1.10	3 (11%)
1	5MU	1A	1939	56,1	19,22,23	1.43	4 (21%)	27,32,35	2.22	6 (22%)
54	PSU	2w	55	54	18,21,22	1.41	2 (11%)	21,30,33	1.99	3 (14%)
32	UR3	2a	1498	32,56	19,22,23	1.02	2 (10%)	26,32,35	1.72	3 (11%)
54	4SU	1y	8	54	18,21,22	1.84	5 (27%)	25,30,33	1.84	4 (16%)
55	PSU	1x	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.06	4 (19%)
1	OMU	1A	2552	56,1	19,22,23	1.22	3 (15%)	25,31,34	1.80	5 (20%)
1	5MU	2A	1939	56,1	19,22,23	1.44	6 (31%)	27,32,35	2.38	6 (22%)
1	2MA	1A	2503	56,1	22,25,26	1.48	4 (18%)	32,37,40	2.38	9 (28%)
1	5MC	2A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.13	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.77	0	25,32,35	1.04	3 (12%)
54	PSU	1y	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.00	5 (23%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.85	5 (15%)
32	5MC	2a	967	32	19,22,23	1.63	3 (15%)	26,32,35	1.13	2 (7%)
1	5MU	2A	1915	56,1	19,22,23	1.44	5 (26%)	27,32,35	2.15	6 (22%)
1	PSU	1A	1917	1	18,21,22	1.41	2 (11%)	21,30,33	2.03	3 (14%)
32	G7M	2a	527	32,56	23,26,27	1.46	4 (17%)	34,39,42	1.66	5 (14%)
55	31H	1x	76	55,56	31,34,35	1.19	3 (9%)	35,47,50	1.93	10 (28%)
54	PSU	1y	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.96	4 (19%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.82	6 (18%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	2.02	5 (23%)
55	5MC	1x	32	55	19,22,23	1.66	3 (15%)	26,32,35	1.23	2 (7%)
54	5MU	1y	54	54	19,22,23	1.41	5 (26%)	27,32,35	1.85	7 (25%)
54	5MU	2y	54	54	19,22,23	1.45	4 (21%)	27,32,35	2.01	6 (22%)
32	2MG	1a	1207	32	23,26,27	1.21	2 (8%)	33,38,41	2.23	8 (24%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.05	9 (27%)
32	5MC	2a	1400	32	19,22,23	1.63	3 (15%)	26,32,35	1.25	3 (11%)
54	PSU	2y	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.15	5 (23%)
1	5MU	1A	1915	1	19,22,23	1.44	5 (26%)	27,32,35	2.19	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.98	3 (14%)
54	PSU	1w	32	56,54	18,21,22	1.33	2 (11%)	21,30,33	1.94	3 (14%)
54	4SU	2w	8	54	18,21,22	1.76	5 (27%)	25,30,33	1.94	4 (16%)
55	4SU	2x	8	55	18,21,22	2.15	6 (33%)	25,30,33	1.29	6 (24%)
1	PSU	1A	2605	56,1	18,21,22	1.42	4 (22%)	21,30,33	2.00	4 (19%)
54	MIA	2y	37	54	21,24,32	1.65	4 (19%)	30,35,47	2.01	7 (23%)
54	PSU	2w	39	54	18,21,22	1.40	2 (11%)	21,30,33	1.69	3 (14%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.00	9 (27%)
1	OMC	2A	1920	1	19,22,23	0.78	0	25,31,34	0.85	0
55	31H	2x	76	55,57,56	31,34,35	1.20	3 (9%)	35,47,50	1.92	9 (25%)
32	5MC	2a	1407	32,56	19,22,23	1.48	3 (15%)	26,32,35	1.22	3 (11%)
1	OMU	2A	2552	56,1	19,22,23	1.23	2 (10%)	25,31,34	1.76	5 (20%)
32	2MG	2a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.26	7 (21%)
54	5MU	1w	54	54	19,22,23	1.37	5 (26%)	27,32,35	2.02	6 (22%)
55	5MC	2x	32	55	19,22,23	1.66	3 (15%)	26,32,35	1.19	3 (11%)
54	PSU	2y	32	54	18,21,22	1.35	2 (11%)	21,30,33	1.94	3 (14%)
1	2MA	2A	2503	56,1	22,25,26	1.53	5 (22%)	32,37,40	2.32	8 (25%)
54	G7M	1y	46	54	23,26,27	1.53	4 (17%)	34,39,42	1.71	5 (14%)
1	PSU	2A	2605	1	18,21,22	1.32	2 (11%)	21,30,33	2.10	4 (19%)
32	5MC	1a	1404	32	19,22,23	1.57	3 (15%)	26,32,35	1.18	3 (11%)
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.96	3 (14%)
54	4SU	1w	8	54	18,21,22	1.81	5 (27%)	25,30,33	2.00	5 (20%)
54	5MU	2w	54	54	19,22,23	1.37	4 (21%)	27,32,35	1.93	7 (25%)
55	5MU	2x	54	55	19,22,23	1.40	5 (26%)	27,32,35	2.11	6 (22%)
54	MIA	1y	37	54	21,24,32	1.66	4 (19%)	30,35,47	1.98	7 (23%)
1	5MC	1A	1942	56,1	19,22,23	1.53	3 (15%)	26,32,35	1.12	2 (7%)
54	PSU	1w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.00	3 (14%)
32	4OC	2a	1402	32	20,23,24	0.74	0	25,32,35	0.97	1 (4%)
32	5MC	1a	967	32	19,22,23	1.55	3 (15%)	26,32,35	1.09	2 (7%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.06	9 (27%)
1	OMG	2A	2251	56,55,1	23,26,27	1.20	3 (13%)	32,38,41	2.08	7 (21%)
32	MA6	2a	1519	32	23,26,27	0.40	0	33,38,41	2.06	9 (27%)
32	PSU	1a	516	32	18,21,22	1.36	3 (16%)	21,30,33	2.07	5 (23%)
43	0TD	2l	92	43	8,9,10	4.63	1 (12%)	6,11,13	2.01	3 (50%)
54	PSU	1w	39	54	18,21,22	1.35	2 (11%)	21,30,33	1.90	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	UR3	1a	1498	32	19,22,23	0.98	1 (5%)	26,32,35	1.84	4 (15%)
32	5MC	2a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.17	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.20	3 (11%)
54	MIA	1w	37	54	28,31,32	2.32	6 (21%)	38,44,47	2.75	12 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	G7M	2y	46	54	-	1/7/25/26	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	56,55,1	-	0/9/27/28	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,56	-	3/7/25/26	0/3/3/3
1	5MC	2A	1962	56,1	-	2/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	53,54	-	4/11/29/34	0/3/3/3
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32,56	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
1	5MU	2A	1939	56,1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	56,1	-	1/7/25/26	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	56,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,56	-	3/7/25/26	0/3/3/3
55	31H	1x	76	55,56	-	4/22/40/41	0/3/3/3
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	1/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	56,54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/7/25/34	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
55	31H	2x	76	55,57,56	-	4/22/40/41	0/3/3/3
32	5MC	2a	1407	32,56	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	56,1	-	2/7/25/26	0/3/3/3
54	G7M	1y	46	54	-	2/7/25/26	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
1	5MC	1A	1942	56,1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	OMG	2A	2251	56,55,1	-	0/9/27/28	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	2/15/33/34	0/3/3/3

The worst 5 of 253 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.80	1.69	1.82
43	1l	92	0TD	CB-SB	-12.14	1.70	1.82
54	2w	37	MIA	C2-S10	-7.41	1.69	1.75
54	1w	37	MIA	C13-C14	6.97	1.53	1.32
1	1A	1962	5MC	C5-C4	6.64	1.49	1.44

The worst 5 of 414 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-11.56	81.59	102.36
54	2w	37	MIA	C5-C4-N3	-8.96	117.74	127.18
54	1w	37	MIA	C12-C13-C14	-8.86	111.11	127.01
1	1A	2503	2MA	C5-C4-N3	-8.56	118.16	127.18
54	1w	37	MIA	C5-C4-N3	-8.27	118.47	127.18

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
54	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1207	2MG	N1-C2-N2-CM2
32	2a	1207	2MG	N3-C2-N2-CM2

There are no ring outliers.

31 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2x	55	PSU	1	0
54	2y	8	4SU	1	0
54	1w	46	G7M	1	0
54	1y	39	PSU	1	0
43	1l	92	0TD	1	0
55	1x	8	4SU	2	0
1	1A	1939	5MU	2	0
54	1y	8	4SU	2	0
1	2A	1939	5MU	1	0
1	1A	2503	2MA	1	0
32	1a	1402	4OC	1	0
54	1y	55	PSU	1	0
32	2a	966	M2G	1	0
1	1A	1917	PSU	1	0
32	1a	966	M2G	2	0
54	2y	54	5MU	1	0
32	1a	1519	MA6	1	0
54	2y	55	PSU	7	0
55	2x	8	4SU	1	0
32	2a	1518	MA6	2	0
1	2A	2552	OMU	1	0
32	2a	1207	2MG	1	0
1	2A	2503	2MA	1	0
54	1w	8	4SU	1	0
54	1y	37	MIA	1	0
54	1w	55	PSU	1	0
32	2a	1402	4OC	3	0
32	1a	1518	MA6	1	0
32	2a	1519	MA6	2	0
43	2l	92	0TD	1	0
32	2a	1404	5MC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2589 ligands modelled in this entry, 2585 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	WC9	2A	3772	-	34,37,37	1.31	2 (5%)	31,53,53	1.07	3 (9%)
60	SF4	2d	302	35	0,12,12	-	-	-		
60	SF4	1d	302	35	0,12,12	-	-	-		
58	WC9	1A	4061	-	34,37,37	1.30	3 (8%)	31,53,53	1.30	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	WC9	2A	3772	-	-	2/28/71/71	0/3/4/4
60	SF4	2d	302	35	-	-	0/6/5/5
60	SF4	1d	302	35	-	-	0/6/5/5
58	WC9	1A	4061	-	-	3/28/71/71	0/3/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4061	WC9	CAM-CBF	-4.99	1.39	1.51
58	2A	3772	WC9	CAM-CBF	-4.86	1.39	1.51
58	2A	3772	WC9	OAW-CB	2.94	1.45	1.42
58	1A	4061	WC9	CD2-CAZ	-2.94	1.50	1.53
58	1A	4061	WC9	CBF-CBH	2.09	1.40	1.31

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	1A	4061	WC9	CBC-CBB-CAZ	-3.84	109.23	116.68
58	1A	4061	WC9	CAF-OAA-CAB	-3.49	109.60	114.17
58	2A	3772	WC9	CAF-OAA-CAB	-3.14	110.06	114.17
58	2A	3772	WC9	CBC-CBB-CAZ	-3.07	110.73	116.68
58	1A	4061	WC9	CD2-CAZ-CAY	-2.69	109.76	113.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	4061	WC9	O-C-CA-CB
58	1A	4061	WC9	NAL-C-CA-CB
58	2A	3772	WC9	O-C-CA-CB
58	2A	3772	WC9	NAL-C-CA-CB
58	1A	4061	WC9	O-C-CA-N

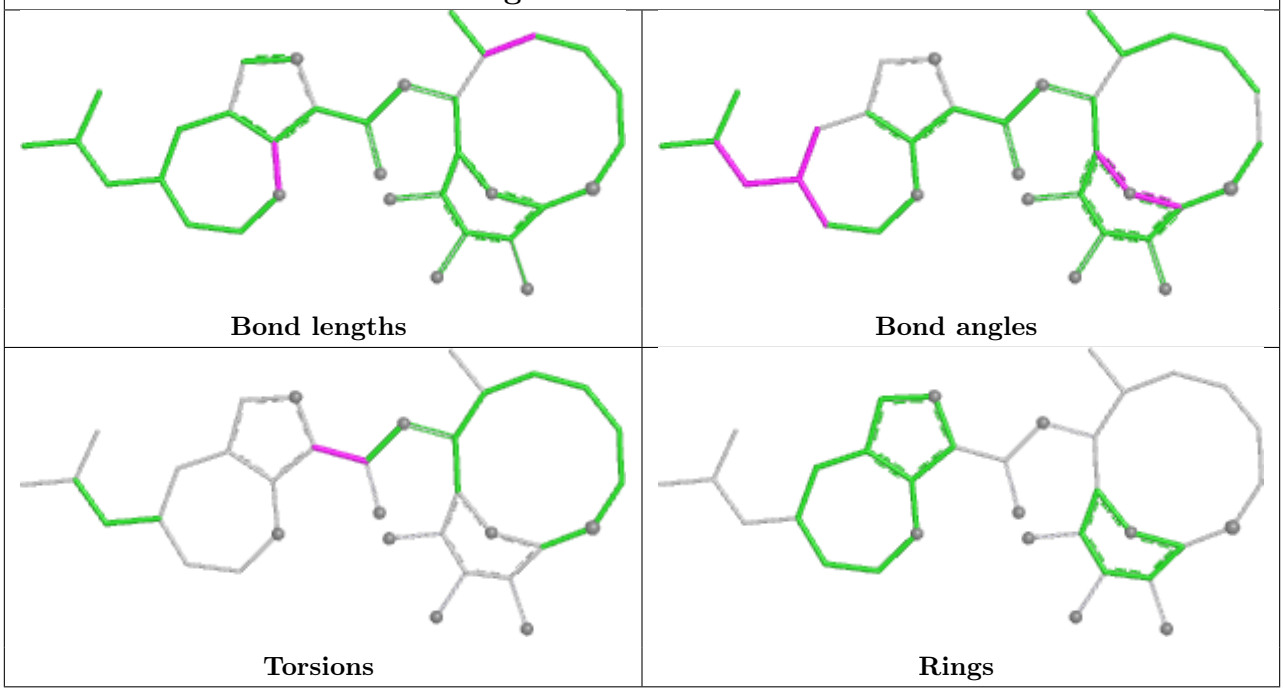
There are no ring outliers.

3 monomers are involved in 3 short contacts:

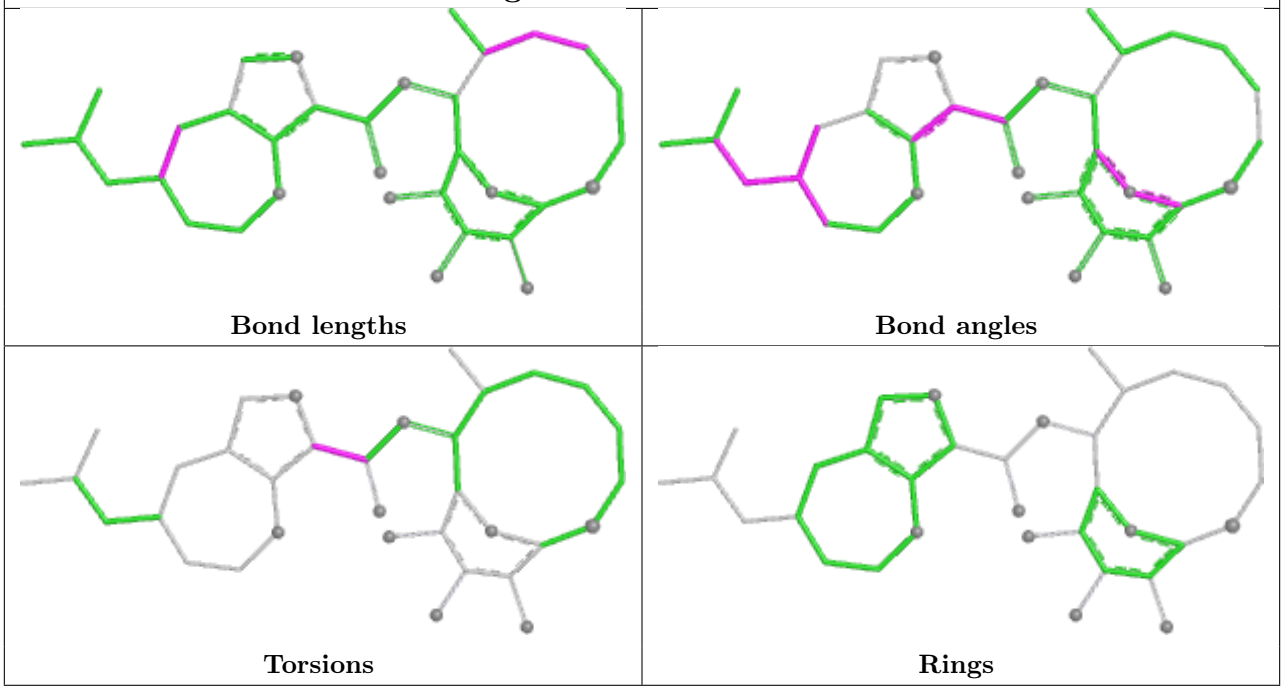
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	2A	3772	WC9	1	0
60	2d	302	SF4	1	0
58	1A	4061	WC9	1	0

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 WC9 2A 3772



Ligand WC9 1A 4061



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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%)	-0.54	119 (4%)	40	37	25, 41, 102, 117	0
1	2A	2789/2915 (95%)	-0.02	119 (4%)	40	36	36, 62, 101, 117	0
2	1B	120/121 (99%)	-0.35	0	100	100	37, 56, 70, 99	0
2	2B	120/121 (99%)	0.97	4 (3%)	49	45	69, 87, 93, 104	0
3	1D	275/276 (99%)	-0.26	4 (1%)	72	70	27, 40, 56, 86	0
3	2D	275/276 (99%)	0.08	3 (1%)	78	76	34, 53, 66, 88	0
4	1E	204/206 (99%)	-0.30	1 (0%)	87	86	25, 43, 64, 81	0
4	2E	204/206 (99%)	0.22	2 (0%)	79	78	39, 62, 77, 89	0
5	1F	203/210 (96%)	-0.10	1 (0%)	87	86	24, 47, 73, 94	0
5	2F	203/210 (96%)	0.45	2 (0%)	79	78	39, 73, 87, 94	0
6	1G	181/182 (99%)	0.55	11 (6%)	27	24	46, 66, 82, 96	0
6	2G	181/182 (99%)	1.39	40 (22%)	2	2	76, 87, 94, 103	0
7	1H	174/180 (96%)	0.17	2 (1%)	78	76	45, 59, 72, 81	0
7	2H	174/180 (96%)	1.28	30 (17%)	4	3	76, 90, 98, 103	0
8	1I	146/148 (98%)	0.73	7 (4%)	35	32	47, 79, 89, 93	0
8	2I	146/148 (98%)	0.83	7 (4%)	35	32	56, 79, 89, 93	0
9	1N	140/140 (100%)	-0.18	0	100	100	31, 43, 69, 82	0
9	2N	140/140 (100%)	0.51	5 (3%)	46	42	52, 69, 83, 93	0
10	1O	122/122 (100%)	-0.21	0	100	100	35, 45, 63, 67	0
10	2O	122/122 (100%)	0.24	0	100	100	49, 60, 75, 80	0
11	1P	149/150 (99%)	0.00	2 (1%)	75	73	27, 50, 74, 84	0
11	2P	149/150 (99%)	0.54	5 (3%)	48	44	43, 74, 91, 99	0
12	1Q	141/141 (100%)	-0.11	1 (0%)	84	83	33, 47, 63, 84	0
12	2Q	141/141 (100%)	1.00	19 (13%)	7	6	55, 73, 86, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.43	0	100	100	30, 39, 58, 66	0
13	2R	118/118 (100%)	0.11	0	100	100	43, 56, 68, 78	0
14	1S	110/112 (98%)	0.15	2 (1%)	67	65	46, 56, 70, 71	0
14	2S	110/112 (98%)	1.21	14 (12%)	8	7	71, 81, 90, 93	0
15	1T	131/146 (89%)	0.01	4 (3%)	51	48	38, 49, 77, 84	0
15	2T	131/146 (89%)	0.41	4 (3%)	51	48	54, 64, 83, 89	0
16	1U	116/118 (98%)	-0.49	1 (0%)	81	80	27, 35, 49, 70	0
16	2U	116/118 (98%)	0.49	1 (0%)	81	80	50, 66, 83, 89	0
17	1V	101/101 (100%)	-0.36	0	100	100	27, 45, 62, 73	0
17	2V	101/101 (100%)	0.67	1 (0%)	79	78	49, 77, 86, 97	0
18	1W	112/113 (99%)	-0.33	2 (1%)	67	65	26, 37, 56, 94	0
18	2W	112/113 (99%)	0.06	2 (1%)	67	65	44, 53, 74, 92	0
19	1X	95/96 (98%)	-0.14	2 (2%)	63	61	29, 44, 69, 87	0
19	2X	95/96 (98%)	0.56	5 (5%)	32	28	50, 65, 80, 93	0
20	1Y	107/110 (97%)	0.16	2 (1%)	66	63	42, 55, 76, 83	0
20	2Y	107/110 (97%)	1.14	17 (15%)	5	4	65, 78, 90, 100	0
21	1Z	154/206 (74%)	0.71	18 (11%)	9	7	48, 70, 94, 99	0
21	2Z	160/206 (77%)	1.65	40 (25%)	2	1	72, 89, 102, 106	0
22	10	83/85 (97%)	0.28	7 (8%)	17	14	34, 44, 76, 95	0
22	20	83/85 (97%)	1.25	11 (13%)	7	6	53, 71, 87, 96	0
23	11	97/98 (98%)	0.08	1 (1%)	79	78	34, 49, 76, 81	0
23	21	97/98 (98%)	0.39	1 (1%)	79	78	42, 59, 81, 84	0
24	12	70/72 (97%)	0.11	1 (1%)	73	72	41, 54, 66, 79	0
24	22	70/72 (97%)	0.62	0	100	100	64, 76, 86, 88	0
25	13	59/60 (98%)	-0.22	1 (1%)	69	67	31, 43, 66, 82	0
25	23	59/60 (98%)	0.67	4 (6%)	23	20	62, 71, 85, 94	0
26	14	69/71 (97%)	0.89	8 (11%)	9	8	59, 82, 99, 102	0
26	24	69/71 (97%)	1.73	22 (31%)	1	1	86, 94, 103, 104	0
27	15	59/60 (98%)	-0.46	1 (1%)	69	67	24, 37, 60, 66	0
27	25	59/60 (98%)	0.05	1 (1%)	69	67	40, 56, 72, 88	0
28	16	53/54 (98%)	-0.28	0	100	100	39, 47, 62, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.59	1 (1%) 66 63	57, 68, 76, 84	0
29	17	48/49 (97%)	-0.22	2 (4%) 40 37	28, 34, 64, 69	0
29	27	48/49 (97%)	0.07	2 (4%) 40 37	38, 44, 71, 78	0
30	18	64/65 (98%)	-0.37	0 100 100	31, 38, 47, 57	0
30	28	64/65 (98%)	0.47	1 (1%) 70 68	53, 59, 68, 74	0
31	19	37/37 (100%)	-0.29	0 100 100	36, 45, 63, 69	0
31	29	37/37 (100%)	1.05	3 (8%) 18 15	66, 73, 83, 89	0
32	1a	1488/1521 (97%)	0.28	61 (4%) 41 37	40, 71, 101, 118	0
32	2a	1491/1521 (98%)	0.76	166 (11%) 10 8	49, 82, 104, 116	0
33	1b	231/256 (90%)	1.10	32 (13%) 6 5	68, 85, 96, 101	0
33	2b	231/256 (90%)	1.70	72 (31%) 1 1	81, 93, 99, 105	0
34	1c	206/239 (86%)	0.84	12 (5%) 29 25	63, 77, 91, 98	0
34	2c	206/239 (86%)	1.86	90 (43%) 0 0	79, 92, 98, 101	0
35	1d	208/209 (99%)	0.96	15 (7%) 21 18	58, 75, 86, 90	0
35	2d	208/209 (99%)	0.82	10 (4%) 35 32	66, 75, 84, 92	0
36	1e	148/162 (91%)	0.50	2 (1%) 73 72	50, 68, 79, 87	0
36	2e	148/162 (91%)	1.22	20 (13%) 7 6	67, 82, 89, 96	0
37	1f	100/101 (99%)	0.58	3 (3%) 52 49	60, 72, 82, 85	0
37	2f	100/101 (99%)	0.66	3 (3%) 52 49	60, 73, 84, 89	0
38	1g	155/156 (99%)	0.68	9 (5%) 29 25	65, 75, 91, 95	0
38	2g	155/156 (99%)	1.05	17 (10%) 10 9	74, 85, 94, 98	0
39	1h	137/138 (99%)	0.48	2 (1%) 72 70	58, 71, 78, 84	0
39	2h	137/138 (99%)	1.14	12 (8%) 15 13	72, 82, 88, 94	0
40	1i	127/128 (99%)	1.14	19 (14%) 5 4	60, 82, 91, 94	0
40	2i	127/128 (99%)	1.75	43 (33%) 1 1	79, 91, 97, 100	0
41	1j	97/105 (92%)	1.23	14 (14%) 6 5	64, 83, 95, 100	0
41	2j	96/105 (91%)	2.29	55 (57%) 0 0	86, 93, 101, 103	0
42	1k	114/129 (88%)	0.57	4 (3%) 47 43	47, 70, 83, 90	0
42	2k	114/129 (88%)	0.77	8 (7%) 22 19	59, 78, 88, 94	0
43	1l	121/132 (91%)	0.25	5 (4%) 41 37	47, 58, 72, 79	0
43	2l	121/132 (91%)	0.99	12 (9%) 13 10	61, 75, 84, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.75	7 (5%)	29	26	60, 76, 86, 95	0
44	2m	122/126 (96%)	1.85	47 (38%)	1	0	77, 91, 97, 100	0
45	1n	60/61 (98%)	0.87	3 (5%)	34	30	63, 72, 80, 82	0
45	2n	60/61 (98%)	2.74	47 (78%)	0	0	85, 93, 97, 102	0
46	1o	88/89 (98%)	0.66	4 (4%)	38	34	52, 71, 81, 87	0
46	2o	88/89 (98%)	0.83	3 (3%)	48	44	64, 78, 86, 94	0
47	1p	82/88 (93%)	1.40	10 (12%)	8	7	61, 76, 85, 91	0
47	2p	82/88 (93%)	0.91	7 (8%)	16	14	63, 74, 84, 92	0
48	1q	99/105 (94%)	0.61	1 (1%)	79	78	58, 73, 83, 85	0
48	2q	99/105 (94%)	0.68	6 (6%)	27	24	69, 78, 88, 90	0
49	1r	68/88 (77%)	0.41	1 (1%)	72	70	61, 70, 84, 86	0
49	2r	68/88 (77%)	0.68	1 (1%)	72	70	62, 76, 87, 93	0
50	1s	83/93 (89%)	0.68	3 (3%)	46	42	69, 80, 88, 91	0
50	2s	83/93 (89%)	2.11	37 (44%)	0	0	87, 95, 100, 104	0
51	1t	96/106 (90%)	0.90	5 (5%)	33	29	65, 76, 85, 90	0
51	2t	96/106 (90%)	0.85	9 (9%)	14	12	63, 75, 89, 91	0
52	1u	23/27 (85%)	1.15	3 (13%)	7	6	68, 71, 78, 81	0
52	2u	23/27 (85%)	2.46	16 (69%)	0	0	82, 87, 94, 94	0
53	1v	13/24 (54%)	0.42	1 (7%)	19	17	52, 64, 85, 101	0
53	2v	13/24 (54%)	1.61	5 (38%)	1	0	73, 88, 100, 107	0
54	1w	65/76 (85%)	0.97	9 (13%)	6	5	65, 93, 107, 112	0
54	1y	67/76 (88%)	1.03	11 (16%)	4	4	43, 100, 108, 112	0
54	2w	63/76 (82%)	1.37	12 (19%)	3	3	86, 102, 111, 116	0
54	2y	66/76 (86%)	1.35	16 (24%)	2	1	59, 106, 111, 114	0
55	1x	71/77 (92%)	0.29	3 (4%)	40	37	33, 66, 90, 97	0
55	2x	71/77 (92%)	0.66	2 (2%)	55	51	49, 85, 97, 106	0
All	All	20869/21748 (95%)	0.37	1521 (7%)	21	18	24, 68, 97, 118	0

The worst 5 of 1521 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	10	6	GLY	8.5
45	1n	2	ALA	7.9

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Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	7.8
22	10	3	HIS	7.4
45	2n	2	ALA	7.3

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	PSU	2y	55	20/21	0.54	0.17	106,112,122,123	0
54	G7M	2w	46	24/25	0.57	0.16	92,104,115,130	0
54	4SU	2y	8	20/21	0.62	0.15	103,107,116,123	0
54	G7M	1w	46	24/25	0.62	0.18	81,92,115,135	0
54	G7M	2y	46	24/25	0.68	0.15	100,107,114,133	0
54	G7M	1y	46	24/25	0.68	0.15	96,105,111,121	0
54	5MU	2y	54	21/22	0.71	0.15	101,106,114,134	0
54	PSU	1y	55	20/21	0.71	0.15	96,104,113,126	0
54	MIA	2y	37	22/30	0.73	0.15	92,101,108,121	0
54	4SU	1y	8	20/21	0.75	0.13	96,103,106,113	0
54	5MU	1y	54	21/22	0.76	0.15	92,98,113,125	0
54	PSU	2y	32	20/21	0.76	0.14	89,97,108,112	0
54	PSU	2y	39	20/21	0.78	0.13	93,95,108,119	0
54	MIA	1y	37	22/30	0.79	0.14	89,94,98,103	0
54	PSU	1y	39	20/21	0.82	0.13	90,93,102,104	0
54	4SU	2w	8	20/21	0.82	0.12	98,101,108,119	0
54	MIA	2w	37	25/30	0.83	0.14	81,90,97,108	0
32	2MG	2a	1207	24/25	0.83	0.15	90,96,99,100	0
54	PSU	1w	55	20/21	0.83	0.11	73,88,94,96	0
54	PSU	2w	55	20/21	0.84	0.12	78,99,106,107	0
54	PSU	1y	32	20/21	0.86	0.11	90,93,105,107	0
54	5MU	2w	54	21/22	0.86	0.11	77,88,94,96	0
54	PSU	2w	32	20/21	0.88	0.11	91,96,106,114	0
54	4SU	1w	8	20/21	0.88	0.12	87,90,97,99	0
55	4SU	2x	8	20/21	0.89	0.12	81,88,93,95	0
55	5MU	2x	54	21/22	0.89	0.12	78,89,92,97	0
32	PSU	2a	516	20/21	0.89	0.11	80,87,91,91	0
43	0TD	2l	92	10/11	0.90	0.14	71,74,79,88	0
32	M2G	2a	966	25/26	0.91	0.18	67,76,90,98	0
55	PSU	2x	55	20/21	0.91	0.10	81,87,92,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MU	2A	1915	21/22	0.91	0.11	75,79,84,87	0
54	MIA	1w	37	29/30	0.92	0.14	54,64,77,101	0
32	5MC	2a	1404	21/22	0.92	0.11	56,61,70,74	0
55	5MC	2x	32	21/22	0.92	0.13	76,79,86,89	0
54	PSU	2w	39	20/21	0.92	0.08	79,91,95,96	0
32	G7M	2a	527	24/25	0.92	0.14	66,74,83,86	0
55	PSU	1x	55	20/21	0.92	0.11	68,73,85,86	0
55	5MU	1x	54	21/22	0.93	0.10	69,75,81,85	0
32	5MC	2a	967	21/22	0.93	0.14	71,79,91,92	0
54	5MU	1w	54	21/22	0.93	0.09	64,76,83,87	0
32	5MC	2a	1400	21/22	0.93	0.15	71,79,82,83	0
32	4OC	2a	1402	22/23	0.93	0.11	60,69,74,78	0
1	PSU	2A	1917	20/21	0.94	0.09	68,74,79,82	0
54	PSU	1w	32	20/21	0.94	0.11	73,78,87,88	0
43	0TD	1l	92	10/11	0.94	0.10	51,56,58,66	0
1	5MU	1A	1915	21/22	0.94	0.10	53,59,63,68	0
55	31H	2x	76	32/33	0.95	0.09	42,50,61,65	0
32	UR3	2a	1498	21/22	0.95	0.10	58,62,68,73	0
32	MA6	2a	1519	24/25	0.95	0.12	56,68,73,76	0
32	2MG	1a	1207	24/25	0.95	0.09	67,76,78,79	0
55	4SU	1x	8	20/21	0.95	0.09	55,68,73,77	0
55	5MC	1x	32	21/22	0.95	0.13	56,62,68,74	0
54	PSU	1w	39	20/21	0.95	0.08	69,75,83,87	0
1	PSU	2A	1911	20/21	0.95	0.08	65,69,75,79	0
32	MA6	2a	1518	24/25	0.96	0.11	55,69,74,76	0
1	2MA	2A	2503	23/24	0.96	0.10	33,42,46,48	0
1	PSU	1A	1917	20/21	0.96	0.08	48,55,60,63	0
32	MA6	1a	1519	24/25	0.96	0.09	39,46,49,52	0
32	PSU	1a	516	20/21	0.96	0.08	58,64,67,69	0
32	G7M	1a	527	24/25	0.96	0.09	44,52,61,64	0
32	M2G	1a	966	25/26	0.96	0.10	50,57,64,72	0
32	5MC	1a	967	21/22	0.96	0.09	49,57,67,68	0
1	OMC	2A	1920	21/22	0.96	0.09	53,67,71,72	0
1	5MC	2A	1942	21/22	0.96	0.09	50,60,63,66	0
1	OMG	2A	2251	24/25	0.96	0.08	41,45,49,51	0
1	PSU	1A	1911	20/21	0.97	0.07	43,50,53,53	0
1	5MU	1A	1939	21/22	0.97	0.07	27,33,37,39	0
1	5MU	2A	1939	21/22	0.97	0.08	35,40,45,54	0
32	5MC	1a	1400	21/22	0.97	0.09	46,54,56,59	0
1	5MC	2A	1962	21/22	0.97	0.07	41,53,59,65	0
32	5MC	1a	1404	21/22	0.97	0.07	37,41,46,47	0
32	5MC	2a	1407	21/22	0.97	0.10	56,60,66,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	5MC	1a	1407	21/22	0.97	0.07	32,42,46,49	0
32	MA6	1a	1518	24/25	0.97	0.08	36,43,49,51	0
1	5MC	1A	1942	21/22	0.97	0.08	37,42,46,49	0
32	4OC	1a	1402	22/23	0.98	0.07	43,46,51,62	0
1	OMU	1A	2552	21/22	0.98	0.07	28,32,37,42	0
1	OMU	2A	2552	21/22	0.98	0.07	41,47,50,56	0
1	PSU	2A	2605	20/21	0.98	0.06	37,41,47,50	0
1	PSU	1A	2605	20/21	0.98	0.06	27,31,35,38	0
32	UR3	1a	1498	21/22	0.98	0.06	38,44,50,53	0
1	OMC	1A	1920	21/22	0.98	0.07	37,47,51,54	0
1	5MC	1A	1962	21/22	0.98	0.06	33,42,49,56	0
55	31H	1x	76	32/33	0.98	0.07	22,32,39,45	10
1	2MA	1A	2503	23/24	0.99	0.05	24,27,32,33	0
1	OMG	1A	2251	24/25	0.99	0.05	26,30,34,36	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	221	1/1	0.37	0.26	84,84,84,84	0
56	MG	1A	4060	1/1	0.43	0.16	129,129,129,129	0
56	MG	1a	1671	1/1	0.47	0.32	80,80,80,80	0
56	MG	2i	202	1/1	0.50	0.36	88,88,88,88	0
56	MG	2A	3313	1/1	0.51	0.39	91,91,91,91	0
56	MG	2a	1758	1/1	0.51	0.38	83,83,83,83	0
56	MG	1B	229	1/1	0.51	0.18	86,86,86,86	0
56	MG	1A	3721	1/1	0.52	0.28	86,86,86,86	0
56	MG	2A	3589	1/1	0.57	0.20	83,83,83,83	0
56	MG	2A	3621	1/1	0.57	0.36	90,90,90,90	0
56	MG	2q	203	1/1	0.57	0.18	89,89,89,89	0
56	MG	2A	3257	1/1	0.58	0.27	81,81,81,81	0
56	MG	2a	1789	1/1	0.59	0.29	77,77,77,77	0
56	MG	1a	1803	1/1	0.59	0.22	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3861	1/1	0.59	0.25	62,62,62,62	0
56	MG	1A	3969	1/1	0.61	0.16	92,92,92,92	0
56	MG	2a	1642	1/1	0.61	0.32	89,89,89,89	0
56	MG	2A	3659	1/1	0.62	0.25	85,85,85,85	0
56	MG	2A	3676	1/1	0.63	0.29	60,60,60,60	0
56	MG	2A	3277	1/1	0.65	0.30	94,94,94,94	0
56	MG	2a	1790	1/1	0.65	0.22	85,85,85,85	0
56	MG	2A	3641	1/1	0.65	0.27	76,76,76,76	0
56	MG	2A	3278	1/1	0.65	0.28	91,91,91,91	0
56	MG	1A	3907	1/1	0.66	0.20	80,80,80,80	0
56	MG	2A	3762	1/1	0.66	0.29	78,78,78,78	0
56	MG	1a	1712	1/1	0.67	0.34	86,86,86,86	0
56	MG	1a	1660	1/1	0.67	0.28	87,87,87,87	0
56	MG	2a	1708	1/1	0.67	0.39	91,91,91,91	0
56	MG	2A	3168	1/1	0.67	0.30	81,81,81,81	0
56	MG	2G	201	1/1	0.68	0.22	81,81,81,81	0
56	MG	2A	3300	1/1	0.68	0.27	74,74,74,74	0
56	MG	1A	3956	1/1	0.68	0.19	76,76,76,76	0
56	MG	2A	3455	1/1	0.68	0.29	71,71,71,71	0
56	MG	2A	3569	1/1	0.69	0.28	68,68,68,68	0
56	MG	1A	3757	1/1	0.69	0.12	83,83,83,83	0
56	MG	2A	3742	1/1	0.69	0.29	81,81,81,81	0
56	MG	2a	1779	1/1	0.69	0.36	77,77,77,77	0
56	MG	1a	1753	1/1	0.69	0.31	81,81,81,81	0
56	MG	2B	214	1/1	0.69	0.36	84,84,84,84	0
56	MG	2F	305	1/1	0.69	0.25	78,78,78,78	0
56	MG	2A	3256	1/1	0.69	0.19	83,83,83,83	0
56	MG	1a	1732	1/1	0.70	0.25	90,90,90,90	0
56	MG	2a	1713	1/1	0.70	0.27	87,87,87,87	0
56	MG	2A	3599	1/1	0.70	0.25	61,61,61,61	0
56	MG	2A	3258	1/1	0.70	0.31	77,77,77,77	0
56	MG	2B	216	1/1	0.70	0.28	74,74,74,74	0
56	MG	2A	3238	1/1	0.70	0.17	66,66,66,66	0
56	MG	2A	3015	1/1	0.70	0.36	85,85,85,85	0
56	MG	2A	3582	1/1	0.70	0.40	81,81,81,81	0
56	MG	1A	4005	1/1	0.71	0.17	67,67,67,67	0
56	MG	2A	3162	1/1	0.71	0.27	87,87,87,87	0
56	MG	2A	3167	1/1	0.71	0.22	61,61,61,61	0
56	MG	2A	3692	1/1	0.71	0.28	91,91,91,91	0
56	MG	28	102	1/1	0.71	0.39	71,71,71,71	0
56	MG	1A	3472	1/1	0.71	0.15	74,74,74,74	0
56	MG	2A	3276	1/1	0.71	0.40	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4034	1/1	0.72	0.21	83,83,83,83	0
56	MG	2A	3080	1/1	0.72	0.26	83,83,83,83	0
56	MG	1A	3955	1/1	0.72	0.22	88,88,88,88	0
56	MG	1a	1793	1/1	0.72	0.21	76,76,76,76	0
56	MG	2A	3424	1/1	0.72	0.30	76,76,76,76	0
56	MG	2a	1698	1/1	0.72	0.31	91,91,91,91	0
56	MG	2j	201	1/1	0.72	0.17	81,81,81,81	0
56	MG	1B	232	1/1	0.72	0.34	89,89,89,89	0
56	MG	1B	215	1/1	0.73	0.25	68,68,68,68	0
56	MG	1A	3490	1/1	0.73	0.28	65,65,65,65	0
56	MG	2A	3022	1/1	0.73	0.29	81,81,81,81	0
56	MG	2A	3193	1/1	0.73	0.26	79,79,79,79	0
56	MG	2A	3235	1/1	0.73	0.39	80,80,80,80	0
56	MG	2i	201	1/1	0.73	0.25	85,85,85,85	0
56	MG	1a	1649	1/1	0.73	0.33	83,83,83,83	0
56	MG	2a	1706	1/1	0.73	0.35	79,79,79,79	0
56	MG	2A	3081	1/1	0.73	0.18	75,75,75,75	0
56	MG	2v	101	1/1	0.73	0.37	87,87,87,87	0
56	MG	1x	107	1/1	0.74	0.24	86,86,86,86	0
56	MG	1A	3277	1/1	0.74	0.18	50,50,50,50	0
56	MG	2B	218	1/1	0.74	0.27	80,80,80,80	0
56	MG	1a	1759	1/1	0.74	0.23	87,87,87,87	0
56	MG	2A	3184	1/1	0.74	0.34	82,82,82,82	0
56	MG	2a	1796	1/1	0.74	0.23	91,91,91,91	0
56	MG	2a	1797	1/1	0.74	0.36	81,81,81,81	0
56	MG	1A	4052	1/1	0.74	0.25	84,84,84,84	0
56	MG	2A	3577	1/1	0.74	0.35	87,87,87,87	0
56	MG	2A	3231	1/1	0.74	0.27	85,85,85,85	0
56	MG	1A	3823	1/1	0.74	0.32	46,46,46,46	0
56	MG	2A	3768	1/1	0.74	0.15	89,89,89,89	0
56	MG	2V	202	1/1	0.75	0.23	72,72,72,72	0
56	MG	1A	3838	1/1	0.75	0.22	62,62,62,62	0
56	MG	2a	1608	1/1	0.75	0.29	77,77,77,77	0
56	MG	1a	1691	1/1	0.75	0.24	80,80,80,80	0
56	MG	2a	1672	1/1	0.75	0.34	78,78,78,78	0
56	MG	2A	3620	1/1	0.75	0.17	94,94,94,94	0
56	MG	1A	3847	1/1	0.75	0.18	43,43,43,43	0
56	MG	2A	3267	1/1	0.75	0.23	68,68,68,68	0
56	MG	2A	3160	1/1	0.75	0.29	71,71,71,71	0
56	MG	1a	1716	1/1	0.75	0.41	76,76,76,76	0
56	MG	1A	4001	1/1	0.75	0.17	83,83,83,83	0
56	MG	1B	226	1/1	0.75	0.22	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3332	1/1	0.75	0.23	65,65,65,65	0
56	MG	2A	3321	1/1	0.75	0.21	80,80,80,80	0
56	MG	2B	203	1/1	0.75	0.33	86,86,86,86	0
56	MG	1A	4026	1/1	0.75	0.23	53,53,53,53	0
56	MG	11	102	1/1	0.75	0.20	56,56,56,56	0
56	MG	1A	3812	1/1	0.75	0.15	69,69,69,69	0
56	MG	2A	3236	1/1	0.75	0.18	91,91,91,91	0
56	MG	1A	3208	1/1	0.75	0.22	76,76,76,76	0
56	MG	2A	3618	1/1	0.76	0.20	71,71,71,71	0
56	MG	2a	1602	1/1	0.76	0.23	88,88,88,88	0
56	MG	1A	3094	1/1	0.76	0.24	69,69,69,69	0
56	MG	2a	1617	1/1	0.76	0.20	79,79,79,79	0
56	MG	2A	3340	1/1	0.76	0.42	73,73,73,73	0
56	MG	1a	1799	1/1	0.76	0.21	75,75,75,75	0
56	MG	2a	1683	1/1	0.76	0.28	88,88,88,88	0
56	MG	1B	222	1/1	0.76	0.20	69,69,69,69	0
56	MG	2a	1701	1/1	0.76	0.26	85,85,85,85	0
56	MG	2A	3462	1/1	0.76	0.21	69,69,69,69	0
56	MG	2A	3501	1/1	0.76	0.17	80,80,80,80	0
56	MG	2A	3725	1/1	0.76	0.20	68,68,68,68	0
56	MG	2A	3511	1/1	0.76	0.28	72,72,72,72	0
56	MG	2a	1772	1/1	0.76	0.30	82,82,82,82	0
56	MG	2A	3552	1/1	0.76	0.21	69,69,69,69	0
56	MG	2A	3240	1/1	0.76	0.26	68,68,68,68	0
56	MG	2A	3242	1/1	0.76	0.26	82,82,82,82	0
56	MG	2a	1794	1/1	0.76	0.25	83,83,83,83	0
56	MG	2A	3290	1/1	0.76	0.31	82,82,82,82	0
56	MG	2A	3587	1/1	0.76	0.14	62,62,62,62	0
56	MG	1A	3781	1/1	0.76	0.30	74,74,74,74	0
56	MG	2B	220	1/1	0.76	0.19	77,77,77,77	0
56	MG	1a	1783	1/1	0.76	0.24	70,70,70,70	0
56	MG	2A	3603	1/1	0.76	0.19	77,77,77,77	0
56	MG	2A	3617	1/1	0.76	0.24	77,77,77,77	0
56	MG	2y	101	1/1	0.76	0.12	99,99,99,99	0
56	MG	2A	3055	1/1	0.77	0.30	78,78,78,78	0
56	MG	2E	301	1/1	0.77	0.28	75,75,75,75	0
56	MG	2a	1724	1/1	0.77	0.37	78,78,78,78	0
56	MG	2a	1737	1/1	0.77	0.11	78,78,78,78	0
56	MG	2A	3640	1/1	0.77	0.19	74,74,74,74	0
56	MG	2a	1771	1/1	0.77	0.20	73,73,73,73	0
56	MG	1A	4032	1/1	0.77	0.25	82,82,82,82	0
56	MG	1a	1789	1/1	0.77	0.24	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3091	1/1	0.77	0.36	85,85,85,85	0
56	MG	2A	3109	1/1	0.77	0.34	78,78,78,78	0
56	MG	1A	3828	1/1	0.77	0.23	81,81,81,81	0
56	MG	1a	1724	1/1	0.77	0.25	69,69,69,69	0
56	MG	1A	3547	1/1	0.77	0.32	56,56,56,56	0
56	MG	2a	1643	1/1	0.77	0.17	79,79,79,79	0
56	MG	2A	3601	1/1	0.77	0.21	82,82,82,82	0
56	MG	1A	3843	1/1	0.77	0.26	76,76,76,76	0
56	MG	1A	3181	1/1	0.77	0.27	63,63,63,63	0
56	MG	2A	3476	1/1	0.77	0.21	56,56,56,56	0
56	MG	1a	1762	1/1	0.77	0.21	82,82,82,82	0
56	MG	1A	3470	1/1	0.78	0.25	79,79,79,79	0
56	MG	1A	3927	1/1	0.78	0.24	82,82,82,82	0
56	MG	1A	3744	1/1	0.78	0.13	28,28,28,28	0
56	MG	2a	1709	1/1	0.78	0.46	73,73,73,73	0
56	MG	2A	3200	1/1	0.78	0.31	79,79,79,79	0
56	MG	2A	3219	1/1	0.78	0.18	77,77,77,77	0
56	MG	2A	3298	1/1	0.78	0.20	75,75,75,75	0
56	MG	2A	3224	1/1	0.78	0.35	76,76,76,76	0
56	MG	15	107	1/1	0.78	0.14	59,59,59,59	0
56	MG	2A	3319	1/1	0.78	0.14	75,75,75,75	0
56	MG	1A	3274	1/1	0.78	0.20	75,75,75,75	0
56	MG	1A	3775	1/1	0.78	0.20	62,62,62,62	0
56	MG	1A	3231	1/1	0.78	0.21	71,71,71,71	0
56	MG	2A	3634	1/1	0.78	0.28	70,70,70,70	0
56	MG	1A	3242	1/1	0.78	0.16	55,55,55,55	0
56	MG	2A	3141	1/1	0.78	0.19	62,62,62,62	0
56	MG	2a	1630	1/1	0.78	0.41	82,82,82,82	0
56	MG	2A	3247	1/1	0.78	0.32	72,72,72,72	0
56	MG	1a	1794	1/1	0.78	0.19	64,64,64,64	0
56	MG	1A	3866	1/1	0.78	0.14	54,54,54,54	0
56	MG	2A	3529	1/1	0.78	0.31	71,71,71,71	0
56	MG	1B	228	1/1	0.78	0.14	80,80,80,80	0
56	MG	2a	1670	1/1	0.79	0.30	83,83,83,83	0
56	MG	2A	3005	1/1	0.79	0.37	69,69,69,69	0
56	MG	1A	3933	1/1	0.79	0.14	70,70,70,70	0
56	MG	2A	3199	1/1	0.79	0.23	67,67,67,67	0
56	MG	1a	1629	1/1	0.79	0.34	69,69,69,69	0
56	MG	2A	3583	1/1	0.79	0.20	88,88,88,88	0
56	MG	2B	211	1/1	0.79	0.30	84,84,84,84	0
56	MG	1a	1757	1/1	0.79	0.25	78,78,78,78	0
56	MG	1a	1638	1/1	0.79	0.29	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3718	1/1	0.79	0.14	33,33,33,33	0
56	MG	1A	3765	1/1	0.79	0.31	69,69,69,69	0
56	MG	2D	306	1/1	0.79	0.28	71,71,71,71	0
56	MG	1A	4045	1/1	0.79	0.30	75,75,75,75	0
56	MG	2A	3122	1/1	0.79	0.20	73,73,73,73	0
56	MG	2A	3407	1/1	0.79	0.27	86,86,86,86	0
56	MG	2A	3135	1/1	0.79	0.32	81,81,81,81	0
56	MG	1a	1688	1/1	0.79	0.32	81,81,81,81	0
56	MG	2A	3155	1/1	0.79	0.49	81,81,81,81	0
56	MG	2a	1607	1/1	0.79	0.33	86,86,86,86	0
56	MG	1A	3619	1/1	0.79	0.23	67,67,67,67	0
56	MG	1A	3683	1/1	0.79	0.21	58,58,58,58	0
56	MG	1A	3782	1/1	0.79	0.20	62,62,62,62	0
56	MG	2a	1641	1/1	0.79	0.21	72,72,72,72	0
56	MG	14	101	1/1	0.79	0.22	83,83,83,83	0
56	MG	2A	3545	1/1	0.79	0.21	76,76,76,76	0
56	MG	2a	1668	1/1	0.79	0.29	71,71,71,71	0
56	MG	1A	3088	1/1	0.80	0.18	71,71,71,71	0
56	MG	1A	3392	1/1	0.80	0.22	65,65,65,65	0
56	MG	2A	3306	1/1	0.80	0.26	73,73,73,73	0
56	MG	2A	3309	1/1	0.80	0.24	82,82,82,82	0
56	MG	2A	3607	1/1	0.80	0.15	71,71,71,71	0
56	MG	2A	3312	1/1	0.80	0.30	72,72,72,72	0
56	MG	1a	1664	1/1	0.80	0.21	63,63,63,63	0
56	MG	2A	3619	1/1	0.80	0.14	89,89,89,89	0
56	MG	2A	3318	1/1	0.80	0.20	77,77,77,77	0
56	MG	1a	1767	1/1	0.80	0.27	73,73,73,73	0
56	MG	2A	3626	1/1	0.80	0.20	75,75,75,75	0
56	MG	2a	1678	1/1	0.80	0.32	84,84,84,84	0
56	MG	1A	3426	1/1	0.80	0.31	81,81,81,81	0
56	MG	2a	1692	1/1	0.80	0.15	80,80,80,80	0
56	MG	2A	3324	1/1	0.80	0.24	64,64,64,64	0
56	MG	1A	4042	1/1	0.80	0.17	75,75,75,75	0
56	MG	2A	3647	1/1	0.80	0.15	61,61,61,61	0
56	MG	2A	3343	1/1	0.80	0.41	65,65,65,65	0
56	MG	2A	3667	1/1	0.80	0.22	60,60,60,60	0
56	MG	1A	3976	1/1	0.80	0.18	71,71,71,71	0
56	MG	2a	1714	1/1	0.80	0.27	78,78,78,78	0
56	MG	1a	1693	1/1	0.80	0.33	73,73,73,73	0
56	MG	2a	1735	1/1	0.80	0.25	80,80,80,80	0
56	MG	2A	3143	1/1	0.80	0.24	77,77,77,77	0
56	MG	2a	1744	1/1	0.80	0.31	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1756	1/1	0.80	0.24	76,76,76,76	0
56	MG	2A	3243	1/1	0.80	0.26	80,80,80,80	0
56	MG	2A	3467	1/1	0.80	0.31	68,68,68,68	0
56	MG	1A	4050	1/1	0.80	0.23	78,78,78,78	0
56	MG	2A	3488	1/1	0.80	0.24	56,56,56,56	0
56	MG	1A	3983	1/1	0.80	0.15	64,64,64,64	0
56	MG	2A	3508	1/1	0.80	0.21	86,86,86,86	0
56	MG	2A	3161	1/1	0.80	0.30	74,74,74,74	0
56	MG	1x	101	1/1	0.80	0.21	80,80,80,80	0
56	MG	2A	3263	1/1	0.80	0.19	70,70,70,70	0
56	MG	2a	1812	1/1	0.80	0.41	85,85,85,85	0
56	MG	1A	3574	1/1	0.80	0.15	65,65,65,65	0
56	MG	1x	108	1/1	0.80	0.36	83,83,83,83	0
56	MG	1A	3252	1/1	0.80	0.17	76,76,76,76	0
56	MG	1a	1750	1/1	0.80	0.34	73,73,73,73	0
56	MG	1A	4020	1/1	0.80	0.15	60,60,60,60	0
56	MG	2A	3297	1/1	0.80	0.34	76,76,76,76	0
56	MG	2A	3170	1/1	0.81	0.17	66,66,66,66	0
56	MG	2A	3635	1/1	0.81	0.15	53,53,53,53	0
56	MG	2A	3472	1/1	0.81	0.18	54,54,54,54	0
56	MG	2a	1657	1/1	0.81	0.19	72,72,72,72	0
56	MG	1x	112	1/1	0.81	0.33	83,83,83,83	0
56	MG	2A	3485	1/1	0.81	0.19	55,55,55,55	0
56	MG	2A	3655	1/1	0.81	0.10	86,86,86,86	0
56	MG	2A	3658	1/1	0.81	0.17	88,88,88,88	0
56	MG	1P	205	1/1	0.81	0.13	65,65,65,65	0
56	MG	2A	3197	1/1	0.81	0.21	68,68,68,68	0
56	MG	2a	1697	1/1	0.81	0.22	82,82,82,82	0
56	MG	1A	3291	1/1	0.81	0.32	66,66,66,66	0
56	MG	2A	3680	1/1	0.81	0.24	86,86,86,86	0
56	MG	1A	3458	1/1	0.81	0.20	57,57,57,57	0
56	MG	1A	3763	1/1	0.81	0.25	78,78,78,78	0
56	MG	2A	3532	1/1	0.81	0.21	74,74,74,74	0
56	MG	2A	3746	1/1	0.81	0.24	78,78,78,78	0
56	MG	1a	1602	1/1	0.81	0.39	79,79,79,79	0
56	MG	2A	3763	1/1	0.81	0.28	72,72,72,72	0
56	MG	2a	1733	1/1	0.81	0.33	80,80,80,80	0
56	MG	1A	3317	1/1	0.81	0.29	69,69,69,69	0
56	MG	1A	3773	1/1	0.81	0.17	66,66,66,66	0
56	MG	1A	3053	1/1	0.81	0.17	59,59,59,59	0
56	MG	2A	3317	1/1	0.81	0.18	87,87,87,87	0
56	MG	1A	3707	1/1	0.81	0.24	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1759	1/1	0.81	0.36	76,76,76,76	0
56	MG	1A	3026	1/1	0.81	0.20	64,64,64,64	0
56	MG	1a	1665	1/1	0.81	0.31	71,71,71,71	0
56	MG	2a	1774	1/1	0.81	0.20	70,70,70,70	0
56	MG	1a	1666	1/1	0.81	0.34	69,69,69,69	0
56	MG	2a	1784	1/1	0.81	0.27	80,80,80,80	0
56	MG	2a	1785	1/1	0.81	0.30	80,80,80,80	0
56	MG	1A	3914	1/1	0.81	0.23	63,63,63,63	0
56	MG	2A	3342	1/1	0.81	0.29	74,74,74,74	0
56	MG	1a	1684	1/1	0.81	0.31	58,58,58,58	0
56	MG	2A	3611	1/1	0.81	0.14	80,80,80,80	0
56	MG	2W	202	1/1	0.81	0.22	80,80,80,80	0
56	MG	2a	1802	1/1	0.81	0.26	76,76,76,76	0
56	MG	2A	3353	1/1	0.81	0.24	67,67,67,67	0
56	MG	2g	201	1/1	0.81	0.24	80,80,80,80	0
56	MG	2A	3390	1/1	0.81	0.23	75,75,75,75	0
56	MG	1A	3540	1/1	0.81	0.15	42,42,42,42	0
56	MG	1A	3819	1/1	0.81	0.12	70,70,70,70	0
56	MG	1A	4039	1/1	0.81	0.14	77,77,77,77	0
56	MG	2a	1629	1/1	0.81	0.39	69,69,69,69	0
56	MG	1D	308	1/1	0.81	0.15	60,60,60,60	0
56	MG	1a	1640	1/1	0.82	0.34	78,78,78,78	0
56	MG	2A	3177	1/1	0.82	0.33	81,81,81,81	0
56	MG	2a	1635	1/1	0.82	0.29	73,73,73,73	0
56	MG	1A	4054	1/1	0.82	0.28	65,65,65,65	0
56	MG	2A	3188	1/1	0.82	0.12	66,66,66,66	0
56	MG	1A	3987	1/1	0.82	0.22	62,62,62,62	0
56	MG	2a	1651	1/1	0.82	0.29	77,77,77,77	0
56	MG	1B	201	1/1	0.82	0.21	68,68,68,68	0
56	MG	2a	1666	1/1	0.82	0.20	83,83,83,83	0
56	MG	2A	3625	1/1	0.82	0.22	79,79,79,79	0
56	MG	1A	3904	1/1	0.82	0.21	76,76,76,76	0
56	MG	1a	1806	1/1	0.82	0.18	64,64,64,64	0
56	MG	2A	3347	1/1	0.82	0.44	71,71,71,71	0
56	MG	1l	201	1/1	0.82	0.21	82,82,82,82	0
56	MG	2A	3362	1/1	0.82	0.23	60,60,60,60	0
56	MG	2A	3385	1/1	0.82	0.18	73,73,73,73	0
56	MG	1A	4003	1/1	0.82	0.23	64,64,64,64	0
56	MG	1A	3328	1/1	0.82	0.36	67,67,67,67	0
56	MG	2a	1704	1/1	0.82	0.29	80,80,80,80	0
56	MG	1A	4006	1/1	0.82	0.22	50,50,50,50	0
56	MG	1A	3474	1/1	0.82	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1690	1/1	0.82	0.61	77,77,77,77	0
56	MG	1A	4021	1/1	0.82	0.10	60,60,60,60	0
56	MG	2A	3684	1/1	0.82	0.14	62,62,62,62	0
56	MG	1B	231	1/1	0.82	0.24	71,71,71,71	0
56	MG	2A	3709	1/1	0.82	0.26	70,70,70,70	0
56	MG	2A	3029	1/1	0.82	0.12	61,61,61,61	0
56	MG	2A	3038	1/1	0.82	0.39	74,74,74,74	0
56	MG	2a	1742	1/1	0.82	0.14	100,100,100,100	0
56	MG	2a	1743	1/1	0.82	0.30	81,81,81,81	0
56	MG	1a	1700	1/1	0.82	0.15	74,74,74,74	0
56	MG	2A	3070	1/1	0.82	0.21	63,63,63,63	0
56	MG	2A	3507	1/1	0.82	0.19	72,72,72,72	0
56	MG	1a	1701	1/1	0.82	0.32	70,70,70,70	0
56	MG	1a	1704	1/1	0.82	0.36	77,77,77,77	0
56	MG	2A	3527	1/1	0.82	0.30	86,86,86,86	0
56	MG	2a	1773	1/1	0.82	0.27	84,84,84,84	0
56	MG	2B	212	1/1	0.82	0.23	89,89,89,89	0
56	MG	1A	3307	1/1	0.82	0.22	65,65,65,65	0
56	MG	1A	3928	1/1	0.82	0.16	83,83,83,83	0
56	MG	1E	315	1/1	0.82	0.16	71,71,71,71	0
56	MG	1A	4033	1/1	0.82	0.22	80,80,80,80	0
56	MG	2D	305	1/1	0.82	0.40	55,55,55,55	0
56	MG	2A	3279	1/1	0.82	0.18	89,89,89,89	0
56	MG	2A	3573	1/1	0.82	0.17	70,70,70,70	0
56	MG	2A	3285	1/1	0.82	0.36	75,75,75,75	0
56	MG	1A	3534	1/1	0.82	0.20	76,76,76,76	0
56	MG	1A	3355	1/1	0.82	0.17	58,58,58,58	0
56	MG	1A	3375	1/1	0.82	0.22	69,69,69,69	0
56	MG	18	106	1/1	0.82	0.21	78,78,78,78	0
56	MG	1A	3572	1/1	0.82	0.32	73,73,73,73	0
56	MG	1a	1764	1/1	0.82	0.19	80,80,80,80	0
56	MG	1A	3787	1/1	0.82	0.23	76,76,76,76	0
56	MG	1A	3804	1/1	0.82	0.18	68,68,68,68	0
56	MG	2x	103	1/1	0.82	0.39	89,89,89,89	0
56	MG	2a	1620	1/1	0.82	0.35	73,73,73,73	0
56	MG	2y	102	1/1	0.82	0.23	88,88,88,88	0
56	MG	1A	3379	1/1	0.83	0.45	49,49,49,49	0
56	MG	2A	3287	1/1	0.83	0.19	70,70,70,70	0
56	MG	2A	3205	1/1	0.83	0.21	78,78,78,78	0
56	MG	2A	3294	1/1	0.83	0.22	62,62,62,62	0
56	MG	2A	3212	1/1	0.83	0.24	85,85,85,85	0
56	MG	1F	310	1/1	0.83	0.21	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1F	312	1/1	0.83	0.29	67,67,67,67	0
56	MG	1a	1648	1/1	0.83	0.31	76,76,76,76	0
56	MG	2A	3234	1/1	0.83	0.30	83,83,83,83	0
56	MG	1A	3192	1/1	0.83	0.17	58,58,58,58	0
56	MG	1A	3901	1/1	0.83	0.14	38,38,38,38	0
56	MG	2A	3522	1/1	0.83	0.16	74,74,74,74	0
56	MG	1a	1661	1/1	0.83	0.15	68,68,68,68	0
56	MG	1a	1707	1/1	0.83	0.29	63,63,63,63	0
56	MG	12	101	1/1	0.83	0.16	61,61,61,61	0
56	MG	2a	1764	1/1	0.83	0.19	53,53,53,53	0
56	MG	2A	3031	1/1	0.83	0.17	58,58,58,58	0
56	MG	2a	1633	1/1	0.83	0.38	74,74,74,74	0
56	MG	1A	3578	1/1	0.83	0.21	64,64,64,64	0
56	MG	2a	1637	1/1	0.83	0.27	75,75,75,75	0
56	MG	2A	3333	1/1	0.83	0.45	68,68,68,68	0
56	MG	2A	3337	1/1	0.83	0.18	65,65,65,65	0
56	MG	2A	3248	1/1	0.83	0.24	79,79,79,79	0
56	MG	2a	1648	1/1	0.83	0.16	90,90,90,90	0
56	MG	2A	3169	1/1	0.83	0.25	75,75,75,75	0
56	MG	2A	3044	1/1	0.83	0.14	68,68,68,68	0
56	MG	1A	3423	1/1	0.83	0.18	40,40,40,40	0
56	MG	1a	1800	1/1	0.83	0.33	80,80,80,80	0
56	MG	2A	3764	1/1	0.83	0.15	79,79,79,79	0
56	MG	2a	1811	1/1	0.83	0.30	91,91,91,91	0
56	MG	1A	3338	1/1	0.83	0.16	63,63,63,63	0
56	MG	2a	1677	1/1	0.83	0.36	78,78,78,78	0
56	MG	2A	3375	1/1	0.83	0.17	63,63,63,63	0
56	MG	2a	1682	1/1	0.83	0.27	80,80,80,80	0
56	MG	2A	3383	1/1	0.83	0.18	74,74,74,74	0
56	MG	1A	3857	1/1	0.83	0.10	52,52,52,52	0
56	MG	1a	1807	1/1	0.83	0.24	78,78,78,78	0
56	MG	2A	3198	1/1	0.83	0.31	75,75,75,75	0
56	MG	2B	217	1/1	0.83	0.33	79,79,79,79	0
56	MG	2A	3100	1/1	0.83	0.28	90,90,90,90	0
56	MG	2a	1686	1/1	0.84	0.23	79,79,79,79	0
56	MG	1A	3799	1/1	0.84	0.30	71,71,71,71	0
56	MG	2B	213	1/1	0.84	0.34	79,79,79,79	0
56	MG	1A	3263	1/1	0.84	0.20	65,65,65,65	0
56	MG	2A	3613	1/1	0.84	0.17	75,75,75,75	0
56	MG	1A	3805	1/1	0.84	0.21	64,64,64,64	0
56	MG	2A	3083	1/1	0.84	0.20	55,55,55,55	0
56	MG	1A	3309	1/1	0.84	0.19	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	1A	3024	1/1	0.84	0.28	69,69,69,69	0
56	MG	1a	1605	1/1	0.84	0.13	67,67,67,67	0
56	MG	1A	3822	1/1	0.84	0.19	72,72,72,72	0
56	MG	2E	303	1/1	0.84	0.13	70,70,70,70	0
56	MG	2a	1725	1/1	0.84	0.36	71,71,71,71	0
56	MG	1a	1632	1/1	0.84	0.19	79,79,79,79	0
56	MG	2A	3497	1/1	0.84	0.25	47,47,47,47	0
56	MG	2A	3311	1/1	0.84	0.17	65,65,65,65	0
56	MG	2A	3140	1/1	0.84	0.21	71,71,71,71	0
56	MG	20	101	1/1	0.84	0.28	62,62,62,62	0
56	MG	1A	3163	1/1	0.84	0.26	73,73,73,73	0
56	MG	2A	3643	1/1	0.84	0.29	77,77,77,77	0
56	MG	1a	1713	1/1	0.84	0.41	80,80,80,80	0
56	MG	2A	3516	1/1	0.84	0.23	78,78,78,78	0
56	MG	2a	1615	1/1	0.84	0.29	80,80,80,80	0
56	MG	2a	1770	1/1	0.84	0.18	88,88,88,88	0
56	MG	1A	3167	1/1	0.84	0.31	47,47,47,47	0
56	MG	2a	1619	1/1	0.84	0.16	78,78,78,78	0
56	MG	1A	3943	1/1	0.84	0.16	47,47,47,47	0
56	MG	2a	1626	1/1	0.84	0.36	72,72,72,72	0
56	MG	2a	1776	1/1	0.84	0.36	82,82,82,82	0
56	MG	1A	3949	1/1	0.84	0.18	37,37,37,37	0
56	MG	2a	1783	1/1	0.84	0.18	77,77,77,77	0
56	MG	2A	3003	1/1	0.84	0.36	72,72,72,72	0
56	MG	2a	1632	1/1	0.84	0.28	71,71,71,71	0
56	MG	1a	1653	1/1	0.84	0.33	78,78,78,78	0
56	MG	1A	3700	1/1	0.84	0.16	53,53,53,53	0
56	MG	2A	3687	1/1	0.84	0.26	87,87,87,87	0
56	MG	1A	3292	1/1	0.84	0.20	76,76,76,76	0
56	MG	2A	3700	1/1	0.84	0.14	54,54,54,54	0
56	MG	1A	3844	1/1	0.84	0.15	30,30,30,30	0
56	MG	2a	1804	1/1	0.84	0.28	71,71,71,71	0
56	MG	2A	3576	1/1	0.84	0.15	76,76,76,76	0
56	MG	2A	3737	1/1	0.84	0.20	74,74,74,74	0
56	MG	2A	3174	1/1	0.84	0.25	70,70,70,70	0
56	MG	1A	3544	1/1	0.84	0.32	71,71,71,71	0
56	MG	2A	3273	1/1	0.84	0.19	68,68,68,68	0
56	MG	1O	205	1/1	0.84	0.13	73,73,73,73	0
56	MG	1A	3783	1/1	0.84	0.11	46,46,46,46	0
56	MG	1A	3349	1/1	0.84	0.15	72,72,72,72	0
56	MG	2A	3058	1/1	0.84	0.30	73,73,73,73	0
56	MG	2B	204	1/1	0.84	0.19	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3283	1/1	0.84	0.23	75,75,75,75	0
56	MG	2A	3307	1/1	0.85	0.28	79,79,79,79	0
56	MG	1A	3378	1/1	0.85	0.31	71,71,71,71	0
56	MG	2a	1631	1/1	0.85	0.36	80,80,80,80	0
56	MG	1a	1771	1/1	0.85	0.16	71,71,71,71	0
56	MG	1B	212	1/1	0.85	0.25	77,77,77,77	0
56	MG	1A	3351	1/1	0.85	0.15	62,62,62,62	0
56	MG	1A	3719	1/1	0.85	0.33	73,73,73,73	0
56	MG	1A	3478	1/1	0.85	0.25	75,75,75,75	0
56	MG	1A	3486	1/1	0.85	0.20	78,78,78,78	0
56	MG	1a	1657	1/1	0.85	0.25	81,81,81,81	0
56	MG	1A	3388	1/1	0.85	0.24	72,72,72,72	0
56	MG	2a	1650	1/1	0.85	0.15	87,87,87,87	0
56	MG	1A	3510	1/1	0.85	0.23	69,69,69,69	0
56	MG	2A	3336	1/1	0.85	0.22	58,58,58,58	0
56	MG	1A	3205	1/1	0.85	0.21	68,68,68,68	0
56	MG	2A	3639	1/1	0.85	0.29	60,60,60,60	0
56	MG	2a	1669	1/1	0.85	0.45	82,82,82,82	0
56	MG	1A	3399	1/1	0.85	0.26	70,70,70,70	0
56	MG	1A	4009	1/1	0.85	0.16	69,69,69,69	0
56	MG	1x	106	1/1	0.85	0.31	71,71,71,71	0
56	MG	1D	312	1/1	0.85	0.33	49,49,49,49	0
56	MG	2A	3654	1/1	0.85	0.24	77,77,77,77	0
56	MG	2A	3350	1/1	0.85	0.34	72,72,72,72	0
56	MG	1a	1679	1/1	0.85	0.30	77,77,77,77	0
56	MG	2A	3354	1/1	0.85	0.15	69,69,69,69	0
56	MG	2A	3357	1/1	0.85	0.26	64,64,64,64	0
56	MG	2A	3360	1/1	0.85	0.26	61,61,61,61	0
56	MG	1a	1680	1/1	0.85	0.09	69,69,69,69	0
56	MG	2A	3222	1/1	0.85	0.33	70,70,70,70	0
56	MG	1E	307	1/1	0.85	0.18	60,60,60,60	0
56	MG	2A	3226	1/1	0.85	0.20	70,70,70,70	0
56	MG	2A	3229	1/1	0.85	0.33	80,80,80,80	0
56	MG	2A	3394	1/1	0.85	0.38	67,67,67,67	0
56	MG	2A	3401	1/1	0.85	0.27	70,70,70,70	0
56	MG	2a	1717	1/1	0.85	0.39	78,78,78,78	0
56	MG	2A	3405	1/1	0.85	0.25	73,73,73,73	0
56	MG	1a	1685	1/1	0.85	0.31	65,65,65,65	0
56	MG	2a	1729	1/1	0.85	0.42	79,79,79,79	0
56	MG	2A	3419	1/1	0.85	0.26	65,65,65,65	0
56	MG	1E	310	1/1	0.85	0.25	71,71,71,71	0
56	MG	1E	313	1/1	0.85	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3408	1/1	0.85	0.27	76,76,76,76	0
56	MG	1A	3359	1/1	0.85	0.25	64,64,64,64	0
56	MG	1a	1697	1/1	0.85	0.13	66,66,66,66	0
56	MG	1A	3903	1/1	0.85	0.19	73,73,73,73	0
56	MG	2B	205	1/1	0.85	0.22	74,74,74,74	0
56	MG	1G	203	1/1	0.85	0.21	75,75,75,75	0
56	MG	1O	201	1/1	0.85	0.11	68,68,68,68	0
56	MG	1A	3360	1/1	0.85	0.40	67,67,67,67	0
56	MG	2A	3252	1/1	0.85	0.18	70,70,70,70	0
56	MG	2A	3253	1/1	0.85	0.23	74,74,74,74	0
56	MG	2A	3073	1/1	0.85	0.28	73,73,73,73	0
56	MG	1A	3444	1/1	0.85	0.17	65,65,65,65	0
56	MG	2B	219	1/1	0.85	0.36	77,77,77,77	0
56	MG	1O	108	1/1	0.85	0.16	72,72,72,72	0
56	MG	2a	1782	1/1	0.85	0.27	84,84,84,84	0
56	MG	1a	1714	1/1	0.85	0.36	76,76,76,76	0
56	MG	1A	3454	1/1	0.85	0.14	63,63,63,63	0
56	MG	1A	3602	1/1	0.85	0.20	58,58,58,58	0
56	MG	2a	1788	1/1	0.85	0.32	71,71,71,71	0
56	MG	2A	3101	1/1	0.85	0.34	70,70,70,70	0
56	MG	2A	3104	1/1	0.85	0.40	79,79,79,79	0
56	MG	1A	3373	1/1	0.85	0.28	35,35,35,35	0
56	MG	2O	201	1/1	0.85	0.19	67,67,67,67	0
56	MG	1a	1741	1/1	0.85	0.32	85,85,85,85	0
56	MG	2a	1798	1/1	0.85	0.26	71,71,71,71	0
56	MG	2a	1799	1/1	0.85	0.20	67,67,67,67	0
56	MG	2A	3127	1/1	0.85	0.33	71,71,71,71	0
56	MG	1A	3469	1/1	0.85	0.12	68,68,68,68	0
56	MG	2O	102	1/1	0.85	0.28	75,75,75,75	0
56	MG	1A	3935	1/1	0.85	0.24	81,81,81,81	0
56	MG	1O	101	1/1	0.85	0.13	56,56,56,56	0
56	MG	1A	3809	1/1	0.85	0.16	64,64,64,64	0
56	MG	2A	3152	1/1	0.85	0.42	75,75,75,75	0
56	MG	2a	1609	1/1	0.85	0.23	77,77,77,77	0
56	MG	1A	3697	1/1	0.85	0.17	63,63,63,63	0
56	MG	2A	3592	1/1	0.85	0.14	58,58,58,58	0
56	MG	2A	3596	1/1	0.85	0.13	55,55,55,55	0
56	MG	2x	105	1/1	0.85	0.34	82,82,82,82	0
56	MG	1a	1763	1/1	0.85	0.29	80,80,80,80	0
56	MG	1A	3318	1/1	0.85	0.41	74,74,74,74	0
56	MG	1A	3327	1/1	0.86	0.26	65,65,65,65	0
56	MG	1A	3992	1/1	0.86	0.12	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	3329	1/1	0.86	0.31	55,55,55,55	0
56	MG	1A	3018	1/1	0.86	0.12	43,43,43,43	0
56	MG	2A	3203	1/1	0.86	0.28	74,74,74,74	0
56	MG	2A	3204	1/1	0.86	0.26	55,55,55,55	0
56	MG	1a	1613	1/1	0.86	0.33	64,64,64,64	0
56	MG	1a	1614	1/1	0.86	0.16	72,72,72,72	0
56	MG	1A	3616	1/1	0.86	0.19	65,65,65,65	0
56	MG	2A	3036	1/1	0.86	0.23	76,76,76,76	0
56	MG	2A	3223	1/1	0.86	0.24	77,77,77,77	0
56	MG	2A	3352	1/1	0.86	0.35	66,66,66,66	0
56	MG	2a	1644	1/1	0.86	0.15	78,78,78,78	0
56	MG	1A	3243	1/1	0.86	0.27	63,63,63,63	0
56	MG	1A	3875	1/1	0.86	0.17	47,47,47,47	0
56	MG	2A	3355	1/1	0.86	0.26	61,61,61,61	0
56	MG	2a	1652	1/1	0.86	0.28	54,54,54,54	0
56	MG	1A	3626	1/1	0.86	0.16	63,63,63,63	0
56	MG	2A	3056	1/1	0.86	0.26	68,68,68,68	0
56	MG	1a	1739	1/1	0.86	0.15	61,61,61,61	0
56	MG	1a	1643	1/1	0.86	0.39	80,80,80,80	0
56	MG	1A	3655	1/1	0.86	0.18	60,60,60,60	0
56	MG	2A	3078	1/1	0.86	0.28	70,70,70,70	0
56	MG	1D	310	1/1	0.86	0.19	68,68,68,68	0
56	MG	1A	3673	1/1	0.86	0.12	30,30,30,30	0
56	MG	1A	3674	1/1	0.86	0.23	68,68,68,68	0
56	MG	2A	3245	1/1	0.86	0.29	72,72,72,72	0
56	MG	2A	3688	1/1	0.86	0.27	73,73,73,73	0
56	MG	2a	1688	1/1	0.86	0.25	76,76,76,76	0
56	MG	1A	3494	1/1	0.86	0.14	69,69,69,69	0
56	MG	2a	1693	1/1	0.86	0.35	80,80,80,80	0
56	MG	2a	1695	1/1	0.86	0.18	76,76,76,76	0
56	MG	2a	1696	1/1	0.86	0.29	75,75,75,75	0
56	MG	2A	3095	1/1	0.86	0.23	77,77,77,77	0
56	MG	2A	3705	1/1	0.86	0.16	83,83,83,83	0
56	MG	1A	3509	1/1	0.86	0.20	72,72,72,72	0
56	MG	2A	3719	1/1	0.86	0.16	57,57,57,57	0
56	MG	2A	3720	1/1	0.86	0.20	46,46,46,46	0
56	MG	2a	1707	1/1	0.86	0.27	67,67,67,67	0
56	MG	2A	3433	1/1	0.86	0.32	75,75,75,75	0
56	MG	2A	3733	1/1	0.86	0.12	57,57,57,57	0
56	MG	1A	3698	1/1	0.86	0.16	59,59,59,59	0
56	MG	2A	3738	1/1	0.86	0.10	66,66,66,66	0
56	MG	2a	1716	1/1	0.86	0.40	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3103	1/1	0.86	0.15	59,59,59,59	0
56	MG	2a	1721	1/1	0.86	0.41	69,69,69,69	0
56	MG	1a	1766	1/1	0.86	0.27	71,71,71,71	0
56	MG	2A	3758	1/1	0.86	0.26	69,69,69,69	0
56	MG	1A	4037	1/1	0.86	0.21	50,50,50,50	0
56	MG	2A	3261	1/1	0.86	0.23	81,81,81,81	0
56	MG	1A	3188	1/1	0.86	0.25	68,68,68,68	0
56	MG	2a	1736	1/1	0.86	0.31	83,83,83,83	0
56	MG	1a	1780	1/1	0.86	0.28	81,81,81,81	0
56	MG	2A	3272	1/1	0.86	0.39	73,73,73,73	0
56	MG	1a	1667	1/1	0.86	0.31	80,80,80,80	0
56	MG	1A	3389	1/1	0.86	0.22	51,51,51,51	0
56	MG	2B	206	1/1	0.86	0.23	82,82,82,82	0
56	MG	2B	210	1/1	0.86	0.13	83,83,83,83	0
56	MG	1a	1674	1/1	0.86	0.22	83,83,83,83	0
56	MG	1a	1677	1/1	0.86	0.19	71,71,71,71	0
56	MG	2a	1765	1/1	0.86	0.29	67,67,67,67	0
56	MG	1A	3365	1/1	0.86	0.30	69,69,69,69	0
56	MG	2A	3518	1/1	0.86	0.21	58,58,58,58	0
56	MG	2A	3519	1/1	0.86	0.28	68,68,68,68	0
56	MG	1A	4048	1/1	0.86	0.16	66,66,66,66	0
56	MG	1a	1802	1/1	0.86	0.16	68,68,68,68	0
56	MG	1A	3945	1/1	0.86	0.16	78,78,78,78	0
56	MG	2A	3288	1/1	0.86	0.32	73,73,73,73	0
56	MG	1a	1804	1/1	0.86	0.26	66,66,66,66	0
56	MG	2A	3291	1/1	0.86	0.37	84,84,84,84	0
56	MG	2A	3553	1/1	0.86	0.27	52,52,52,52	0
56	MG	2E	302	1/1	0.86	0.27	71,71,71,71	0
56	MG	2A	3561	1/1	0.86	0.17	58,58,58,58	0
56	MG	2E	304	1/1	0.86	0.34	76,76,76,76	0
56	MG	1T	202	1/1	0.86	0.14	65,65,65,65	0
56	MG	1A	3541	1/1	0.86	0.12	44,44,44,44	0
56	MG	1A	3397	1/1	0.86	0.24	68,68,68,68	0
56	MG	1r	101	1/1	0.86	0.20	80,80,80,80	0
56	MG	2A	3302	1/1	0.86	0.25	67,67,67,67	0
56	MG	1A	3398	1/1	0.86	0.15	68,68,68,68	0
56	MG	2A	3175	1/1	0.86	0.26	70,70,70,70	0
56	MG	1a	1692	1/1	0.86	0.33	69,69,69,69	0
56	MG	2A	3178	1/1	0.86	0.46	81,81,81,81	0
56	MG	2a	1603	1/1	0.86	0.21	72,72,72,72	0
56	MG	2a	1606	1/1	0.86	0.40	80,80,80,80	0
56	MG	1A	3840	1/1	0.86	0.16	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3185	1/1	0.86	0.14	61,61,61,61	0
56	MG	2A	3600	1/1	0.86	0.28	82,82,82,82	0
56	MG	2q	201	1/1	0.86	0.14	67,67,67,67	0
56	MG	2a	1611	1/1	0.86	0.38	78,78,78,78	0
56	MG	2a	1614	1/1	0.86	0.24	79,79,79,79	0
56	MG	1A	3131	1/1	0.86	0.13	58,58,58,58	0
56	MG	2a	1616	1/1	0.86	0.24	68,68,68,68	0
56	MG	1A	3402	1/1	0.86	0.28	63,63,63,63	0
56	MG	1x	113	1/1	0.86	0.15	70,70,70,70	0
56	MG	1a	1738	1/1	0.87	0.12	64,64,64,64	0
56	MG	1A	4011	1/1	0.87	0.19	58,58,58,58	0
56	MG	2A	3107	1/1	0.87	0.18	58,58,58,58	0
56	MG	2A	3565	1/1	0.87	0.17	41,41,41,41	0
56	MG	1a	1740	1/1	0.87	0.12	70,70,70,70	0
56	MG	2A	3119	1/1	0.87	0.18	76,76,76,76	0
56	MG	2A	3574	1/1	0.87	0.29	74,74,74,74	0
56	MG	1A	3680	1/1	0.87	0.13	31,31,31,31	0
56	MG	2A	3292	1/1	0.87	0.24	87,87,87,87	0
56	MG	1a	1745	1/1	0.87	0.09	74,74,74,74	0
56	MG	1a	1748	1/1	0.87	0.26	63,63,63,63	0
56	MG	2a	1624	1/1	0.87	0.38	73,73,73,73	0
56	MG	13	103	1/1	0.87	0.21	61,61,61,61	0
56	MG	1A	3183	1/1	0.87	0.15	59,59,59,59	0
56	MG	1A	3833	1/1	0.87	0.09	46,46,46,46	0
56	MG	2A	3305	1/1	0.87	0.39	69,69,69,69	0
56	MG	1A	4031	1/1	0.87	0.10	66,66,66,66	0
56	MG	1A	3835	1/1	0.87	0.19	43,43,43,43	0
56	MG	1A	3685	1/1	0.87	0.20	62,62,62,62	0
56	MG	1a	1603	1/1	0.87	0.14	70,70,70,70	0
56	MG	1A	3687	1/1	0.87	0.14	68,68,68,68	0
56	MG	2A	3610	1/1	0.87	0.19	63,63,63,63	0
56	MG	1A	3688	1/1	0.87	0.23	60,60,60,60	0
56	MG	2A	3316	1/1	0.87	0.16	71,71,71,71	0
56	MG	1A	3690	1/1	0.87	0.22	77,77,77,77	0
56	MG	1a	1778	1/1	0.87	0.27	65,65,65,65	0
56	MG	1a	1624	1/1	0.87	0.27	60,60,60,60	0
56	MG	1a	1628	1/1	0.87	0.14	63,63,63,63	0
56	MG	1A	3692	1/1	0.87	0.25	75,75,75,75	0
56	MG	2a	1664	1/1	0.87	0.23	71,71,71,71	0
56	MG	1a	1790	1/1	0.87	0.33	61,61,61,61	0
56	MG	1a	1631	1/1	0.87	0.38	67,67,67,67	0
56	MG	1A	3346	1/1	0.87	0.26	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1635	1/1	0.87	0.26	75,75,75,75	0
56	MG	1A	4047	1/1	0.87	0.15	65,65,65,65	0
56	MG	1A	3083	1/1	0.87	0.23	48,48,48,48	0
56	MG	1A	3497	1/1	0.87	0.32	62,62,62,62	0
56	MG	1A	3706	1/1	0.87	0.12	76,76,76,76	0
56	MG	2A	3645	1/1	0.87	0.24	72,72,72,72	0
56	MG	2A	3348	1/1	0.87	0.20	68,68,68,68	0
56	MG	2A	3651	1/1	0.87	0.22	60,60,60,60	0
56	MG	2a	1691	1/1	0.87	0.21	80,80,80,80	0
56	MG	1A	3507	1/1	0.87	0.18	73,73,73,73	0
56	MG	1A	3713	1/1	0.87	0.18	76,76,76,76	0
56	MG	1A	3001	1/1	0.87	0.13	48,48,48,48	0
56	MG	1l	202	1/1	0.87	0.13	72,72,72,72	0
56	MG	2A	3660	1/1	0.87	0.19	93,93,93,93	0
56	MG	1A	3295	1/1	0.87	0.39	65,65,65,65	0
56	MG	2A	3211	1/1	0.87	0.22	65,65,65,65	0
56	MG	2A	3359	1/1	0.87	0.14	59,59,59,59	0
56	MG	2A	3682	1/1	0.87	0.24	73,73,73,73	0
56	MG	1A	3358	1/1	0.87	0.16	60,60,60,60	0
56	MG	1x	103	1/1	0.87	0.24	72,72,72,72	0
56	MG	2A	3363	1/1	0.87	0.36	72,72,72,72	0
56	MG	2a	1710	1/1	0.87	0.28	66,66,66,66	0
56	MG	2a	1712	1/1	0.87	0.25	64,64,64,64	0
56	MG	2A	3365	1/1	0.87	0.27	72,72,72,72	0
56	MG	2A	3367	1/1	0.87	0.29	75,75,75,75	0
56	MG	1A	3409	1/1	0.87	0.34	80,80,80,80	0
56	MG	2A	3706	1/1	0.87	0.29	77,77,77,77	0
56	MG	2A	3377	1/1	0.87	0.18	63,63,63,63	0
56	MG	2A	3710	1/1	0.87	0.21	74,74,74,74	0
56	MG	2A	3711	1/1	0.87	0.09	52,52,52,52	0
56	MG	1A	3753	1/1	0.87	0.16	45,45,45,45	0
56	MG	1A	3415	1/1	0.87	0.13	69,69,69,69	0
56	MG	1A	3542	1/1	0.87	0.15	66,66,66,66	0
56	MG	1A	3939	1/1	0.87	0.14	45,45,45,45	0
56	MG	2A	3400	1/1	0.87	0.15	66,66,66,66	0
56	MG	2a	1741	1/1	0.87	0.19	85,85,85,85	0
56	MG	1x	114	1/1	0.87	0.22	66,66,66,66	0
56	MG	2A	3403	1/1	0.87	0.26	69,69,69,69	0
56	MG	1A	3249	1/1	0.87	0.17	70,70,70,70	0
56	MG	2A	3757	1/1	0.87	0.12	71,71,71,71	0
56	MG	1A	3546	1/1	0.87	0.26	61,61,61,61	0
56	MG	2A	3761	1/1	0.87	0.24	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3414	1/1	0.87	0.20	65,65,65,65	0
56	MG	1A	3425	1/1	0.87	0.38	81,81,81,81	0
56	MG	2a	1766	1/1	0.87	0.27	81,81,81,81	0
56	MG	2A	3237	1/1	0.87	0.11	74,74,74,74	0
56	MG	1A	3180	1/1	0.87	0.23	46,46,46,46	0
56	MG	2A	3769	1/1	0.87	0.19	72,72,72,72	0
56	MG	2A	3438	1/1	0.87	0.12	60,60,60,60	0
56	MG	1A	3260	1/1	0.87	0.20	71,71,71,71	0
56	MG	1A	3957	1/1	0.87	0.13	54,54,54,54	0
56	MG	1A	3368	1/1	0.87	0.24	59,59,59,59	0
56	MG	2A	3470	1/1	0.87	0.16	69,69,69,69	0
56	MG	1A	3974	1/1	0.87	0.14	70,70,70,70	0
56	MG	2A	3474	1/1	0.87	0.12	50,50,50,50	0
56	MG	1A	3586	1/1	0.87	0.14	65,65,65,65	0
56	MG	2A	3054	1/1	0.87	0.16	73,73,73,73	0
56	MG	1A	3156	1/1	0.87	0.12	44,44,44,44	0
56	MG	2A	3495	1/1	0.87	0.10	39,39,39,39	0
56	MG	1A	3459	1/1	0.87	0.28	65,65,65,65	0
56	MG	1A	3322	1/1	0.87	0.29	64,64,64,64	0
56	MG	1G	204	1/1	0.87	0.10	75,75,75,75	0
56	MG	1A	3326	1/1	0.87	0.36	69,69,69,69	0
56	MG	1A	3266	1/1	0.87	0.27	71,71,71,71	0
56	MG	2a	1801	1/1	0.87	0.23	68,68,68,68	0
56	MG	1A	3813	1/1	0.87	0.17	60,60,60,60	0
56	MG	1R	202	1/1	0.87	0.21	67,67,67,67	0
56	MG	1S	201	1/1	0.87	0.13	58,58,58,58	0
56	MG	2A	3521	1/1	0.87	0.15	43,43,43,43	0
56	MG	2d	301	1/1	0.87	0.09	67,67,67,67	0
56	MG	2A	3086	1/1	0.87	0.20	73,73,73,73	0
56	MG	1A	3272	1/1	0.87	0.16	62,62,62,62	0
56	MG	2A	3528	1/1	0.87	0.23	72,72,72,72	0
56	MG	2P	201	1/1	0.87	0.17	64,64,64,64	0
56	MG	1O	104	1/1	0.87	0.15	68,68,68,68	0
56	MG	2A	3531	1/1	0.87	0.24	74,74,74,74	0
56	MG	1O	105	1/1	0.87	0.14	63,63,63,63	0
56	MG	2w	101	1/1	0.87	0.19	78,78,78,78	0
56	MG	2A	3541	1/1	0.87	0.17	51,51,51,51	0
56	MG	1A	3218	1/1	0.87	0.23	52,52,52,52	0
56	MG	2A	3546	1/1	0.87	0.21	57,57,57,57	0
56	MG	2A	3550	1/1	0.87	0.25	67,67,67,67	0
56	MG	1X	104	1/1	0.88	0.15	53,53,53,53	0
56	MG	2A	3399	1/1	0.88	0.27	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1634	1/1	0.88	0.40	83,83,83,83	0
56	MG	2A	3105	1/1	0.88	0.23	74,74,74,74	0
56	MG	2A	3106	1/1	0.88	0.52	78,78,78,78	0
56	MG	2a	1639	1/1	0.88	0.15	70,70,70,70	0
56	MG	1A	3244	1/1	0.88	0.21	77,77,77,77	0
56	MG	1A	3617	1/1	0.88	0.10	31,31,31,31	0
56	MG	2A	3116	1/1	0.88	0.10	67,67,67,67	0
56	MG	1a	1682	1/1	0.88	0.28	52,52,52,52	0
56	MG	2A	3417	1/1	0.88	0.41	75,75,75,75	0
56	MG	2A	3121	1/1	0.88	0.22	56,56,56,56	0
56	MG	2A	3422	1/1	0.88	0.22	57,57,57,57	0
56	MG	2A	3662	1/1	0.88	0.23	52,52,52,52	0
56	MG	2A	3269	1/1	0.88	0.21	74,74,74,74	0
56	MG	2A	3426	1/1	0.88	0.46	70,70,70,70	0
56	MG	2A	3428	1/1	0.88	0.24	67,67,67,67	0
56	MG	2a	1667	1/1	0.88	0.17	64,64,64,64	0
56	MG	2A	3432	1/1	0.88	0.28	77,77,77,77	0
56	MG	10	107	1/1	0.88	0.09	62,62,62,62	0
56	MG	2A	3123	1/1	0.88	0.13	83,83,83,83	0
56	MG	1A	3501	1/1	0.88	0.36	72,72,72,72	0
56	MG	2a	1673	1/1	0.88	0.18	61,61,61,61	0
56	MG	1a	1687	1/1	0.88	0.34	72,72,72,72	0
56	MG	2A	3465	1/1	0.88	0.19	56,56,56,56	0
56	MG	2A	3704	1/1	0.88	0.12	89,89,89,89	0
56	MG	1B	210	1/1	0.88	0.15	60,60,60,60	0
56	MG	2a	1684	1/1	0.88	0.37	74,74,74,74	0
56	MG	1a	1689	1/1	0.88	0.24	67,67,67,67	0
56	MG	1A	3977	1/1	0.88	0.15	65,65,65,65	0
56	MG	2A	3284	1/1	0.88	0.31	60,60,60,60	0
56	MG	1b	301	1/1	0.88	0.19	84,84,84,84	0
56	MG	1A	3620	1/1	0.88	0.18	80,80,80,80	0
56	MG	2a	1694	1/1	0.88	0.18	64,64,64,64	0
56	MG	2A	3159	1/1	0.88	0.14	71,71,71,71	0
56	MG	2A	3490	1/1	0.88	0.18	66,66,66,66	0
56	MG	2A	3730	1/1	0.88	0.14	43,43,43,43	0
56	MG	1B	218	1/1	0.88	0.10	50,50,50,50	0
56	MG	2a	1700	1/1	0.88	0.43	78,78,78,78	0
56	MG	1A	3437	1/1	0.88	0.32	70,70,70,70	0
56	MG	1A	3232	1/1	0.88	0.14	55,55,55,55	0
56	MG	2a	1705	1/1	0.88	0.24	63,63,63,63	0
56	MG	2A	3502	1/1	0.88	0.17	55,55,55,55	0
56	MG	1A	3122	1/1	0.88	0.20	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	2A	3295	1/1	0.88	0.11	77,77,77,77	0
56	MG	2A	3296	1/1	0.88	0.13	77,77,77,77	0
56	MG	1B	227	1/1	0.88	0.13	48,48,48,48	0
56	MG	1A	3517	1/1	0.88	0.23	44,44,44,44	0
56	MG	1a	1705	1/1	0.88	0.17	59,59,59,59	0
56	MG	1x	109	1/1	0.88	0.23	72,72,72,72	0
56	MG	2A	3304	1/1	0.88	0.36	60,60,60,60	0
56	MG	1A	3678	1/1	0.88	0.20	65,65,65,65	0
56	MG	2a	1718	1/1	0.88	0.41	73,73,73,73	0
56	MG	2a	1719	1/1	0.88	0.44	82,82,82,82	0
56	MG	1A	3895	1/1	0.88	0.15	60,60,60,60	0
56	MG	1A	3518	1/1	0.88	0.22	62,62,62,62	0
56	MG	2A	3181	1/1	0.88	0.21	68,68,68,68	0
56	MG	1a	1623	1/1	0.88	0.17	59,59,59,59	0
56	MG	1A	3456	1/1	0.88	0.11	62,62,62,62	0
56	MG	2A	3007	1/1	0.88	0.21	64,64,64,64	0
56	MG	1a	1718	1/1	0.88	0.32	69,69,69,69	0
56	MG	1A	3103	1/1	0.88	0.10	43,43,43,43	0
56	MG	1A	3788	1/1	0.88	0.14	49,49,49,49	0
56	MG	2B	215	1/1	0.88	0.14	74,74,74,74	0
56	MG	1A	3262	1/1	0.88	0.17	64,64,64,64	0
56	MG	1A	4029	1/1	0.88	0.29	68,68,68,68	0
56	MG	2a	1748	1/1	0.88	0.19	71,71,71,71	0
56	MG	1A	3333	1/1	0.88	0.23	60,60,60,60	0
56	MG	2A	3568	1/1	0.88	0.18	71,71,71,71	0
56	MG	1A	3372	1/1	0.88	0.16	55,55,55,55	0
56	MG	2A	3051	1/1	0.88	0.18	63,63,63,63	0
56	MG	2A	3207	1/1	0.88	0.21	64,64,64,64	0
56	MG	2A	3210	1/1	0.88	0.25	54,54,54,54	0
56	MG	2a	1769	1/1	0.88	0.21	54,54,54,54	0
56	MG	1A	3932	1/1	0.88	0.11	62,62,62,62	0
56	MG	2A	3341	1/1	0.88	0.27	71,71,71,71	0
56	MG	1A	3311	1/1	0.88	0.24	67,67,67,67	0
56	MG	2E	308	1/1	0.88	0.19	81,81,81,81	0
56	MG	1A	3316	1/1	0.88	0.27	70,70,70,70	0
56	MG	2A	3588	1/1	0.88	0.15	53,53,53,53	0
56	MG	1A	3285	1/1	0.88	0.17	61,61,61,61	0
56	MG	1I	201	1/1	0.88	0.15	77,77,77,77	0
56	MG	2R	202	1/1	0.88	0.13	53,53,53,53	0
56	MG	2A	3595	1/1	0.88	0.19	58,58,58,58	0
56	MG	2A	3072	1/1	0.88	0.15	60,60,60,60	0
56	MG	2A	3598	1/1	0.88	0.24	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1656	1/1	0.88	0.25	68,68,68,68	0
56	MG	21	102	1/1	0.88	0.14	65,65,65,65	0
56	MG	2A	3076	1/1	0.88	0.14	63,63,63,63	0
56	MG	2a	1795	1/1	0.88	0.29	83,83,83,83	0
56	MG	1A	3290	1/1	0.88	0.17	52,52,52,52	0
56	MG	2A	3233	1/1	0.88	0.35	84,84,84,84	0
56	MG	2a	1604	1/1	0.88	0.14	85,85,85,85	0
56	MG	1O	204	1/1	0.88	0.13	59,59,59,59	0
56	MG	1A	3488	1/1	0.88	0.14	64,64,64,64	0
56	MG	1A	3424	1/1	0.88	0.12	54,54,54,54	0
56	MG	2A	3361	1/1	0.88	0.28	75,75,75,75	0
56	MG	2A	3084	1/1	0.88	0.14	60,60,60,60	0
56	MG	2a	1612	1/1	0.88	0.25	71,71,71,71	0
56	MG	1A	3587	1/1	0.88	0.16	37,37,37,37	0
56	MG	1A	3598	1/1	0.88	0.10	34,34,34,34	0
56	MG	1A	3382	1/1	0.88	0.17	56,56,56,56	0
56	MG	2A	3098	1/1	0.88	0.15	64,64,64,64	0
56	MG	2A	3376	1/1	0.88	0.23	72,72,72,72	0
56	MG	1T	203	1/1	0.88	0.15	61,61,61,61	0
56	MG	2a	1622	1/1	0.88	0.25	77,77,77,77	0
56	MG	2r	102	1/1	0.88	0.32	81,81,81,81	0
56	MG	2A	3632	1/1	0.88	0.17	45,45,45,45	0
56	MG	1V	202	1/1	0.88	0.25	47,47,47,47	0
56	MG	2a	1627	1/1	0.88	0.27	61,61,61,61	0
56	MG	1a	1675	1/1	0.88	0.27	67,67,67,67	0
56	MG	2x	106	1/1	0.88	0.25	69,69,69,69	0
56	MG	2A	3637	1/1	0.88	0.15	73,73,73,73	0
56	MG	2A	3250	1/1	0.88	0.13	68,68,68,68	0
56	MG	1A	3724	1/1	0.89	0.11	67,67,67,67	0
56	MG	2A	3249	1/1	0.89	0.28	74,74,74,74	0
56	MG	1a	1770	1/1	0.89	0.39	73,73,73,73	0
56	MG	1A	3735	1/1	0.89	0.10	24,24,24,24	0
56	MG	1A	3741	1/1	0.89	0.20	55,55,55,55	0
56	MG	2A	3255	1/1	0.89	0.21	64,64,64,64	0
56	MG	1A	3082	1/1	0.89	0.27	55,55,55,55	0
56	MG	2A	3415	1/1	0.89	0.34	79,79,79,79	0
56	MG	1a	1781	1/1	0.89	0.21	68,68,68,68	0
56	MG	2A	3418	1/1	0.89	0.41	72,72,72,72	0
56	MG	1A	3671	1/1	0.89	0.09	32,32,32,32	0
56	MG	2A	3421	1/1	0.89	0.51	65,65,65,65	0
56	MG	2a	1649	1/1	0.89	0.28	74,74,74,74	0
56	MG	2A	3657	1/1	0.89	0.13	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3260	1/1	0.89	0.23	70,70,70,70	0
56	MG	1N	203	1/1	0.89	0.10	56,56,56,56	0
56	MG	1A	3207	1/1	0.89	0.12	65,65,65,65	0
56	MG	2a	1658	1/1	0.89	0.17	68,68,68,68	0
56	MG	2a	1662	1/1	0.89	0.29	70,70,70,70	0
56	MG	2A	3108	1/1	0.89	0.36	70,70,70,70	0
56	MG	2A	3666	1/1	0.89	0.30	55,55,55,55	0
56	MG	1O	203	1/1	0.89	0.26	69,69,69,69	0
56	MG	2A	3672	1/1	0.89	0.16	74,74,74,74	0
56	MG	1A	3325	1/1	0.89	0.26	62,62,62,62	0
56	MG	2A	3434	1/1	0.89	0.21	76,76,76,76	0
56	MG	2A	3117	1/1	0.89	0.12	82,82,82,82	0
56	MG	2A	3441	1/1	0.89	0.19	77,77,77,77	0
56	MG	2A	3444	1/1	0.89	0.12	32,32,32,32	0
56	MG	2A	3445	1/1	0.89	0.30	65,65,65,65	0
56	MG	2A	3454	1/1	0.89	0.13	55,55,55,55	0
56	MG	2A	3694	1/1	0.89	0.23	69,69,69,69	0
56	MG	2A	3274	1/1	0.89	0.14	60,60,60,60	0
56	MG	2A	3701	1/1	0.89	0.12	78,78,78,78	0
56	MG	1A	3876	1/1	0.89	0.16	49,49,49,49	0
56	MG	2a	1689	1/1	0.89	0.21	70,70,70,70	0
56	MG	1A	3764	1/1	0.89	0.21	64,64,64,64	0
56	MG	1A	3259	1/1	0.89	0.37	74,74,74,74	0
56	MG	1A	3361	1/1	0.89	0.31	63,63,63,63	0
56	MG	1S	202	1/1	0.89	0.19	67,67,67,67	0
56	MG	2A	3129	1/1	0.89	0.18	66,66,66,66	0
56	MG	2A	3713	1/1	0.89	0.13	62,62,62,62	0
56	MG	1a	1805	1/1	0.89	0.21	61,61,61,61	0
56	MG	1A	3682	1/1	0.89	0.18	50,50,50,50	0
56	MG	2A	3724	1/1	0.89	0.16	47,47,47,47	0
56	MG	1A	3776	1/1	0.89	0.07	30,30,30,30	0
56	MG	2A	3728	1/1	0.89	0.14	56,56,56,56	0
56	MG	2A	3489	1/1	0.89	0.17	58,58,58,58	0
56	MG	1a	1808	1/1	0.89	0.23	68,68,68,68	0
56	MG	1A	3909	1/1	0.89	0.14	60,60,60,60	0
56	MG	1W	207	1/1	0.89	0.16	35,35,35,35	0
56	MG	2A	3498	1/1	0.89	0.30	70,70,70,70	0
56	MG	1A	3168	1/1	0.89	0.27	68,68,68,68	0
56	MG	2A	3756	1/1	0.89	0.16	74,74,74,74	0
56	MG	1m	3002	1/1	0.89	0.28	71,71,71,71	0
56	MG	1p	101	1/1	0.89	0.11	69,69,69,69	0
56	MG	1O	103	1/1	0.89	0.22	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3163	1/1	0.89	0.31	68,68,68,68	0
56	MG	1A	3684	1/1	0.89	0.13	76,76,76,76	0
56	MG	1A	3045	1/1	0.89	0.11	46,46,46,46	0
56	MG	2a	1720	1/1	0.89	0.35	65,65,65,65	0
56	MG	1A	3786	1/1	0.89	0.12	75,75,75,75	0
56	MG	1A	3057	1/1	0.89	0.11	54,54,54,54	0
56	MG	2A	3771	1/1	0.89	0.30	75,75,75,75	0
56	MG	2a	1727	1/1	0.89	0.27	73,73,73,73	0
56	MG	1A	3059	1/1	0.89	0.14	53,53,53,53	0
56	MG	2a	1732	1/1	0.89	0.37	66,66,66,66	0
56	MG	2A	3525	1/1	0.89	0.21	68,68,68,68	0
56	MG	2A	3526	1/1	0.89	0.11	48,48,48,48	0
56	MG	11	103	1/1	0.89	0.26	67,67,67,67	0
56	MG	1A	3798	1/1	0.89	0.23	63,63,63,63	0
56	MG	1A	3416	1/1	0.89	0.08	69,69,69,69	0
56	MG	1B	211	1/1	0.89	0.23	69,69,69,69	0
56	MG	1A	3944	1/1	0.89	0.12	66,66,66,66	0
56	MG	1A	3800	1/1	0.89	0.11	71,71,71,71	0
56	MG	2A	3186	1/1	0.89	0.30	74,74,74,74	0
56	MG	2a	1749	1/1	0.89	0.33	84,84,84,84	0
56	MG	2A	3006	1/1	0.89	0.19	61,61,61,61	0
56	MG	2A	3547	1/1	0.89	0.22	67,67,67,67	0
56	MG	2A	3192	1/1	0.89	0.12	78,78,78,78	0
56	MG	1A	3802	1/1	0.89	0.13	58,58,58,58	0
56	MG	1a	1601	1/1	0.89	0.15	68,68,68,68	0
56	MG	2A	3327	1/1	0.89	0.29	60,60,60,60	0
56	MG	2A	3019	1/1	0.89	0.14	68,68,68,68	0
56	MG	2A	3566	1/1	0.89	0.13	53,53,53,53	0
56	MG	1A	3310	1/1	0.89	0.15	57,57,57,57	0
56	MG	2A	3334	1/1	0.89	0.36	72,72,72,72	0
56	MG	2A	3571	1/1	0.89	0.23	53,53,53,53	0
56	MG	2A	3027	1/1	0.89	0.16	75,75,75,75	0
56	MG	2F	303	1/1	0.89	0.21	68,68,68,68	0
56	MG	2a	1778	1/1	0.89	0.26	77,77,77,77	0
56	MG	2A	3028	1/1	0.89	0.23	57,57,57,57	0
56	MG	1A	3157	1/1	0.89	0.12	57,57,57,57	0
56	MG	1A	3102	1/1	0.89	0.29	76,76,76,76	0
56	MG	2A	3579	1/1	0.89	0.11	77,77,77,77	0
56	MG	2R	201	1/1	0.89	0.12	67,67,67,67	0
56	MG	2A	3580	1/1	0.89	0.15	71,71,71,71	0
56	MG	1A	3699	1/1	0.89	0.21	67,67,67,67	0
56	MG	1A	3380	1/1	0.89	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	2A	3039	1/1	0.89	0.26	59,59,59,59	0
56	MG	1A	3603	1/1	0.89	0.22	62,62,62,62	0
56	MG	2A	3213	1/1	0.89	0.11	60,60,60,60	0
56	MG	1A	3429	1/1	0.89	0.11	55,55,55,55	0
56	MG	2A	3221	1/1	0.89	0.17	66,66,66,66	0
56	MG	2A	3052	1/1	0.89	0.20	67,67,67,67	0
56	MG	1a	1626	1/1	0.89	0.27	63,63,63,63	0
56	MG	2a	1605	1/1	0.89	0.33	70,70,70,70	0
56	MG	1A	3711	1/1	0.89	0.14	56,56,56,56	0
56	MG	2a	1810	1/1	0.89	0.20	78,78,78,78	0
56	MG	1A	3196	1/1	0.89	0.36	68,68,68,68	0
56	MG	1A	3830	1/1	0.89	0.14	52,52,52,52	0
56	MG	1D	311	1/1	0.89	0.17	53,53,53,53	0
56	MG	1a	1749	1/1	0.89	0.38	82,82,82,82	0
56	MG	1a	1634	1/1	0.89	0.39	78,78,78,78	0
56	MG	1A	3385	1/1	0.89	0.10	50,50,50,50	0
56	MG	1a	1755	1/1	0.89	0.14	67,67,67,67	0
56	MG	2A	3371	1/1	0.89	0.34	79,79,79,79	0
56	MG	1a	1636	1/1	0.89	0.15	56,56,56,56	0
56	MG	1A	4002	1/1	0.89	0.08	22,22,22,22	0
56	MG	2t	201	1/1	0.89	0.24	57,57,57,57	0
56	MG	1A	3447	1/1	0.89	0.24	62,62,62,62	0
56	MG	1A	3353	1/1	0.89	0.11	56,56,56,56	0
56	MG	2x	102	1/1	0.89	0.20	77,77,77,77	0
56	MG	2A	3622	1/1	0.89	0.15	68,68,68,68	0
56	MG	1a	1645	1/1	0.89	0.18	64,64,64,64	0
56	MG	2A	3087	1/1	0.89	0.18	81,81,81,81	0
56	MG	2A	3628	1/1	0.89	0.16	71,71,71,71	0
56	MG	1A	3723	1/1	0.89	0.11	47,47,47,47	0
56	MG	2A	3339	1/1	0.90	0.38	69,69,69,69	0
56	MG	1A	3253	1/1	0.90	0.17	81,81,81,81	0
56	MG	1A	3614	1/1	0.90	0.11	52,52,52,52	0
56	MG	1F	307	1/1	0.90	0.14	60,60,60,60	0
56	MG	1e	201	1/1	0.90	0.16	76,76,76,76	0
56	MG	1e	202	1/1	0.90	0.20	56,56,56,56	0
56	MG	1a	1662	1/1	0.90	0.24	72,72,72,72	0
56	MG	1A	3990	1/1	0.90	0.10	52,52,52,52	0
56	MG	2A	3608	1/1	0.90	0.12	52,52,52,52	0
56	MG	1A	3240	1/1	0.90	0.28	50,50,50,50	0
56	MG	1n	101	1/1	0.90	0.14	59,59,59,59	0
56	MG	1A	3995	1/1	0.90	0.11	39,39,39,39	0
56	MG	2A	3615	1/1	0.90	0.19	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3498	1/1	0.90	0.24	48,48,48,48	0
56	MG	1A	3060	1/1	0.90	0.19	59,59,59,59	0
56	MG	1N	202	1/1	0.90	0.15	57,57,57,57	0
56	MG	2a	1636	1/1	0.90	0.23	76,76,76,76	0
56	MG	2A	3194	1/1	0.90	0.25	81,81,81,81	0
56	MG	1A	3505	1/1	0.90	0.33	76,76,76,76	0
56	MG	1A	3624	1/1	0.90	0.09	34,34,34,34	0
56	MG	1A	3352	1/1	0.90	0.11	69,69,69,69	0
56	MG	2A	3364	1/1	0.90	0.30	68,68,68,68	0
56	MG	1A	3746	1/1	0.90	0.14	29,29,29,29	0
56	MG	1A	3639	1/1	0.90	0.10	65,65,65,65	0
56	MG	1A	4015	1/1	0.90	0.13	27,27,27,27	0
56	MG	1Q	203	1/1	0.90	0.14	69,69,69,69	0
56	MG	1a	1686	1/1	0.90	0.32	56,56,56,56	0
56	MG	1A	3651	1/1	0.90	0.13	34,34,34,34	0
56	MG	2a	1653	1/1	0.90	0.21	66,66,66,66	0
56	MG	2a	1656	1/1	0.90	0.25	70,70,70,70	0
56	MG	1R	206	1/1	0.90	0.20	44,44,44,44	0
56	MG	1A	3759	1/1	0.90	0.09	43,43,43,43	0
56	MG	2a	1660	1/1	0.90	0.22	62,62,62,62	0
56	MG	2A	3386	1/1	0.90	0.21	64,64,64,64	0
56	MG	2A	3388	1/1	0.90	0.21	60,60,60,60	0
56	MG	1A	3868	1/1	0.90	0.11	60,60,60,60	0
56	MG	2A	3392	1/1	0.90	0.36	81,81,81,81	0
56	MG	1A	3871	1/1	0.90	0.23	41,41,41,41	0
56	MG	2A	3396	1/1	0.90	0.16	45,45,45,45	0
56	MG	1A	3761	1/1	0.90	0.09	48,48,48,48	0
56	MG	2A	3026	1/1	0.90	0.22	59,59,59,59	0
56	MG	1U	203	1/1	0.90	0.17	60,60,60,60	0
56	MG	1A	3319	1/1	0.90	0.15	64,64,64,64	0
56	MG	2A	3225	1/1	0.90	0.19	64,64,64,64	0
56	MG	2a	1679	1/1	0.90	0.33	72,72,72,72	0
56	MG	2A	3663	1/1	0.90	0.17	75,75,75,75	0
56	MG	1a	1698	1/1	0.90	0.22	60,60,60,60	0
56	MG	1a	1699	1/1	0.90	0.28	71,71,71,71	0
56	MG	2a	1685	1/1	0.90	0.20	73,73,73,73	0
56	MG	2A	3230	1/1	0.90	0.19	68,68,68,68	0
56	MG	2A	3416	1/1	0.90	0.15	61,61,61,61	0
56	MG	2A	3033	1/1	0.90	0.14	49,49,49,49	0
56	MG	1W	205	1/1	0.90	0.17	47,47,47,47	0
56	MG	1A	3884	1/1	0.90	0.12	30,30,30,30	0
56	MG	1a	1703	1/1	0.90	0.31	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3890	1/1	0.90	0.14	70,70,70,70	0
56	MG	2A	3046	1/1	0.90	0.17	73,73,73,73	0
56	MG	2A	3048	1/1	0.90	0.19	66,66,66,66	0
56	MG	2A	3696	1/1	0.90	0.21	65,65,65,65	0
56	MG	1A	3664	1/1	0.90	0.14	32,32,32,32	0
56	MG	2a	1699	1/1	0.90	0.16	69,69,69,69	0
56	MG	2A	3429	1/1	0.90	0.46	77,77,77,77	0
56	MG	1A	3134	1/1	0.90	0.17	53,53,53,53	0
56	MG	1A	3293	1/1	0.90	0.22	58,58,58,58	0
56	MG	1A	4044	1/1	0.90	0.17	65,65,65,65	0
56	MG	1A	3150	1/1	0.90	0.13	44,44,44,44	0
56	MG	1A	3299	1/1	0.90	0.25	56,56,56,56	0
56	MG	1A	3245	1/1	0.90	0.18	52,52,52,52	0
56	MG	1a	1719	1/1	0.90	0.23	63,63,63,63	0
56	MG	2A	3449	1/1	0.90	0.15	60,60,60,60	0
56	MG	2a	1711	1/1	0.90	0.32	72,72,72,72	0
56	MG	2A	3453	1/1	0.90	0.20	74,74,74,74	0
56	MG	2A	3251	1/1	0.90	0.43	66,66,66,66	0
56	MG	1a	1721	1/1	0.90	0.19	60,60,60,60	0
56	MG	1A	3913	1/1	0.90	0.15	70,70,70,70	0
56	MG	2A	3729	1/1	0.90	0.21	75,75,75,75	0
56	MG	2A	3077	1/1	0.90	0.13	60,60,60,60	0
56	MG	1A	3364	1/1	0.90	0.10	55,55,55,55	0
56	MG	2A	3734	1/1	0.90	0.12	47,47,47,47	0
56	MG	1A	3464	1/1	0.90	0.18	53,53,53,53	0
56	MG	2a	1723	1/1	0.90	0.18	65,65,65,65	0
56	MG	1A	3400	1/1	0.90	0.13	55,55,55,55	0
56	MG	18	101	1/1	0.90	0.16	67,67,67,67	0
56	MG	2A	3744	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	3929	1/1	0.90	0.10	43,43,43,43	0
56	MG	2a	1731	1/1	0.90	0.48	70,70,70,70	0
56	MG	2A	3482	1/1	0.90	0.24	58,58,58,58	0
56	MG	2A	3262	1/1	0.90	0.28	74,74,74,74	0
56	MG	1B	203	1/1	0.90	0.19	59,59,59,59	0
56	MG	1A	3401	1/1	0.90	0.13	59,59,59,59	0
56	MG	1A	3040	1/1	0.90	0.20	64,64,64,64	0
56	MG	2A	3092	1/1	0.90	0.32	73,73,73,73	0
56	MG	1A	3934	1/1	0.90	0.22	67,67,67,67	0
56	MG	1B	214	1/1	0.90	0.26	66,66,66,66	0
56	MG	2A	3499	1/1	0.90	0.26	75,75,75,75	0
56	MG	1A	3558	1/1	0.90	0.21	51,51,51,51	0
56	MG	2B	201	1/1	0.90	0.23	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2B	202	1/1	0.90	0.11	75,75,75,75	0
56	MG	1A	3559	1/1	0.90	0.23	61,61,61,61	0
56	MG	1a	1616	1/1	0.90	0.13	62,62,62,62	0
56	MG	2a	1762	1/1	0.90	0.16	59,59,59,59	0
56	MG	1a	1619	1/1	0.90	0.15	61,61,61,61	0
56	MG	1B	219	1/1	0.90	0.21	59,59,59,59	0
56	MG	1A	3940	1/1	0.90	0.16	37,37,37,37	0
56	MG	1A	3568	1/1	0.90	0.40	68,68,68,68	0
56	MG	2A	3286	1/1	0.90	0.10	73,73,73,73	0
56	MG	1A	3250	1/1	0.90	0.13	54,54,54,54	0
56	MG	1a	1768	1/1	0.90	0.17	52,52,52,52	0
56	MG	2A	3524	1/1	0.90	0.19	70,70,70,70	0
56	MG	2A	3115	1/1	0.90	0.18	65,65,65,65	0
56	MG	1a	1769	1/1	0.90	0.10	65,65,65,65	0
56	MG	2a	1777	1/1	0.90	0.23	75,75,75,75	0
56	MG	1A	3476	1/1	0.90	0.15	62,62,62,62	0
56	MG	1A	3577	1/1	0.90	0.10	59,59,59,59	0
56	MG	1a	1772	1/1	0.90	0.19	55,55,55,55	0
56	MG	2D	301	1/1	0.90	0.20	54,54,54,54	0
56	MG	1A	3950	1/1	0.90	0.12	25,25,25,25	0
56	MG	1B	230	1/1	0.90	0.21	77,77,77,77	0
56	MG	2A	3533	1/1	0.90	0.18	62,62,62,62	0
56	MG	2A	3534	1/1	0.90	0.23	60,60,60,60	0
56	MG	2A	3126	1/1	0.90	0.14	57,57,57,57	0
56	MG	2a	1791	1/1	0.90	0.28	78,78,78,78	0
56	MG	1A	3807	1/1	0.90	0.25	66,66,66,66	0
56	MG	2E	307	1/1	0.90	0.10	38,38,38,38	0
56	MG	1A	3371	1/1	0.90	0.14	61,61,61,61	0
56	MG	2F	302	1/1	0.90	0.09	50,50,50,50	0
56	MG	2A	3131	1/1	0.90	0.23	70,70,70,70	0
56	MG	2A	3134	1/1	0.90	0.14	54,54,54,54	0
56	MG	1a	1785	1/1	0.90	0.17	76,76,76,76	0
56	MG	2A	3136	1/1	0.90	0.29	71,71,71,71	0
56	MG	1a	1637	1/1	0.90	0.26	65,65,65,65	0
56	MG	1B	233	1/1	0.90	0.24	70,70,70,70	0
56	MG	2A	3142	1/1	0.90	0.29	64,64,64,64	0
56	MG	2T	201	1/1	0.90	0.27	74,74,74,74	0
56	MG	1a	1792	1/1	0.90	0.16	57,57,57,57	0
56	MG	2A	3315	1/1	0.90	0.33	84,84,84,84	0
56	MG	2A	3570	1/1	0.90	0.17	70,70,70,70	0
56	MG	2A	3145	1/1	0.90	0.12	63,63,63,63	0
56	MG	2A	3149	1/1	0.90	0.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1639	1/1	0.90	0.19	68,68,68,68	0
56	MG	1A	3129	1/1	0.90	0.09	78,78,78,78	0
56	MG	1A	3487	1/1	0.90	0.19	80,80,80,80	0
56	MG	1A	3970	1/1	0.90	0.14	72,72,72,72	0
56	MG	1a	1647	1/1	0.90	0.18	64,64,64,64	0
56	MG	1A	3339	1/1	0.90	0.23	66,66,66,66	0
56	MG	2A	3331	1/1	0.90	0.20	57,57,57,57	0
56	MG	2A	3585	1/1	0.90	0.14	71,71,71,71	0
56	MG	1A	3712	1/1	0.90	0.10	56,56,56,56	0
56	MG	2A	3165	1/1	0.90	0.13	70,70,70,70	0
56	MG	1E	309	1/1	0.90	0.12	64,64,64,64	0
56	MG	1A	3342	1/1	0.90	0.20	57,57,57,57	0
56	MG	2A	3349	1/1	0.91	0.29	63,63,63,63	0
56	MG	1A	3387	1/1	0.91	0.60	81,81,81,81	0
56	MG	2A	3351	1/1	0.91	0.34	64,64,64,64	0
56	MG	2A	3605	1/1	0.91	0.15	73,73,73,73	0
56	MG	1A	3226	1/1	0.91	0.29	71,71,71,71	0
56	MG	1A	3789	1/1	0.91	0.18	63,63,63,63	0
56	MG	2A	3187	1/1	0.91	0.29	69,69,69,69	0
56	MG	1A	3794	1/1	0.91	0.07	38,38,38,38	0
56	MG	2A	3356	1/1	0.91	0.18	54,54,54,54	0
56	MG	2A	3614	1/1	0.91	0.13	62,62,62,62	0
56	MG	2A	3189	1/1	0.91	0.20	80,80,80,80	0
56	MG	2A	3358	1/1	0.91	0.34	65,65,65,65	0
56	MG	1A	3972	1/1	0.91	0.10	69,69,69,69	0
56	MG	1x	111	1/1	0.91	0.27	71,71,71,71	0
56	MG	1N	201	1/1	0.91	0.17	63,63,63,63	0
56	MG	1A	3795	1/1	0.91	0.16	56,56,56,56	0
56	MG	2a	1638	1/1	0.91	0.33	75,75,75,75	0
56	MG	1A	3027	1/1	0.91	0.18	78,78,78,78	0
56	MG	2A	3623	1/1	0.91	0.12	81,81,81,81	0
56	MG	1A	3275	1/1	0.91	0.22	44,44,44,44	0
56	MG	1A	3169	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3627	1/1	0.91	0.33	70,70,70,70	0
56	MG	2a	1647	1/1	0.91	0.29	75,75,75,75	0
56	MG	1A	3087	1/1	0.91	0.27	49,49,49,49	0
56	MG	2A	3368	1/1	0.91	0.10	46,46,46,46	0
56	MG	2A	3369	1/1	0.91	0.10	68,68,68,68	0
56	MG	1A	3803	1/1	0.91	0.16	69,69,69,69	0
56	MG	1O	206	1/1	0.91	0.21	68,68,68,68	0
56	MG	1A	3340	1/1	0.91	0.38	40,40,40,40	0
56	MG	2a	1655	1/1	0.91	0.38	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3208	1/1	0.91	0.17	48,48,48,48	0
56	MG	1A	3006	1/1	0.91	0.18	67,67,67,67	0
56	MG	1A	3138	1/1	0.91	0.18	49,49,49,49	0
56	MG	2A	3644	1/1	0.91	0.09	51,51,51,51	0
56	MG	1A	3508	1/1	0.91	0.24	73,73,73,73	0
56	MG	1a	1694	1/1	0.91	0.24	61,61,61,61	0
56	MG	2A	3648	1/1	0.91	0.12	72,72,72,72	0
56	MG	1A	3810	1/1	0.91	0.23	63,63,63,63	0
56	MG	2A	3391	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3220	1/1	0.91	0.19	77,77,77,77	0
56	MG	2A	3030	1/1	0.91	0.12	52,52,52,52	0
56	MG	1A	4004	1/1	0.91	0.18	49,49,49,49	0
56	MG	1T	201	1/1	0.91	0.24	51,51,51,51	0
56	MG	2a	1675	1/1	0.91	0.16	73,73,73,73	0
56	MG	2a	1676	1/1	0.91	0.19	63,63,63,63	0
56	MG	1A	3811	1/1	0.91	0.14	59,59,59,59	0
56	MG	1A	3347	1/1	0.91	0.20	62,62,62,62	0
56	MG	1A	3148	1/1	0.91	0.24	39,39,39,39	0
56	MG	2A	3227	1/1	0.91	0.17	62,62,62,62	0
56	MG	2A	3041	1/1	0.91	0.21	63,63,63,63	0
56	MG	2A	3412	1/1	0.91	0.19	51,51,51,51	0
56	MG	1U	204	1/1	0.91	0.17	39,39,39,39	0
56	MG	1U	210	1/1	0.91	0.17	55,55,55,55	0
56	MG	1A	3004	1/1	0.91	0.10	37,37,37,37	0
56	MG	2A	3049	1/1	0.91	0.22	75,75,75,75	0
56	MG	2a	1690	1/1	0.91	0.10	81,81,81,81	0
56	MG	2A	3686	1/1	0.91	0.18	74,74,74,74	0
56	MG	1A	4012	1/1	0.91	0.09	49,49,49,49	0
56	MG	1A	3413	1/1	0.91	0.09	58,58,58,58	0
56	MG	1A	3526	1/1	0.91	0.20	53,53,53,53	0
56	MG	1A	3246	1/1	0.91	0.22	46,46,46,46	0
56	MG	1A	4023	1/1	0.91	0.17	50,50,50,50	0
56	MG	1A	3695	1/1	0.91	0.14	50,50,50,50	0
56	MG	2A	3065	1/1	0.91	0.20	71,71,71,71	0
56	MG	1A	3696	1/1	0.91	0.11	34,34,34,34	0
56	MG	2A	3430	1/1	0.91	0.10	69,69,69,69	0
56	MG	1A	3834	1/1	0.91	0.18	45,45,45,45	0
56	MG	2a	1702	1/1	0.91	0.18	64,64,64,64	0
56	MG	1a	1731	1/1	0.91	0.23	52,52,52,52	0
56	MG	1A	3298	1/1	0.91	0.17	38,38,38,38	0
56	MG	1A	3247	1/1	0.91	0.09	78,78,78,78	0
56	MG	1A	3303	1/1	0.91	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3248	1/1	0.91	0.10	53,53,53,53	0
56	MG	13	104	1/1	0.91	0.09	50,50,50,50	0
56	MG	1a	1743	1/1	0.91	0.23	57,57,57,57	0
56	MG	1A	3100	1/1	0.91	0.26	74,74,74,74	0
56	MG	1A	3197	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	3856	1/1	0.91	0.16	74,74,74,74	0
56	MG	2A	3090	1/1	0.91	0.27	68,68,68,68	0
56	MG	2a	1715	1/1	0.91	0.28	73,73,73,73	0
56	MG	1A	3708	1/1	0.91	0.10	67,67,67,67	0
56	MG	1a	1751	1/1	0.91	0.26	57,57,57,57	0
56	MG	1A	3548	1/1	0.91	0.19	73,73,73,73	0
56	MG	2A	3266	1/1	0.91	0.22	70,70,70,70	0
56	MG	1A	3865	1/1	0.91	0.21	66,66,66,66	0
56	MG	1A	3550	1/1	0.91	0.29	71,71,71,71	0
56	MG	1A	3431	1/1	0.91	0.11	69,69,69,69	0
56	MG	2A	3483	1/1	0.91	0.16	46,46,46,46	0
56	MG	1A	3716	1/1	0.91	0.14	36,36,36,36	0
56	MG	2a	1726	1/1	0.91	0.32	70,70,70,70	0
56	MG	1a	1609	1/1	0.91	0.17	65,65,65,65	0
56	MG	2A	3759	1/1	0.91	0.18	66,66,66,66	0
56	MG	1A	4056	1/1	0.91	0.19	48,48,48,48	0
56	MG	1A	3435	1/1	0.91	0.20	62,62,62,62	0
56	MG	1A	3362	1/1	0.91	0.13	63,63,63,63	0
56	MG	1A	3877	1/1	0.91	0.20	66,66,66,66	0
56	MG	1B	207	1/1	0.91	0.13	64,64,64,64	0
56	MG	1A	3570	1/1	0.91	0.17	52,52,52,52	0
56	MG	2A	3500	1/1	0.91	0.11	49,49,49,49	0
56	MG	1A	3046	1/1	0.91	0.17	44,44,44,44	0
56	MG	1a	1627	1/1	0.91	0.26	65,65,65,65	0
56	MG	1a	1774	1/1	0.91	0.22	64,64,64,64	0
56	MG	2a	1745	1/1	0.91	0.17	83,83,83,83	0
56	MG	1A	3162	1/1	0.91	0.20	63,63,63,63	0
56	MG	2A	3289	1/1	0.91	0.23	71,71,71,71	0
56	MG	2a	1751	1/1	0.91	0.21	72,72,72,72	0
56	MG	1a	1779	1/1	0.91	0.12	48,48,48,48	0
56	MG	2a	1757	1/1	0.91	0.16	65,65,65,65	0
56	MG	2B	208	1/1	0.91	0.31	77,77,77,77	0
56	MG	1A	3726	1/1	0.91	0.15	53,53,53,53	0
56	MG	1A	3453	1/1	0.91	0.14	64,64,64,64	0
56	MG	1A	3256	1/1	0.91	0.10	49,49,49,49	0
56	MG	1a	1784	1/1	0.91	0.24	59,59,59,59	0
56	MG	1A	3064	1/1	0.91	0.19	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1768	1/1	0.91	0.28	80,80,80,80	0
56	MG	1a	1788	1/1	0.91	0.12	63,63,63,63	0
56	MG	1A	3457	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3216	1/1	0.91	0.21	48,48,48,48	0
56	MG	2A	3137	1/1	0.91	0.33	66,66,66,66	0
56	MG	2A	3303	1/1	0.91	0.22	71,71,71,71	0
56	MG	1a	1791	1/1	0.91	0.17	72,72,72,72	0
56	MG	1A	3320	1/1	0.91	0.35	64,64,64,64	0
56	MG	1A	3924	1/1	0.91	0.20	66,66,66,66	0
56	MG	1A	3261	1/1	0.91	0.14	66,66,66,66	0
56	MG	2D	307	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3308	1/1	0.91	0.13	78,78,78,78	0
56	MG	2A	3542	1/1	0.91	0.18	46,46,46,46	0
56	MG	1A	3467	1/1	0.91	0.09	55,55,55,55	0
56	MG	2A	3310	1/1	0.91	0.17	68,68,68,68	0
56	MG	2a	1786	1/1	0.91	0.29	71,71,71,71	0
56	MG	1a	1642	1/1	0.91	0.23	64,64,64,64	0
56	MG	2A	3150	1/1	0.91	0.10	58,58,58,58	0
56	MG	2E	310	1/1	0.91	0.19	62,62,62,62	0
56	MG	1A	3376	1/1	0.91	0.44	53,53,53,53	0
56	MG	2A	3154	1/1	0.91	0.17	53,53,53,53	0
56	MG	1A	3323	1/1	0.91	0.13	45,45,45,45	0
56	MG	2A	3564	1/1	0.91	0.20	64,64,64,64	0
56	MG	1A	3324	1/1	0.91	0.20	67,67,67,67	0
56	MG	1A	3770	1/1	0.91	0.11	22,22,22,22	0
56	MG	1A	3771	1/1	0.91	0.08	45,45,45,45	0
56	MG	1A	3217	1/1	0.91	0.11	62,62,62,62	0
56	MG	1A	3050	1/1	0.91	0.23	44,44,44,44	0
56	MG	2U	201	1/1	0.91	0.20	60,60,60,60	0
56	MG	2a	1809	1/1	0.91	0.20	84,84,84,84	0
56	MG	2A	3164	1/1	0.91	0.21	74,74,74,74	0
56	MG	2A	3328	1/1	0.91	0.25	57,57,57,57	0
56	MG	1A	3384	1/1	0.91	0.13	61,61,61,61	0
56	MG	2A	3330	1/1	0.91	0.24	51,51,51,51	0
56	MG	1a	1659	1/1	0.91	0.18	62,62,62,62	0
56	MG	2A	3578	1/1	0.91	0.14	61,61,61,61	0
56	MG	1E	302	1/1	0.91	0.12	55,55,55,55	0
56	MG	1A	3780	1/1	0.91	0.40	36,36,36,36	0
56	MG	2A	3335	1/1	0.91	0.23	44,44,44,44	0
56	MG	1A	3634	1/1	0.91	0.19	50,50,50,50	0
56	MG	2A	3172	1/1	0.91	0.19	64,64,64,64	0
56	MG	1a	1663	1/1	0.91	0.09	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3638	1/1	0.91	0.07	25,25,25,25	0
56	MG	1A	3223	1/1	0.91	0.18	56,56,56,56	0
56	MG	1A	3954	1/1	0.91	0.13	74,74,74,74	0
56	MG	1A	3646	1/1	0.91	0.08	39,39,39,39	0
56	MG	2x	104	1/1	0.91	0.22	74,74,74,74	0
56	MG	2a	1613	1/1	0.91	0.23	66,66,66,66	0
56	MG	2A	3344	1/1	0.91	0.38	79,79,79,79	0
56	MG	2A	3182	1/1	0.91	0.12	58,58,58,58	0
56	MG	2A	3183	1/1	0.91	0.17	66,66,66,66	0
57	K	2x	101	1/1	0.91	0.21	85,85,85,85	0
56	MG	2a	1623	1/1	0.92	0.34	75,75,75,75	0
56	MG	1A	3640	1/1	0.92	0.11	50,50,50,50	0
56	MG	1a	1606	1/1	0.92	0.30	67,67,67,67	0
56	MG	2A	3395	1/1	0.92	0.14	62,62,62,62	0
56	MG	2a	1628	1/1	0.92	0.32	61,61,61,61	0
56	MG	1A	3255	1/1	0.92	0.12	48,48,48,48	0
56	MG	1A	3146	1/1	0.92	0.11	40,40,40,40	0
56	MG	1a	1758	1/1	0.92	0.16	73,73,73,73	0
56	MG	2A	3244	1/1	0.92	0.41	82,82,82,82	0
56	MG	2A	3402	1/1	0.92	0.19	66,66,66,66	0
56	MG	1A	3919	1/1	0.92	0.08	27,27,27,27	0
56	MG	1a	1760	1/1	0.92	0.23	68,68,68,68	0
56	MG	2A	3406	1/1	0.92	0.08	65,65,65,65	0
56	MG	1A	3921	1/1	0.92	0.10	62,62,62,62	0
56	MG	2A	3411	1/1	0.92	0.16	49,49,49,49	0
56	MG	1A	3922	1/1	0.92	0.19	64,64,64,64	0
56	MG	2a	1640	1/1	0.92	0.09	83,83,83,83	0
56	MG	2A	3094	1/1	0.92	0.25	66,66,66,66	0
56	MG	1A	3436	1/1	0.92	0.20	75,75,75,75	0
56	MG	2A	3096	1/1	0.92	0.15	74,74,74,74	0
56	MG	2A	3097	1/1	0.92	0.15	57,57,57,57	0
56	MG	2a	1646	1/1	0.92	0.10	70,70,70,70	0
56	MG	1A	3656	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3650	1/1	0.92	0.19	72,72,72,72	0
56	MG	1A	3125	1/1	0.92	0.28	46,46,46,46	0
56	MG	2A	3420	1/1	0.92	0.25	61,61,61,61	0
56	MG	1A	3172	1/1	0.92	0.07	51,51,51,51	0
56	MG	1A	3445	1/1	0.92	0.13	60,60,60,60	0
56	MG	2A	3423	1/1	0.92	0.32	69,69,69,69	0
56	MG	1A	3519	1/1	0.92	0.34	59,59,59,59	0
56	MG	1A	3390	1/1	0.92	0.24	73,73,73,73	0
56	MG	1A	3452	1/1	0.92	0.09	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3937	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3537	1/1	0.92	0.10	48,48,48,48	0
56	MG	1A	3792	1/1	0.92	0.07	29,29,29,29	0
56	MG	2A	3669	1/1	0.92	0.17	64,64,64,64	0
56	MG	2A	3671	1/1	0.92	0.28	66,66,66,66	0
56	MG	1A	3793	1/1	0.92	0.10	37,37,37,37	0
56	MG	1A	3212	1/1	0.92	0.06	57,57,57,57	0
56	MG	2A	3677	1/1	0.92	0.13	70,70,70,70	0
56	MG	1a	1782	1/1	0.92	0.10	50,50,50,50	0
56	MG	2a	1671	1/1	0.92	0.21	65,65,65,65	0
56	MG	2A	3439	1/1	0.92	0.12	38,38,38,38	0
56	MG	2A	3683	1/1	0.92	0.14	60,60,60,60	0
56	MG	1A	3394	1/1	0.92	0.17	54,54,54,54	0
56	MG	2A	3275	1/1	0.92	0.28	63,63,63,63	0
56	MG	1A	3091	1/1	0.92	0.34	64,64,64,64	0
56	MG	1A	3151	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3690	1/1	0.92	0.18	76,76,76,76	0
56	MG	2A	3450	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3300	1/1	0.92	0.27	59,59,59,59	0
56	MG	2A	3695	1/1	0.92	0.18	87,87,87,87	0
56	MG	2A	3125	1/1	0.92	0.21	61,61,61,61	0
56	MG	2A	3280	1/1	0.92	0.08	68,68,68,68	0
56	MG	2a	1687	1/1	0.92	0.17	57,57,57,57	0
56	MG	1a	1644	1/1	0.92	0.26	66,66,66,66	0
56	MG	1E	303	1/1	0.92	0.20	44,44,44,44	0
56	MG	1A	3104	1/1	0.92	0.25	50,50,50,50	0
56	MG	1A	3461	1/1	0.92	0.10	56,56,56,56	0
56	MG	1A	3694	1/1	0.92	0.16	55,55,55,55	0
56	MG	1a	1650	1/1	0.92	0.16	51,51,51,51	0
56	MG	1a	1798	1/1	0.92	0.28	72,72,72,72	0
56	MG	2A	3479	1/1	0.92	0.16	57,57,57,57	0
56	MG	2A	3716	1/1	0.92	0.17	56,56,56,56	0
56	MG	1A	3967	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3549	1/1	0.92	0.10	67,67,67,67	0
56	MG	1A	3463	1/1	0.92	0.18	76,76,76,76	0
56	MG	1A	3334	1/1	0.92	0.12	66,66,66,66	0
56	MG	1A	3267	1/1	0.92	0.28	58,58,58,58	0
56	MG	1A	3468	1/1	0.92	0.20	52,52,52,52	0
56	MG	2A	3146	1/1	0.92	0.24	67,67,67,67	0
56	MG	1A	3269	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	3121	1/1	0.92	0.18	54,54,54,54	0
56	MG	2A	3736	1/1	0.92	0.29	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3986	1/1	0.92	0.09	61,61,61,61	0
56	MG	1A	3818	1/1	0.92	0.11	70,70,70,70	0
56	MG	1A	3410	1/1	0.92	0.09	58,58,58,58	0
56	MG	2A	3743	1/1	0.92	0.10	65,65,65,65	0
56	MG	2A	3156	1/1	0.92	0.31	65,65,65,65	0
56	MG	1A	3411	1/1	0.92	0.12	65,65,65,65	0
56	MG	2A	3748	1/1	0.92	0.15	54,54,54,54	0
56	MG	2A	3753	1/1	0.92	0.16	60,60,60,60	0
56	MG	2A	3755	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3224	1/1	0.92	0.16	64,64,64,64	0
56	MG	1A	3579	1/1	0.92	0.21	56,56,56,56	0
56	MG	2A	3515	1/1	0.92	0.23	55,55,55,55	0
56	MG	1A	3414	1/1	0.92	0.24	57,57,57,57	0
56	MG	1A	3481	1/1	0.92	0.28	51,51,51,51	0
56	MG	1A	3591	1/1	0.92	0.15	55,55,55,55	0
56	MG	1A	3482	1/1	0.92	0.29	46,46,46,46	0
56	MG	1w	102	1/1	0.92	0.13	73,73,73,73	0
56	MG	1Q	204	1/1	0.92	0.11	59,59,59,59	0
56	MG	1a	1683	1/1	0.92	0.28	52,52,52,52	0
56	MG	2A	3770	1/1	0.92	0.21	54,54,54,54	0
56	MG	2a	1730	1/1	0.92	0.27	66,66,66,66	0
56	MG	1A	3720	1/1	0.92	0.15	61,61,61,61	0
56	MG	2A	3171	1/1	0.92	0.18	72,72,72,72	0
56	MG	1A	3601	1/1	0.92	0.13	42,42,42,42	0
56	MG	1A	3841	1/1	0.92	0.07	37,37,37,37	0
56	MG	1A	3484	1/1	0.92	0.22	64,64,64,64	0
56	MG	2A	3326	1/1	0.92	0.21	46,46,46,46	0
56	MG	2a	1740	1/1	0.92	0.17	78,78,78,78	0
56	MG	1A	3344	1/1	0.92	0.13	47,47,47,47	0
56	MG	2B	207	1/1	0.92	0.12	70,70,70,70	0
56	MG	1A	3136	1/1	0.92	0.31	47,47,47,47	0
56	MG	2B	209	1/1	0.92	0.23	70,70,70,70	0
56	MG	2A	3539	1/1	0.92	0.14	34,34,34,34	0
56	MG	2a	1746	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	3848	1/1	0.92	0.12	56,56,56,56	0
56	MG	1A	3851	1/1	0.92	0.14	33,33,33,33	0
56	MG	2a	1750	1/1	0.92	0.20	69,69,69,69	0
56	MG	1A	3729	1/1	0.92	0.17	64,64,64,64	0
56	MG	2A	3332	1/1	0.92	0.29	61,61,61,61	0
56	MG	1A	4027	1/1	0.92	0.19	61,61,61,61	0
56	MG	1A	3730	1/1	0.92	0.19	61,61,61,61	0
56	MG	1a	1695	1/1	0.92	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3012	1/1	0.92	0.10	55,55,55,55	0
56	MG	2A	3554	1/1	0.92	0.15	64,64,64,64	0
56	MG	2A	3559	1/1	0.92	0.20	52,52,52,52	0
56	MG	1W	202	1/1	0.92	0.16	51,51,51,51	0
56	MG	2D	304	1/1	0.92	0.47	48,48,48,48	0
56	MG	1A	3615	1/1	0.92	0.10	41,41,41,41	0
56	MG	2A	3190	1/1	0.92	0.08	70,70,70,70	0
56	MG	1A	3739	1/1	0.92	0.09	26,26,26,26	0
56	MG	1A	3740	1/1	0.92	0.12	33,33,33,33	0
56	MG	1X	105	1/1	0.92	0.10	54,54,54,54	0
56	MG	2A	3195	1/1	0.92	0.12	66,66,66,66	0
56	MG	1Z	301	1/1	0.92	0.15	65,65,65,65	0
56	MG	2A	3572	1/1	0.92	0.09	52,52,52,52	0
56	MG	10	102	1/1	0.92	0.09	51,51,51,51	0
56	MG	2E	309	1/1	0.92	0.13	50,50,50,50	0
56	MG	2a	1781	1/1	0.92	0.19	67,67,67,67	0
56	MG	1A	3419	1/1	0.92	0.20	48,48,48,48	0
56	MG	2A	3575	1/1	0.92	0.25	66,66,66,66	0
56	MG	1a	1706	1/1	0.92	0.35	57,57,57,57	0
56	MG	2A	3202	1/1	0.92	0.16	66,66,66,66	0
56	MG	1A	4036	1/1	0.92	0.25	64,64,64,64	0
56	MG	2a	1787	1/1	0.92	0.16	69,69,69,69	0
56	MG	1a	1711	1/1	0.92	0.25	54,54,54,54	0
56	MG	1A	3421	1/1	0.92	0.16	52,52,52,52	0
56	MG	1A	3874	1/1	0.92	0.11	24,24,24,24	0
56	MG	1A	3052	1/1	0.92	0.18	56,56,56,56	0
56	MG	2a	1792	1/1	0.92	0.10	82,82,82,82	0
56	MG	11	101	1/1	0.92	0.28	41,41,41,41	0
56	MG	1a	1717	1/1	0.92	0.14	61,61,61,61	0
56	MG	2V	201	1/1	0.92	0.32	57,57,57,57	0
56	MG	2A	3047	1/1	0.92	0.22	68,68,68,68	0
56	MG	1A	4043	1/1	0.92	0.13	51,51,51,51	0
56	MG	2A	3216	1/1	0.92	0.08	55,55,55,55	0
56	MG	2a	1800	1/1	0.92	0.24	69,69,69,69	0
56	MG	1A	3750	1/1	0.92	0.14	46,46,46,46	0
56	MG	21	101	1/1	0.92	0.34	50,50,50,50	0
56	MG	2a	1803	1/1	0.92	0.27	81,81,81,81	0
56	MG	2A	3050	1/1	0.92	0.22	74,74,74,74	0
56	MG	2a	1805	1/1	0.92	0.17	81,81,81,81	0
56	MG	2a	1808	1/1	0.92	0.22	64,64,64,64	0
56	MG	25	101	1/1	0.92	0.18	63,63,63,63	0
56	MG	1A	3496	1/1	0.92	0.20	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	1601	1/1	0.92	0.12	68,68,68,68	0
56	MG	1A	4046	1/1	0.92	0.19	56,56,56,56	0
56	MG	2a	1814	1/1	0.92	0.26	58,58,58,58	0
56	MG	1A	3283	1/1	0.92	0.22	51,51,51,51	0
56	MG	2e	201	1/1	0.92	0.08	87,87,87,87	0
56	MG	1A	3381	1/1	0.92	0.16	51,51,51,51	0
56	MG	1A	3893	1/1	0.92	0.12	42,42,42,42	0
56	MG	16	101	1/1	0.92	0.07	63,63,63,63	0
56	MG	2A	3606	1/1	0.92	0.21	75,75,75,75	0
56	MG	2A	3373	1/1	0.92	0.06	71,71,71,71	0
56	MG	2q	202	1/1	0.92	0.09	81,81,81,81	0
56	MG	2A	3063	1/1	0.92	0.09	58,58,58,58	0
56	MG	2a	1610	1/1	0.92	0.26	75,75,75,75	0
56	MG	2A	3228	1/1	0.92	0.30	78,78,78,78	0
56	MG	1A	3142	1/1	0.92	0.14	61,61,61,61	0
56	MG	18	102	1/1	0.92	0.36	48,48,48,48	0
56	MG	1A	3898	1/1	0.92	0.17	69,69,69,69	0
56	MG	1A	3636	1/1	0.92	0.10	33,33,33,33	0
56	MG	2A	3616	1/1	0.92	0.15	60,60,60,60	0
56	MG	1A	3637	1/1	0.92	0.09	26,26,26,26	0
56	MG	2A	3389	1/1	0.92	0.12	65,65,65,65	0
56	MG	1A	3288	1/1	0.92	0.12	66,66,66,66	0
56	MG	2a	1621	1/1	0.92	0.21	66,66,66,66	0
56	MG	1A	3506	1/1	0.92	0.10	56,56,56,56	0
56	MG	1A	3442	1/1	0.93	0.10	69,69,69,69	0
56	MG	1a	1796	1/1	0.93	0.21	61,61,61,61	0
56	MG	1B	223	1/1	0.93	0.19	71,71,71,71	0
56	MG	2A	3586	1/1	0.93	0.09	38,38,38,38	0
56	MG	1A	3532	1/1	0.93	0.11	42,42,42,42	0
56	MG	1A	3676	1/1	0.93	0.06	27,27,27,27	0
56	MG	2A	3338	1/1	0.93	0.44	66,66,66,66	0
56	MG	1A	3443	1/1	0.93	0.22	70,70,70,70	0
56	MG	1A	3930	1/1	0.93	0.10	65,65,65,65	0
56	MG	1a	1641	1/1	0.93	0.34	73,73,73,73	0
56	MG	1A	3236	1/1	0.93	0.16	56,56,56,56	0
56	MG	1A	3238	1/1	0.93	0.13	42,42,42,42	0
56	MG	1A	3383	1/1	0.93	0.17	54,54,54,54	0
56	MG	1A	3797	1/1	0.93	0.35	72,72,72,72	0
56	MG	2A	3602	1/1	0.93	0.06	49,49,49,49	0
56	MG	1D	302	1/1	0.93	0.22	39,39,39,39	0
56	MG	1A	3448	1/1	0.93	0.17	55,55,55,55	0
56	MG	1A	3938	1/1	0.93	0.09	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1k	201	1/1	0.93	0.18	57,57,57,57	0
56	MG	2A	3180	1/1	0.93	0.22	71,71,71,71	0
56	MG	1A	3055	1/1	0.93	0.28	56,56,56,56	0
56	MG	1A	3545	1/1	0.93	0.12	53,53,53,53	0
56	MG	1a	1654	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	3002	1/1	0.93	0.12	60,60,60,60	0
56	MG	1A	3143	1/1	0.93	0.20	47,47,47,47	0
56	MG	1E	305	1/1	0.93	0.27	40,40,40,40	0
56	MG	1A	3184	1/1	0.93	0.17	75,75,75,75	0
56	MG	1w	103	1/1	0.93	0.30	79,79,79,79	0
56	MG	1A	3187	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	3114	1/1	0.93	0.17	54,54,54,54	0
56	MG	2A	3191	1/1	0.93	0.08	50,50,50,50	0
56	MG	1E	311	1/1	0.93	0.10	27,27,27,27	0
56	MG	1A	3951	1/1	0.93	0.18	50,50,50,50	0
56	MG	1A	3953	1/1	0.93	0.13	41,41,41,41	0
56	MG	1F	305	1/1	0.93	0.17	40,40,40,40	0
56	MG	1A	3808	1/1	0.93	0.08	74,74,74,74	0
56	MG	1a	1669	1/1	0.93	0.16	67,67,67,67	0
56	MG	1A	3554	1/1	0.93	0.08	49,49,49,49	0
56	MG	1A	3147	1/1	0.93	0.30	45,45,45,45	0
56	MG	2A	3201	1/1	0.93	0.32	68,68,68,68	0
56	MG	1A	3118	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3380	1/1	0.93	0.17	49,49,49,49	0
56	MG	2A	3004	1/1	0.93	0.38	73,73,73,73	0
56	MG	2A	3384	1/1	0.93	0.09	58,58,58,58	0
56	MG	2A	3642	1/1	0.93	0.12	46,46,46,46	0
56	MG	1A	3961	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3016	1/1	0.93	0.23	53,53,53,53	0
56	MG	2A	3387	1/1	0.93	0.25	69,69,69,69	0
56	MG	2a	1665	1/1	0.93	0.37	69,69,69,69	0
56	MG	1A	3968	1/1	0.93	0.09	60,60,60,60	0
56	MG	1A	3089	1/1	0.93	0.17	51,51,51,51	0
56	MG	2A	3649	1/1	0.93	0.25	63,63,63,63	0
56	MG	2A	3209	1/1	0.93	0.33	54,54,54,54	0
56	MG	2A	3013	1/1	0.93	0.12	49,49,49,49	0
56	MG	2A	3653	1/1	0.93	0.09	69,69,69,69	0
56	MG	1A	3571	1/1	0.93	0.20	55,55,55,55	0
56	MG	1N	205	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3656	1/1	0.93	0.14	76,76,76,76	0
56	MG	1A	3154	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3214	1/1	0.93	0.11	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	3397	1/1	0.93	0.11	62,62,62,62	0
56	MG	2A	3398	1/1	0.93	0.18	36,36,36,36	0
56	MG	2a	1681	1/1	0.93	0.27	66,66,66,66	0
56	MG	2A	3023	1/1	0.93	0.15	70,70,70,70	0
56	MG	2A	3218	1/1	0.93	0.20	60,60,60,60	0
56	MG	2A	3665	1/1	0.93	0.11	58,58,58,58	0
56	MG	1O	202	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3973	1/1	0.93	0.20	63,63,63,63	0
56	MG	1A	3029	1/1	0.93	0.09	50,50,50,50	0
56	MG	2A	3404	1/1	0.93	0.07	53,53,53,53	0
56	MG	1A	3576	1/1	0.93	0.29	66,66,66,66	0
56	MG	2A	3675	1/1	0.93	0.20	49,49,49,49	0
56	MG	1A	3824	1/1	0.93	0.14	48,48,48,48	0
56	MG	1A	3305	1/1	0.93	0.09	61,61,61,61	0
56	MG	2A	3678	1/1	0.93	0.15	69,69,69,69	0
56	MG	1A	3306	1/1	0.93	0.26	55,55,55,55	0
56	MG	2A	3035	1/1	0.93	0.17	38,38,38,38	0
56	MG	1A	3831	1/1	0.93	0.08	48,48,48,48	0
56	MG	1R	201	1/1	0.93	0.18	48,48,48,48	0
56	MG	1A	3407	1/1	0.93	0.17	52,52,52,52	0
56	MG	1R	205	1/1	0.93	0.15	28,28,28,28	0
56	MG	1A	3581	1/1	0.93	0.11	41,41,41,41	0
56	MG	2A	3232	1/1	0.93	0.20	63,63,63,63	0
56	MG	1A	3994	1/1	0.93	0.13	45,45,45,45	0
56	MG	2a	1703	1/1	0.93	0.34	76,76,76,76	0
56	MG	1A	3127	1/1	0.93	0.19	57,57,57,57	0
56	MG	1A	3836	1/1	0.93	0.18	37,37,37,37	0
56	MG	1A	3357	1/1	0.93	0.12	55,55,55,55	0
56	MG	1A	3308	1/1	0.93	0.20	61,61,61,61	0
56	MG	2A	3425	1/1	0.93	0.21	57,57,57,57	0
56	MG	2A	3702	1/1	0.93	0.17	74,74,74,74	0
56	MG	1A	3594	1/1	0.93	0.08	14,14,14,14	0
56	MG	1A	3842	1/1	0.93	0.08	50,50,50,50	0
56	MG	1U	205	1/1	0.93	0.17	47,47,47,47	0
56	MG	2A	3707	1/1	0.93	0.12	77,77,77,77	0
56	MG	1a	1710	1/1	0.93	0.32	79,79,79,79	0
56	MG	2A	3431	1/1	0.93	0.20	61,61,61,61	0
56	MG	1A	3595	1/1	0.93	0.20	38,38,38,38	0
56	MG	1A	3213	1/1	0.93	0.18	54,54,54,54	0
56	MG	2A	3715	1/1	0.93	0.18	51,51,51,51	0
56	MG	2A	3246	1/1	0.93	0.37	79,79,79,79	0
56	MG	2A	3437	1/1	0.93	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3059	1/1	0.93	0.20	65,65,65,65	0
56	MG	2A	3722	1/1	0.93	0.18	65,65,65,65	0
56	MG	1W	201	1/1	0.93	0.17	58,58,58,58	0
56	MG	2A	3440	1/1	0.93	0.21	65,65,65,65	0
56	MG	2A	3064	1/1	0.93	0.13	71,71,71,71	0
56	MG	2A	3442	1/1	0.93	0.14	39,39,39,39	0
56	MG	2a	1728	1/1	0.93	0.30	75,75,75,75	0
56	MG	1A	3846	1/1	0.93	0.10	31,31,31,31	0
56	MG	1a	1715	1/1	0.93	0.33	79,79,79,79	0
56	MG	1A	3258	1/1	0.93	0.19	56,56,56,56	0
56	MG	1A	4014	1/1	0.93	0.09	55,55,55,55	0
56	MG	2A	3254	1/1	0.93	0.09	59,59,59,59	0
56	MG	2A	3074	1/1	0.93	0.21	57,57,57,57	0
56	MG	1A	3128	1/1	0.93	0.12	45,45,45,45	0
56	MG	2A	3460	1/1	0.93	0.10	43,43,43,43	0
56	MG	2a	1739	1/1	0.93	0.12	75,75,75,75	0
56	MG	1A	4016	1/1	0.93	0.11	69,69,69,69	0
56	MG	2A	3464	1/1	0.93	0.11	73,73,73,73	0
56	MG	1Y	202	1/1	0.93	0.24	56,56,56,56	0
56	MG	2A	3752	1/1	0.93	0.17	62,62,62,62	0
56	MG	2A	3079	1/1	0.93	0.09	57,57,57,57	0
56	MG	1a	1722	1/1	0.93	0.21	65,65,65,65	0
56	MG	1A	3733	1/1	0.93	0.16	54,54,54,54	0
56	MG	1a	1726	1/1	0.93	0.13	41,41,41,41	0
56	MG	2A	3265	1/1	0.93	0.10	64,64,64,64	0
56	MG	1a	1729	1/1	0.93	0.17	67,67,67,67	0
56	MG	1A	3312	1/1	0.93	0.12	46,46,46,46	0
56	MG	2a	1752	1/1	0.93	0.24	68,68,68,68	0
56	MG	2a	1754	1/1	0.93	0.18	70,70,70,70	0
56	MG	2a	1755	1/1	0.93	0.09	84,84,84,84	0
56	MG	1A	3607	1/1	0.93	0.07	37,37,37,37	0
56	MG	2A	3270	1/1	0.93	0.11	64,64,64,64	0
56	MG	2A	3271	1/1	0.93	0.27	73,73,73,73	0
56	MG	2A	3088	1/1	0.93	0.13	56,56,56,56	0
56	MG	1A	3858	1/1	0.93	0.15	42,42,42,42	0
56	MG	2A	3491	1/1	0.93	0.13	44,44,44,44	0
56	MG	2A	3492	1/1	0.93	0.15	58,58,58,58	0
56	MG	1A	3608	1/1	0.93	0.07	25,25,25,25	0
56	MG	2a	1767	1/1	0.93	0.13	72,72,72,72	0
56	MG	1A	4028	1/1	0.93	0.25	59,59,59,59	0
56	MG	1A	3313	1/1	0.93	0.27	41,41,41,41	0
56	MG	1a	1742	1/1	0.93	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3035	1/1	0.93	0.07	48,48,48,48	0
56	MG	1a	1744	1/1	0.93	0.23	65,65,65,65	0
56	MG	1A	3164	1/1	0.93	0.10	46,46,46,46	0
56	MG	2A	3282	1/1	0.93	0.20	62,62,62,62	0
56	MG	1A	3869	1/1	0.93	0.11	52,52,52,52	0
56	MG	2A	3510	1/1	0.93	0.12	63,63,63,63	0
56	MG	11	104	1/1	0.93	0.12	50,50,50,50	0
56	MG	2A	3102	1/1	0.93	0.21	52,52,52,52	0
56	MG	1A	3369	1/1	0.93	0.13	55,55,55,55	0
56	MG	1A	3130	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	3095	1/1	0.93	0.14	60,60,60,60	0
56	MG	1A	3621	1/1	0.93	0.18	31,31,31,31	0
56	MG	1a	1756	1/1	0.93	0.11	59,59,59,59	0
56	MG	15	103	1/1	0.93	0.27	46,46,46,46	0
56	MG	1A	3073	1/1	0.93	0.21	59,59,59,59	0
56	MG	2A	3293	1/1	0.93	0.13	76,76,76,76	0
56	MG	2A	3111	1/1	0.93	0.13	53,53,53,53	0
56	MG	1A	3878	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3879	1/1	0.93	0.24	73,73,73,73	0
56	MG	1a	1761	1/1	0.93	0.19	73,73,73,73	0
56	MG	1A	3883	1/1	0.93	0.06	45,45,45,45	0
56	MG	2A	3299	1/1	0.93	0.28	67,67,67,67	0
56	MG	18	105	1/1	0.93	0.20	58,58,58,58	0
56	MG	2A	3536	1/1	0.93	0.13	72,72,72,72	0
56	MG	2A	3538	1/1	0.93	0.13	39,39,39,39	0
56	MG	1A	3428	1/1	0.93	0.15	62,62,62,62	0
56	MG	1a	1765	1/1	0.93	0.20	51,51,51,51	0
56	MG	1A	3888	1/1	0.93	0.09	51,51,51,51	0
56	MG	2A	3544	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3504	1/1	0.93	0.18	54,54,54,54	0
56	MG	1A	4049	1/1	0.93	0.16	72,72,72,72	0
56	MG	1A	3891	1/1	0.93	0.17	59,59,59,59	0
56	MG	2a	1806	1/1	0.93	0.22	58,58,58,58	0
56	MG	2A	3548	1/1	0.93	0.08	37,37,37,37	0
56	MG	1A	3228	1/1	0.93	0.17	40,40,40,40	0
56	MG	1A	3894	1/1	0.93	0.11	40,40,40,40	0
56	MG	1a	1608	1/1	0.93	0.33	60,60,60,60	0
56	MG	1A	3268	1/1	0.93	0.11	53,53,53,53	0
56	MG	2A	3555	1/1	0.93	0.10	41,41,41,41	0
56	MG	2A	3556	1/1	0.93	0.10	58,58,58,58	0
56	MG	1A	4058	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3138	1/1	0.93	0.22	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	2W	201	1/1	0.93	0.09	63,63,63,63	0
56	MG	1A	3433	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3900	1/1	0.93	0.08	25,25,25,25	0
56	MG	2l	201	1/1	0.93	0.10	72,72,72,72	0
56	MG	2l	202	1/1	0.93	0.11	81,81,81,81	0
56	MG	2l	203	1/1	0.93	0.15	78,78,78,78	0
56	MG	1A	3434	1/1	0.93	0.25	51,51,51,51	0
56	MG	1A	3774	1/1	0.93	0.11	51,51,51,51	0
56	MG	2A	3144	1/1	0.93	0.20	69,69,69,69	0
56	MG	2A	3320	1/1	0.93	0.16	62,62,62,62	0
56	MG	28	101	1/1	0.93	0.16	67,67,67,67	0
56	MG	1A	3170	1/1	0.93	0.32	49,49,49,49	0
56	MG	1a	1625	1/1	0.93	0.20	66,66,66,66	0
56	MG	2A	3325	1/1	0.93	0.26	48,48,48,48	0
56	MG	1A	3025	1/1	0.93	0.18	40,40,40,40	0
56	MG	1A	3512	1/1	0.93	0.15	41,41,41,41	0
56	MG	1A	3513	1/1	0.93	0.17	62,62,62,62	0
56	MG	1A	3235	1/1	0.93	0.19	39,39,39,39	0
56	MG	1A	3440	1/1	0.93	0.21	57,57,57,57	0
56	MG	1A	3784	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	3441	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	3301	1/1	0.94	0.22	58,58,58,58	0
56	MG	1a	1658	1/1	0.94	0.07	61,61,61,61	0
56	MG	2a	1618	1/1	0.94	0.14	80,80,80,80	0
56	MG	2A	3372	1/1	0.94	0.24	52,52,52,52	0
56	MG	1x	110	1/1	0.94	0.09	31,31,31,31	0
56	MG	1A	3925	1/1	0.94	0.27	66,66,66,66	0
56	MG	1A	3926	1/1	0.94	0.24	69,69,69,69	0
56	MG	1A	3777	1/1	0.94	0.10	28,28,28,28	0
56	MG	1A	3779	1/1	0.94	0.10	41,41,41,41	0
56	MG	2A	3001	1/1	0.94	0.33	63,63,63,63	0
56	MG	2A	3206	1/1	0.94	0.11	52,52,52,52	0
56	MG	1A	3622	1/1	0.94	0.08	41,41,41,41	0
56	MG	1A	3190	1/1	0.94	0.14	38,38,38,38	0
56	MG	1A	3030	1/1	0.94	0.27	39,39,39,39	0
56	MG	1A	3631	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3195	1/1	0.94	0.35	42,42,42,42	0
56	MG	2A	3624	1/1	0.94	0.12	40,40,40,40	0
56	MG	1A	3119	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3034	1/1	0.94	0.18	41,41,41,41	0
56	MG	1a	1672	1/1	0.94	0.27	68,68,68,68	0
56	MG	2A	3393	1/1	0.94	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3215	1/1	0.94	0.20	56,56,56,56	0
56	MG	2A	3633	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	3511	1/1	0.94	0.31	45,45,45,45	0
56	MG	2A	3217	1/1	0.94	0.17	60,60,60,60	0
56	MG	2A	3636	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3254	1/1	0.94	0.18	41,41,41,41	0
56	MG	1A	3791	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3024	1/1	0.94	0.20	52,52,52,52	0
56	MG	1a	1678	1/1	0.94	0.23	69,69,69,69	0
56	MG	1E	314	1/1	0.94	0.18	32,32,32,32	0
56	MG	1A	3941	1/1	0.94	0.14	32,32,32,32	0
56	MG	1E	316	1/1	0.94	0.21	46,46,46,46	0
56	MG	1A	3942	1/1	0.94	0.12	38,38,38,38	0
56	MG	1A	3058	1/1	0.94	0.21	63,63,63,63	0
56	MG	1A	3641	1/1	0.94	0.08	40,40,40,40	0
56	MG	1A	3642	1/1	0.94	0.12	27,27,27,27	0
56	MG	2A	3408	1/1	0.94	0.18	64,64,64,64	0
56	MG	2A	3409	1/1	0.94	0.25	62,62,62,62	0
56	MG	1A	3946	1/1	0.94	0.14	46,46,46,46	0
56	MG	2A	3037	1/1	0.94	0.21	65,65,65,65	0
56	MG	2A	3413	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3948	1/1	0.94	0.11	63,63,63,63	0
56	MG	1A	3370	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	3124	1/1	0.94	0.31	42,42,42,42	0
56	MG	2A	3042	1/1	0.94	0.21	56,56,56,56	0
56	MG	1A	3257	1/1	0.94	0.13	49,49,49,49	0
56	MG	2A	3661	1/1	0.94	0.17	60,60,60,60	0
56	MG	1A	3521	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3659	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3664	1/1	0.94	0.10	38,38,38,38	0
56	MG	1A	3523	1/1	0.94	0.12	30,30,30,30	0
56	MG	2a	1674	1/1	0.94	0.29	68,68,68,68	0
56	MG	2A	3239	1/1	0.94	0.10	50,50,50,50	0
56	MG	1A	3048	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3529	1/1	0.94	0.36	44,44,44,44	0
56	MG	1A	3530	1/1	0.94	0.15	53,53,53,53	0
56	MG	1A	3963	1/1	0.94	0.05	37,37,37,37	0
56	MG	2a	1680	1/1	0.94	0.14	41,41,41,41	0
56	MG	2A	3674	1/1	0.94	0.15	55,55,55,55	0
56	MG	1A	3211	1/1	0.94	0.25	43,43,43,43	0
56	MG	1A	3049	1/1	0.94	0.18	35,35,35,35	0
56	MG	1a	1702	1/1	0.94	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	1A	3377	1/1	0.94	0.10	63,63,63,63	0
56	MG	1A	3539	1/1	0.94	0.25	55,55,55,55	0
56	MG	1Q	206	1/1	0.94	0.15	43,43,43,43	0
56	MG	1A	3061	1/1	0.94	0.33	69,69,69,69	0
56	MG	1A	3020	1/1	0.94	0.09	49,49,49,49	0
56	MG	2A	3067	1/1	0.94	0.18	47,47,47,47	0
56	MG	2A	3068	1/1	0.94	0.11	52,52,52,52	0
56	MG	1A	3165	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3975	1/1	0.94	0.13	68,68,68,68	0
56	MG	1A	3817	1/1	0.94	0.17	48,48,48,48	0
56	MG	1A	3686	1/1	0.94	0.15	62,62,62,62	0
56	MG	2A	3259	1/1	0.94	0.21	53,53,53,53	0
56	MG	1A	3980	1/1	0.94	0.15	42,42,42,42	0
56	MG	1A	3321	1/1	0.94	0.40	70,70,70,70	0
56	MG	1A	3166	1/1	0.94	0.07	46,46,46,46	0
56	MG	1A	3099	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3989	1/1	0.94	0.07	32,32,32,32	0
56	MG	1A	3067	1/1	0.94	0.22	66,66,66,66	0
56	MG	1U	209	1/1	0.94	0.13	66,66,66,66	0
56	MG	1A	3827	1/1	0.94	0.05	49,49,49,49	0
56	MG	2A	3708	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3693	1/1	0.94	0.20	54,54,54,54	0
56	MG	2A	3466	1/1	0.94	0.15	53,53,53,53	0
56	MG	1A	3829	1/1	0.94	0.06	29,29,29,29	0
56	MG	2A	3712	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3468	1/1	0.94	0.15	60,60,60,60	0
56	MG	2A	3714	1/1	0.94	0.17	59,59,59,59	0
56	MG	1A	3998	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3471	1/1	0.94	0.10	36,36,36,36	0
56	MG	2A	3718	1/1	0.94	0.08	35,35,35,35	0
56	MG	1a	1730	1/1	0.94	0.11	66,66,66,66	0
56	MG	1A	3455	1/1	0.94	0.18	49,49,49,49	0
56	MG	2A	3475	1/1	0.94	0.07	52,52,52,52	0
56	MG	1A	3225	1/1	0.94	0.18	53,53,53,53	0
56	MG	2A	3478	1/1	0.94	0.10	37,37,37,37	0
56	MG	2A	3727	1/1	0.94	0.10	69,69,69,69	0
56	MG	1a	1734	1/1	0.94	0.25	49,49,49,49	0
56	MG	1a	1736	1/1	0.94	0.12	68,68,68,68	0
56	MG	1A	3832	1/1	0.94	0.14	44,44,44,44	0
56	MG	2A	3732	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3484	1/1	0.94	0.14	44,44,44,44	0
56	MG	1A	3271	1/1	0.94	0.22	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	1Y	201	1/1	0.94	0.25	62,62,62,62	0
56	MG	2A	3281	1/1	0.94	0.09	67,67,67,67	0
56	MG	1A	3551	1/1	0.94	0.22	66,66,66,66	0
56	MG	1A	3552	1/1	0.94	0.22	57,57,57,57	0
56	MG	1A	4007	1/1	0.94	0.05	28,28,28,28	0
56	MG	1A	3553	1/1	0.94	0.10	63,63,63,63	0
56	MG	1A	3132	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3839	1/1	0.94	0.13	38,38,38,38	0
56	MG	10	106	1/1	0.94	0.06	53,53,53,53	0
56	MG	1A	3701	1/1	0.94	0.12	63,63,63,63	0
56	MG	1A	3038	1/1	0.94	0.30	48,48,48,48	0
56	MG	10	109	1/1	0.94	0.06	55,55,55,55	0
56	MG	2A	3506	1/1	0.94	0.11	50,50,50,50	0
56	MG	1a	1754	1/1	0.94	0.23	61,61,61,61	0
56	MG	1A	3330	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3560	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3561	1/1	0.94	0.12	38,38,38,38	0
56	MG	2A	3513	1/1	0.94	0.20	66,66,66,66	0
56	MG	2A	3118	1/1	0.94	0.20	59,59,59,59	0
56	MG	2A	3765	1/1	0.94	0.14	52,52,52,52	0
56	MG	2A	3767	1/1	0.94	0.08	51,51,51,51	0
56	MG	1A	3391	1/1	0.94	0.25	76,76,76,76	0
56	MG	2A	3517	1/1	0.94	0.16	61,61,61,61	0
56	MG	2A	3120	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3171	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3075	1/1	0.94	0.12	35,35,35,35	0
56	MG	1A	3850	1/1	0.94	0.09	44,44,44,44	0
56	MG	2A	3523	1/1	0.94	0.15	55,55,55,55	0
56	MG	1A	3174	1/1	0.94	0.49	43,43,43,43	0
56	MG	2a	1763	1/1	0.94	0.18	52,52,52,52	0
56	MG	15	102	1/1	0.94	0.20	43,43,43,43	0
56	MG	1A	3854	1/1	0.94	0.06	28,28,28,28	0
56	MG	2A	3128	1/1	0.94	0.17	47,47,47,47	0
56	MG	15	104	1/1	0.94	0.21	59,59,59,59	0
56	MG	1A	3336	1/1	0.94	0.17	44,44,44,44	0
56	MG	2A	3133	1/1	0.94	0.21	46,46,46,46	0
56	MG	1A	3337	1/1	0.94	0.19	47,47,47,47	0
56	MG	1A	3471	1/1	0.94	0.10	66,66,66,66	0
56	MG	1A	4035	1/1	0.94	0.19	58,58,58,58	0
56	MG	1A	3176	1/1	0.94	0.08	36,36,36,36	0
56	MG	1A	3286	1/1	0.94	0.17	58,58,58,58	0
56	MG	2a	1775	1/1	0.94	0.22	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3287	1/1	0.94	0.20	56,56,56,56	0
56	MG	1A	3582	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3237	1/1	0.94	0.21	41,41,41,41	0
56	MG	1A	3731	1/1	0.94	0.11	62,62,62,62	0
56	MG	2a	1780	1/1	0.94	0.19	75,75,75,75	0
56	MG	1a	1604	1/1	0.94	0.14	66,66,66,66	0
56	MG	1A	3732	1/1	0.94	0.09	19,19,19,19	0
56	MG	2D	303	1/1	0.94	0.12	38,38,38,38	0
56	MG	1A	3079	1/1	0.94	0.09	66,66,66,66	0
56	MG	1A	3589	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	3141	1/1	0.94	0.12	59,59,59,59	0
56	MG	1A	3182	1/1	0.94	0.23	53,53,53,53	0
56	MG	2D	308	1/1	0.94	0.13	76,76,76,76	0
56	MG	1a	1786	1/1	0.94	0.12	86,86,86,86	0
56	MG	1a	1787	1/1	0.94	0.23	66,66,66,66	0
56	MG	1A	3106	1/1	0.94	0.08	30,30,30,30	0
56	MG	1A	3881	1/1	0.94	0.07	47,47,47,47	0
56	MG	2E	305	1/1	0.94	0.17	48,48,48,48	0
56	MG	1A	4053	1/1	0.94	0.16	66,66,66,66	0
56	MG	1A	3350	1/1	0.94	0.17	66,66,66,66	0
56	MG	1A	4055	1/1	0.94	0.19	64,64,64,64	0
56	MG	1A	3745	1/1	0.94	0.08	68,68,68,68	0
56	MG	1A	3113	1/1	0.94	0.07	46,46,46,46	0
56	MG	2A	3567	1/1	0.94	0.12	58,58,58,58	0
56	MG	1A	3749	1/1	0.94	0.15	74,74,74,74	0
56	MG	1A	3296	1/1	0.94	0.24	51,51,51,51	0
56	MG	1A	3751	1/1	0.94	0.07	32,32,32,32	0
56	MG	1a	1630	1/1	0.94	0.34	63,63,63,63	0
56	MG	2Q	202	1/1	0.94	0.19	56,56,56,56	0
56	MG	1B	206	1/1	0.94	0.21	53,53,53,53	0
56	MG	2a	1807	1/1	0.94	0.14	68,68,68,68	0
56	MG	1A	3491	1/1	0.94	0.13	51,51,51,51	0
56	MG	1B	208	1/1	0.94	0.29	70,70,70,70	0
56	MG	1A	3605	1/1	0.94	0.07	48,48,48,48	0
56	MG	2A	3346	1/1	0.94	0.20	57,57,57,57	0
56	MG	1A	3493	1/1	0.94	0.21	50,50,50,50	0
56	MG	2a	1813	1/1	0.94	0.21	71,71,71,71	0
56	MG	2A	3176	1/1	0.94	0.10	63,63,63,63	0
56	MG	1A	3297	1/1	0.94	0.11	38,38,38,38	0
56	MG	2X	102	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3611	1/1	0.94	0.13	66,66,66,66	0
56	MG	2A	3581	1/1	0.94	0.15	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3417	1/1	0.94	0.20	48,48,48,48	0
56	MG	1B	217	1/1	0.94	0.13	49,49,49,49	0
56	MG	2k	201	1/1	0.94	0.11	67,67,67,67	0
56	MG	1A	3017	1/1	0.94	0.15	69,69,69,69	0
56	MG	1A	3769	1/1	0.94	0.13	28,28,28,28	0
56	MG	1A	3420	1/1	0.94	0.13	46,46,46,46	0
56	MG	1A	3910	1/1	0.94	0.20	67,67,67,67	0
56	MG	1A	3912	1/1	0.94	0.12	55,55,55,55	0
56	MG	1a	1646	1/1	0.94	0.21	57,57,57,57	0
56	MG	2r	101	1/1	0.94	0.22	75,75,75,75	0
56	MG	2A	3593	1/1	0.94	0.13	67,67,67,67	0
56	MG	1B	224	1/1	0.94	0.15	55,55,55,55	0
56	MG	1A	3500	1/1	0.94	0.21	57,57,57,57	0
56	MG	2A	3597	1/1	0.94	0.13	73,73,73,73	0
56	MG	1A	3772	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3618	1/1	0.94	0.09	21,21,21,21	0
56	MG	1A	3920	1/1	0.94	0.08	61,61,61,61	0
56	MG	1A	3117	1/1	0.94	0.17	44,44,44,44	0
56	MG	1x	104	1/1	0.94	0.22	75,75,75,75	0
56	MG	2A	3366	1/1	0.94	0.38	57,57,57,57	0
56	MG	1a	1655	1/1	0.94	0.20	60,60,60,60	0
56	MG	1A	3189	1/1	0.94	0.29	47,47,47,47	0
59	ZN	14	102	1/1	0.94	0.11	123,123,123,123	0
59	ZN	24	501	1/1	0.94	0.17	131,131,131,131	0
56	MG	1A	3403	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3859	1/1	0.95	0.10	61,61,61,61	0
56	MG	2A	3018	1/1	0.95	0.08	43,43,43,43	0
56	MG	1a	1681	1/1	0.95	0.24	54,54,54,54	0
56	MG	2A	3021	1/1	0.95	0.20	46,46,46,46	0
56	MG	1A	3635	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3997	1/1	0.95	0.09	49,49,49,49	0
56	MG	1A	3356	1/1	0.95	0.20	58,58,58,58	0
56	MG	1P	203	1/1	0.95	0.22	35,35,35,35	0
56	MG	1P	204	1/1	0.95	0.54	39,39,39,39	0
56	MG	1A	3999	1/1	0.95	0.14	49,49,49,49	0
56	MG	1A	3028	1/1	0.95	0.17	36,36,36,36	0
56	MG	1A	3126	1/1	0.95	0.35	44,44,44,44	0
56	MG	1Q	205	1/1	0.95	0.12	45,45,45,45	0
56	MG	1A	3315	1/1	0.95	0.14	47,47,47,47	0
56	MG	1A	3870	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3070	1/1	0.95	0.10	39,39,39,39	0
56	MG	2A	3652	1/1	0.95	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	1A	3766	1/1	0.95	0.11	55,55,55,55	0
56	MG	1A	3158	1/1	0.95	0.17	40,40,40,40	0
56	MG	1a	1696	1/1	0.95	0.08	65,65,65,65	0
56	MG	2A	3040	1/1	0.95	0.10	65,65,65,65	0
56	MG	1A	3056	1/1	0.95	0.10	29,29,29,29	0
56	MG	1A	3363	1/1	0.95	0.28	48,48,48,48	0
56	MG	2A	3043	1/1	0.95	0.14	36,36,36,36	0
56	MG	2a	1654	1/1	0.95	0.10	60,60,60,60	0
56	MG	1A	3101	1/1	0.95	0.09	51,51,51,51	0
56	MG	2A	3045	1/1	0.95	0.17	67,67,67,67	0
56	MG	2A	3427	1/1	0.95	0.33	65,65,65,65	0
56	MG	1A	3653	1/1	0.95	0.06	30,30,30,30	0
56	MG	2a	1659	1/1	0.95	0.18	57,57,57,57	0
56	MG	1A	3036	1/1	0.95	0.10	37,37,37,37	0
56	MG	2a	1661	1/1	0.95	0.12	58,58,58,58	0
56	MG	1A	3241	1/1	0.95	0.11	58,58,58,58	0
56	MG	2a	1663	1/1	0.95	0.26	82,82,82,82	0
56	MG	1A	4019	1/1	0.95	0.19	64,64,64,64	0
56	MG	1A	3278	1/1	0.95	0.35	43,43,43,43	0
56	MG	1A	3885	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	4022	1/1	0.95	0.11	43,43,43,43	0
56	MG	2A	3435	1/1	0.95	0.11	45,45,45,45	0
56	MG	2A	3053	1/1	0.95	0.06	48,48,48,48	0
56	MG	1A	3886	1/1	0.95	0.09	51,51,51,51	0
56	MG	1a	1708	1/1	0.95	0.19	52,52,52,52	0
56	MG	1V	203	1/1	0.95	0.35	44,44,44,44	0
56	MG	1A	4025	1/1	0.95	0.16	55,55,55,55	0
56	MG	1A	3008	1/1	0.95	0.12	29,29,29,29	0
56	MG	2A	3061	1/1	0.95	0.12	62,62,62,62	0
56	MG	2A	3062	1/1	0.95	0.15	48,48,48,48	0
56	MG	1A	3666	1/1	0.95	0.07	29,29,29,29	0
56	MG	1A	3667	1/1	0.95	0.11	75,75,75,75	0
56	MG	1A	3198	1/1	0.95	0.14	47,47,47,47	0
56	MG	1A	3556	1/1	0.95	0.07	40,40,40,40	0
56	MG	1X	106	1/1	0.95	0.17	72,72,72,72	0
56	MG	2A	3459	1/1	0.95	0.09	47,47,47,47	0
56	MG	2A	3069	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3201	1/1	0.95	0.07	31,31,31,31	0
56	MG	1A	3896	1/1	0.95	0.07	41,41,41,41	0
56	MG	1a	1720	1/1	0.95	0.21	74,74,74,74	0
56	MG	1A	3897	1/1	0.95	0.13	65,65,65,65	0
56	MG	1Z	302	1/1	0.95	0.24	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3202	1/1	0.95	0.07	48,48,48,48	0
56	MG	1A	3489	1/1	0.95	0.16	52,52,52,52	0
56	MG	2A	3268	1/1	0.95	0.08	61,61,61,61	0
56	MG	1A	3080	1/1	0.95	0.13	45,45,45,45	0
56	MG	1A	3681	1/1	0.95	0.08	41,41,41,41	0
56	MG	1A	3563	1/1	0.95	0.24	57,57,57,57	0
56	MG	2A	3082	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3906	1/1	0.95	0.09	64,64,64,64	0
56	MG	1a	1733	1/1	0.95	0.15	54,54,54,54	0
56	MG	2A	3085	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3564	1/1	0.95	0.08	43,43,43,43	0
56	MG	1A	3427	1/1	0.95	0.08	46,46,46,46	0
56	MG	1a	1737	1/1	0.95	0.17	70,70,70,70	0
56	MG	1A	3569	1/1	0.95	0.29	66,66,66,66	0
56	MG	1A	3492	1/1	0.95	0.25	41,41,41,41	0
56	MG	1A	3133	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3105	1/1	0.95	0.16	45,45,45,45	0
56	MG	1A	3915	1/1	0.95	0.16	57,57,57,57	0
56	MG	12	102	1/1	0.95	0.13	50,50,50,50	0
56	MG	2A	3496	1/1	0.95	0.12	56,56,56,56	0
56	MG	13	102	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3917	1/1	0.95	0.05	32,32,32,32	0
56	MG	1A	3918	1/1	0.95	0.12	76,76,76,76	0
56	MG	1A	3495	1/1	0.95	0.28	50,50,50,50	0
56	MG	15	101	1/1	0.95	0.37	41,41,41,41	0
56	MG	1A	3691	1/1	0.95	0.10	51,51,51,51	0
56	MG	1A	3135	1/1	0.95	0.19	31,31,31,31	0
56	MG	1A	3039	1/1	0.95	0.30	43,43,43,43	0
56	MG	15	106	1/1	0.95	0.15	48,48,48,48	0
56	MG	2A	3739	1/1	0.95	0.09	65,65,65,65	0
56	MG	1A	4059	1/1	0.95	0.33	58,58,58,58	0
56	MG	1A	3251	1/1	0.95	0.11	42,42,42,42	0
56	MG	2A	3512	1/1	0.95	0.15	55,55,55,55	0
56	MG	17	102	1/1	0.95	0.11	40,40,40,40	0
56	MG	1A	3499	1/1	0.95	0.23	49,49,49,49	0
56	MG	2A	3751	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3112	1/1	0.95	0.19	71,71,71,71	0
56	MG	2A	3113	1/1	0.95	0.24	64,64,64,64	0
56	MG	2A	3754	1/1	0.95	0.16	70,70,70,70	0
56	MG	2A	3114	1/1	0.95	0.25	68,68,68,68	0
56	MG	2A	3301	1/1	0.95	0.15	43,43,43,43	0
56	MG	2A	3520	1/1	0.95	0.11	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	3335	1/1	0.95	0.17	49,49,49,49	0
56	MG	18	104	1/1	0.95	0.18	57,57,57,57	0
56	MG	2a	1734	1/1	0.95	0.15	71,71,71,71	0
56	MG	2A	3760	1/1	0.95	0.14	64,64,64,64	0
56	MG	1B	204	1/1	0.95	0.25	67,67,67,67	0
56	MG	1A	3806	1/1	0.95	0.06	44,44,44,44	0
56	MG	2a	1738	1/1	0.95	0.08	86,86,86,86	0
56	MG	1A	3110	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3583	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3502	1/1	0.95	0.08	29,29,29,29	0
56	MG	1A	3931	1/1	0.95	0.12	69,69,69,69	0
56	MG	1A	3051	1/1	0.95	0.09	63,63,63,63	0
56	MG	1B	213	1/1	0.95	0.14	48,48,48,48	0
56	MG	1A	3022	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3703	1/1	0.95	0.08	60,60,60,60	0
56	MG	2a	1747	1/1	0.95	0.28	67,67,67,67	0
56	MG	1B	216	1/1	0.95	0.08	63,63,63,63	0
56	MG	1a	1612	1/1	0.95	0.14	76,76,76,76	0
56	MG	2A	3537	1/1	0.95	0.12	71,71,71,71	0
56	MG	1a	1775	1/1	0.95	0.15	63,63,63,63	0
56	MG	2A	3132	1/1	0.95	0.26	55,55,55,55	0
56	MG	2A	3540	1/1	0.95	0.10	58,58,58,58	0
56	MG	1a	1776	1/1	0.95	0.20	55,55,55,55	0
56	MG	1A	3062	1/1	0.95	0.24	53,53,53,53	0
56	MG	1A	3936	1/1	0.95	0.09	70,70,70,70	0
56	MG	2A	3322	1/1	0.95	0.19	65,65,65,65	0
56	MG	2A	3323	1/1	0.95	0.17	45,45,45,45	0
56	MG	1A	3814	1/1	0.95	0.14	60,60,60,60	0
56	MG	1A	3386	1/1	0.95	0.19	53,53,53,53	0
56	MG	2A	3549	1/1	0.95	0.09	40,40,40,40	0
56	MG	1a	1620	1/1	0.95	0.06	50,50,50,50	0
56	MG	2A	3139	1/1	0.95	0.08	41,41,41,41	0
56	MG	1a	1621	1/1	0.95	0.28	64,64,64,64	0
56	MG	1a	1622	1/1	0.95	0.22	64,64,64,64	0
56	MG	1A	3219	1/1	0.95	0.14	66,66,66,66	0
56	MG	1A	3709	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3710	1/1	0.95	0.13	59,59,59,59	0
56	MG	2A	3560	1/1	0.95	0.15	48,48,48,48	0
56	MG	1B	225	1/1	0.95	0.12	61,61,61,61	0
56	MG	1A	3596	1/1	0.95	0.13	37,37,37,37	0
56	MG	1A	3597	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3825	1/1	0.95	0.08	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	1A	3826	1/1	0.95	0.13	50,50,50,50	0
56	MG	2A	3153	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3341	1/1	0.95	0.17	42,42,42,42	0
56	MG	1A	3599	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	3717	1/1	0.95	0.08	56,56,56,56	0
56	MG	2A	3157	1/1	0.95	0.13	47,47,47,47	0
56	MG	1a	1797	1/1	0.95	0.22	67,67,67,67	0
56	MG	1A	3600	1/1	0.95	0.09	35,35,35,35	0
56	MG	1B	234	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	3220	1/1	0.95	0.13	49,49,49,49	0
56	MG	1D	307	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3952	1/1	0.95	0.10	24,24,24,24	0
56	MG	2F	304	1/1	0.95	0.16	50,50,50,50	0
56	MG	1A	3446	1/1	0.95	0.24	47,47,47,47	0
56	MG	1A	3302	1/1	0.95	0.10	36,36,36,36	0
56	MG	2N	201	1/1	0.95	0.06	62,62,62,62	0
56	MG	1A	3221	1/1	0.95	0.10	61,61,61,61	0
56	MG	1A	3451	1/1	0.95	0.23	48,48,48,48	0
56	MG	1A	3003	1/1	0.95	0.08	28,28,28,28	0
56	MG	1E	304	1/1	0.95	0.15	41,41,41,41	0
56	MG	1d	301	1/1	0.95	0.43	67,67,67,67	0
56	MG	2A	3173	1/1	0.95	0.15	47,47,47,47	0
56	MG	2T	202	1/1	0.95	0.23	59,59,59,59	0
56	MG	1A	3958	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	3959	1/1	0.95	0.07	32,32,32,32	0
56	MG	1f	201	1/1	0.95	0.16	53,53,53,53	0
56	MG	1A	3837	1/1	0.95	0.22	42,42,42,42	0
56	MG	2A	3594	1/1	0.95	0.12	71,71,71,71	0
56	MG	2X	101	1/1	0.95	0.09	72,72,72,72	0
56	MG	1A	3609	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	3348	1/1	0.95	0.13	44,44,44,44	0
56	MG	1m	3001	1/1	0.95	0.09	65,65,65,65	0
56	MG	1E	312	1/1	0.95	0.15	67,67,67,67	0
56	MG	1A	3395	1/1	0.95	0.31	69,69,69,69	0
56	MG	21	103	1/1	0.95	0.12	55,55,55,55	0
56	MG	1A	3522	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3090	1/1	0.95	0.22	60,60,60,60	0
56	MG	1A	3065	1/1	0.95	0.14	45,45,45,45	0
56	MG	1F	302	1/1	0.95	0.15	35,35,35,35	0
56	MG	2f	201	1/1	0.95	0.10	52,52,52,52	0
56	MG	2A	3604	1/1	0.95	0.25	63,63,63,63	0
56	MG	1F	303	1/1	0.95	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	1x	102	1/1	0.95	0.22	69,69,69,69	0
56	MG	1F	304	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3527	1/1	0.95	0.23	48,48,48,48	0
56	MG	2A	3609	1/1	0.95	0.12	65,65,65,65	0
56	MG	1x	105	1/1	0.95	0.20	63,63,63,63	0
56	MG	1A	3845	1/1	0.95	0.10	33,33,33,33	0
56	MG	1F	309	1/1	0.95	0.12	36,36,36,36	0
56	MG	1A	3528	1/1	0.95	0.13	42,42,42,42	0
56	MG	1A	3092	1/1	0.95	0.16	59,59,59,59	0
56	MG	1A	3066	1/1	0.95	0.06	36,36,36,36	0
56	MG	1A	3265	1/1	0.95	0.11	45,45,45,45	0
56	MG	1a	1668	1/1	0.95	0.14	65,65,65,65	0
56	MG	1G	205	1/1	0.95	0.14	69,69,69,69	0
56	MG	1a	1670	1/1	0.95	0.29	64,64,64,64	0
56	MG	1A	3981	1/1	0.95	0.08	27,27,27,27	0
56	MG	1A	3230	1/1	0.95	0.22	52,52,52,52	0
56	MG	1a	1673	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3462	1/1	0.95	0.06	53,53,53,53	0
56	MG	1A	3855	1/1	0.95	0.08	32,32,32,32	0
56	MG	1A	3628	1/1	0.95	0.11	46,46,46,46	0
56	MG	2A	3009	1/1	0.95	0.23	66,66,66,66	0
56	MG	2a	1625	1/1	0.95	0.07	97,97,97,97	0
56	MG	2A	3010	1/1	0.95	0.18	55,55,55,55	0
56	MG	1A	3538	1/1	0.95	0.09	45,45,45,45	0
56	MG	1A	3796	1/1	0.96	0.18	51,51,51,51	0
56	MG	1A	3902	1/1	0.96	0.11	74,74,74,74	0
56	MG	1a	1651	1/1	0.96	0.18	51,51,51,51	0
56	MG	1A	3186	1/1	0.96	0.06	50,50,50,50	0
56	MG	1A	3037	1/1	0.96	0.14	28,28,28,28	0
56	MG	2A	3457	1/1	0.96	0.13	60,60,60,60	0
56	MG	2A	3458	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	4024	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3531	1/1	0.96	0.07	42,42,42,42	0
56	MG	2A	3461	1/1	0.96	0.17	72,72,72,72	0
56	MG	2A	3124	1/1	0.96	0.09	48,48,48,48	0
56	MG	2A	3463	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3473	1/1	0.96	0.15	48,48,48,48	0
56	MG	1A	3908	1/1	0.96	0.09	73,73,73,73	0
56	MG	1Q	201	1/1	0.96	0.17	42,42,42,42	0
56	MG	2a	1645	1/1	0.96	0.30	56,56,56,56	0
56	MG	1Q	202	1/1	0.96	0.07	55,55,55,55	0
56	MG	2A	3668	1/1	0.96	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	3801	1/1	0.96	0.10	38,38,38,38	0
56	MG	2A	3469	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3533	1/1	0.96	0.26	40,40,40,40	0
56	MG	2A	3673	1/1	0.96	0.17	67,67,67,67	0
56	MG	1A	3911	1/1	0.96	0.06	58,58,58,58	0
56	MG	1A	3115	1/1	0.96	0.22	44,44,44,44	0
56	MG	1A	3161	1/1	0.96	0.31	39,39,39,39	0
56	MG	1A	3477	1/1	0.96	0.11	59,59,59,59	0
56	MG	1R	204	1/1	0.96	0.32	45,45,45,45	0
56	MG	1A	3229	1/1	0.96	0.23	42,42,42,42	0
56	MG	1A	3479	1/1	0.96	0.25	35,35,35,35	0
56	MG	2A	3481	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	3613	1/1	0.96	0.07	22,22,22,22	0
56	MG	1A	4038	1/1	0.96	0.08	40,40,40,40	0
56	MG	1A	3304	1/1	0.96	0.28	57,57,57,57	0
56	MG	1A	3081	1/1	0.96	0.13	39,39,39,39	0
56	MG	2A	3689	1/1	0.96	0.08	43,43,43,43	0
56	MG	2A	3486	1/1	0.96	0.16	47,47,47,47	0
56	MG	2A	3691	1/1	0.96	0.25	59,59,59,59	0
56	MG	1A	3483	1/1	0.96	0.28	42,42,42,42	0
56	MG	2A	3693	1/1	0.96	0.05	43,43,43,43	0
56	MG	1U	202	1/1	0.96	0.16	41,41,41,41	0
56	MG	1t	201	1/1	0.96	0.15	67,67,67,67	0
56	MG	1a	1676	1/1	0.96	0.41	77,77,77,77	0
56	MG	2A	3698	1/1	0.96	0.14	50,50,50,50	0
56	MG	2A	3699	1/1	0.96	0.11	57,57,57,57	0
56	MG	2A	3148	1/1	0.96	0.16	60,60,60,60	0
56	MG	2A	3494	1/1	0.96	0.11	37,37,37,37	0
56	MG	1A	3191	1/1	0.96	0.20	41,41,41,41	0
56	MG	1A	3430	1/1	0.96	0.27	65,65,65,65	0
56	MG	1A	3097	1/1	0.96	0.06	42,42,42,42	0
56	MG	1U	207	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	3816	1/1	0.96	0.08	21,21,21,21	0
56	MG	2A	3314	1/1	0.96	0.13	71,71,71,71	0
56	MG	1A	3714	1/1	0.96	0.09	53,53,53,53	0
56	MG	1A	3715	1/1	0.96	0.09	22,22,22,22	0
56	MG	2A	3505	1/1	0.96	0.12	43,43,43,43	0
56	MG	1A	3193	1/1	0.96	0.25	42,42,42,42	0
56	MG	2A	3158	1/1	0.96	0.14	71,71,71,71	0
56	MG	1A	3820	1/1	0.96	0.07	22,22,22,22	0
56	MG	2A	3509	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3821	1/1	0.96	0.15	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	1A	3194	1/1	0.96	0.41	37,37,37,37	0
56	MG	1W	206	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3011	1/1	0.96	0.10	45,45,45,45	0
56	MG	2A	3721	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3514	1/1	0.96	0.17	62,62,62,62	0
56	MG	2A	3723	1/1	0.96	0.06	45,45,45,45	0
56	MG	1X	101	1/1	0.96	0.29	44,44,44,44	0
56	MG	1X	102	1/1	0.96	0.14	46,46,46,46	0
56	MG	1X	103	1/1	0.96	0.08	53,53,53,53	0
56	MG	2A	3002	1/1	0.96	0.28	53,53,53,53	0
56	MG	1A	3623	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3270	1/1	0.96	0.13	60,60,60,60	0
56	MG	2A	3731	1/1	0.96	0.19	62,62,62,62	0
56	MG	1A	3137	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3722	1/1	0.96	0.08	38,38,38,38	0
56	MG	1A	3627	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3438	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3725	1/1	0.96	0.07	46,46,46,46	0
56	MG	2A	3011	1/1	0.96	0.07	48,48,48,48	0
56	MG	1B	205	1/1	0.96	0.09	53,53,53,53	0
56	MG	2A	3740	1/1	0.96	0.15	70,70,70,70	0
56	MG	1A	3629	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3630	1/1	0.96	0.08	41,41,41,41	0
56	MG	2A	3530	1/1	0.96	0.13	62,62,62,62	0
56	MG	2A	3745	1/1	0.96	0.07	43,43,43,43	0
56	MG	2A	3016	1/1	0.96	0.14	46,46,46,46	0
56	MG	2A	3747	1/1	0.96	0.07	61,61,61,61	0
56	MG	2A	3017	1/1	0.96	0.15	63,63,63,63	0
56	MG	2A	3749	1/1	0.96	0.15	65,65,65,65	0
56	MG	2A	3750	1/1	0.96	0.15	67,67,67,67	0
56	MG	1A	3041	1/1	0.96	0.06	35,35,35,35	0
56	MG	1B	209	1/1	0.96	0.06	55,55,55,55	0
56	MG	2A	3535	1/1	0.96	0.16	62,62,62,62	0
56	MG	1A	3633	1/1	0.96	0.14	53,53,53,53	0
56	MG	1A	3314	1/1	0.96	0.10	59,59,59,59	0
56	MG	2A	3345	1/1	0.96	0.39	66,66,66,66	0
56	MG	1A	3139	1/1	0.96	0.20	46,46,46,46	0
56	MG	1A	3085	1/1	0.96	0.21	37,37,37,37	0
56	MG	1A	3736	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3737	1/1	0.96	0.09	32,32,32,32	0
56	MG	1A	3123	1/1	0.96	0.21	42,42,42,42	0
56	MG	11	105	1/1	0.96	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3086	1/1	0.96	0.13	38,38,38,38	0
56	MG	1A	3562	1/1	0.96	0.17	43,43,43,43	0
56	MG	2A	3032	1/1	0.96	0.08	55,55,55,55	0
56	MG	2A	3196	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3742	1/1	0.96	0.07	37,37,37,37	0
56	MG	2A	3034	1/1	0.96	0.18	57,57,57,57	0
56	MG	1B	220	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	3282	1/1	0.96	0.12	48,48,48,48	0
56	MG	1A	3206	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3567	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3557	1/1	0.96	0.18	68,68,68,68	0
56	MG	1A	3643	1/1	0.96	0.06	34,34,34,34	0
56	MG	1A	3644	1/1	0.96	0.06	26,26,26,26	0
56	MG	1a	1723	1/1	0.96	0.15	58,58,58,58	0
56	MG	2A	3562	1/1	0.96	0.13	42,42,42,42	0
56	MG	2A	3563	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	3960	1/1	0.96	0.05	34,34,34,34	0
56	MG	1a	1725	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3042	1/1	0.96	0.19	37,37,37,37	0
56	MG	1a	1727	1/1	0.96	0.11	41,41,41,41	0
56	MG	2a	1753	1/1	0.96	0.15	83,83,83,83	0
56	MG	1A	3962	1/1	0.96	0.05	28,28,28,28	0
56	MG	1A	3647	1/1	0.96	0.06	49,49,49,49	0
56	MG	17	101	1/1	0.96	0.05	34,34,34,34	0
56	MG	1A	3964	1/1	0.96	0.07	49,49,49,49	0
56	MG	17	103	1/1	0.96	0.18	47,47,47,47	0
56	MG	17	104	1/1	0.96	0.08	48,48,48,48	0
56	MG	2a	1760	1/1	0.96	0.24	71,71,71,71	0
56	MG	1a	1735	1/1	0.96	0.21	45,45,45,45	0
56	MG	2A	3378	1/1	0.96	0.16	63,63,63,63	0
56	MG	2A	3379	1/1	0.96	0.40	52,52,52,52	0
56	MG	17	105	1/1	0.96	0.14	62,62,62,62	0
56	MG	2A	3381	1/1	0.96	0.07	59,59,59,59	0
56	MG	1A	3966	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3853	1/1	0.96	0.08	28,28,28,28	0
56	MG	18	103	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	3754	1/1	0.96	0.06	56,56,56,56	0
56	MG	1A	3756	1/1	0.96	0.09	26,26,26,26	0
56	MG	2A	3060	1/1	0.96	0.06	37,37,37,37	0
56	MG	1D	301	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3650	1/1	0.96	0.05	26,26,26,26	0
56	MG	1D	306	1/1	0.96	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	2E	306	1/1	0.96	0.26	67,67,67,67	0
56	MG	1A	3503	1/1	0.96	0.23	51,51,51,51	0
56	MG	2A	3590	1/1	0.96	0.07	49,49,49,49	0
56	MG	2A	3591	1/1	0.96	0.15	65,65,65,65	0
56	MG	1a	1747	1/1	0.96	0.18	49,49,49,49	0
56	MG	2A	3066	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3449	1/1	0.96	0.06	44,44,44,44	0
56	MG	1A	3074	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3173	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3404	1/1	0.96	0.07	46,46,46,46	0
56	MG	1a	1607	1/1	0.96	0.06	59,59,59,59	0
56	MG	1E	301	1/1	0.96	0.21	47,47,47,47	0
56	MG	1A	3663	1/1	0.96	0.09	34,34,34,34	0
56	MG	2Q	201	1/1	0.96	0.10	66,66,66,66	0
56	MG	2A	3075	1/1	0.96	0.08	58,58,58,58	0
56	MG	2Q	203	1/1	0.96	0.09	68,68,68,68	0
56	MG	1a	1611	1/1	0.96	0.08	62,62,62,62	0
56	MG	1A	3575	1/1	0.96	0.26	59,59,59,59	0
56	MG	1A	3665	1/1	0.96	0.09	23,23,23,23	0
56	MG	2A	3241	1/1	0.96	0.16	56,56,56,56	0
56	MG	1A	3406	1/1	0.96	0.21	52,52,52,52	0
56	MG	1a	1615	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3985	1/1	0.96	0.06	57,57,57,57	0
56	MG	2A	3410	1/1	0.96	0.07	38,38,38,38	0
56	MG	1a	1617	1/1	0.96	0.05	47,47,47,47	0
56	MG	1E	308	1/1	0.96	0.13	45,45,45,45	0
56	MG	2A	3612	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3043	1/1	0.96	0.18	39,39,39,39	0
56	MG	1A	3175	1/1	0.96	0.18	37,37,37,37	0
56	MG	1A	3672	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3366	1/1	0.96	0.11	54,54,54,54	0
56	MG	1A	3580	1/1	0.96	0.08	27,27,27,27	0
56	MG	23	101	1/1	0.96	0.13	68,68,68,68	0
56	MG	23	102	1/1	0.96	0.13	59,59,59,59	0
56	MG	2A	3089	1/1	0.96	0.11	60,60,60,60	0
56	MG	27	101	1/1	0.96	0.23	67,67,67,67	0
56	MG	1A	3149	1/1	0.96	0.34	51,51,51,51	0
56	MG	1A	3076	1/1	0.96	0.15	51,51,51,51	0
56	MG	1A	3679	1/1	0.96	0.10	37,37,37,37	0
56	MG	2A	3093	1/1	0.96	0.16	40,40,40,40	0
56	MG	1A	3516	1/1	0.96	0.17	42,42,42,42	0
56	MG	1a	1773	1/1	0.96	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3585	1/1	0.96	0.09	29,29,29,29	0
56	MG	1A	3412	1/1	0.96	0.27	49,49,49,49	0
56	MG	1A	3077	1/1	0.96	0.13	45,45,45,45	0
56	MG	1A	3887	1/1	0.96	0.07	44,44,44,44	0
56	MG	2A	3629	1/1	0.96	0.10	59,59,59,59	0
56	MG	2A	3631	1/1	0.96	0.17	46,46,46,46	0
56	MG	1F	308	1/1	0.96	0.16	52,52,52,52	0
56	MG	1A	3588	1/1	0.96	0.07	54,54,54,54	0
56	MG	1A	3294	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3590	1/1	0.96	0.24	58,58,58,58	0
56	MG	1G	201	1/1	0.96	0.13	47,47,47,47	0
56	MG	1G	202	1/1	0.96	0.19	62,62,62,62	0
56	MG	1A	3111	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	4008	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3790	1/1	0.96	0.26	38,38,38,38	0
56	MG	1A	3465	1/1	0.96	0.18	39,39,39,39	0
56	MG	1A	3155	1/1	0.96	0.24	47,47,47,47	0
56	MG	1A	3374	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3044	1/1	0.96	0.08	40,40,40,40	0
56	MG	2A	3646	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3443	1/1	0.96	0.15	61,61,61,61	0
56	MG	1A	3899	1/1	0.96	0.06	48,48,48,48	0
57	K	1A	3520	1/1	0.96	0.20	85,85,85,85	0
56	MG	1A	3185	1/1	0.96	0.12	39,39,39,39	0
56	MG	2A	3446	1/1	0.96	0.12	42,42,42,42	0
56	MG	2A	3448	1/1	0.96	0.15	69,69,69,69	0
59	ZN	2n	501	1/1	0.96	0.06	107,107,107,107	0
56	MG	1A	3728	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3273	1/1	0.97	0.17	50,50,50,50	0
56	MG	1A	3991	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3096	1/1	0.97	0.17	44,44,44,44	0
56	MG	1A	3480	1/1	0.97	0.11	38,38,38,38	0
56	MG	1A	3815	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3996	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3657	1/1	0.97	0.06	32,32,32,32	0
56	MG	2P	202	1/1	0.97	0.06	65,65,65,65	0
56	MG	1a	1777	1/1	0.97	0.10	64,64,64,64	0
56	MG	1A	3071	1/1	0.97	0.13	42,42,42,42	0
56	MG	2A	3679	1/1	0.97	0.06	54,54,54,54	0
56	MG	1A	3660	1/1	0.97	0.06	35,35,35,35	0
56	MG	2A	3681	1/1	0.97	0.04	63,63,63,63	0
56	MG	1D	304	1/1	0.97	0.06	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3057	1/1	0.97	0.24	54,54,54,54	0
56	MG	1A	3662	1/1	0.97	0.07	28,28,28,28	0
56	MG	2a	1722	1/1	0.97	0.34	54,54,54,54	0
56	MG	2A	3685	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	3593	1/1	0.97	0.05	40,40,40,40	0
56	MG	1A	3209	1/1	0.97	0.07	45,45,45,45	0
56	MG	2A	3179	1/1	0.97	0.07	68,68,68,68	0
56	MG	1D	309	1/1	0.97	0.16	32,32,32,32	0
56	MG	1A	3210	1/1	0.97	0.10	48,48,48,48	0
56	MG	1A	3279	1/1	0.97	0.24	38,38,38,38	0
56	MG	1A	3485	1/1	0.97	0.18	62,62,62,62	0
56	MG	1A	3743	1/1	0.97	0.06	27,27,27,27	0
56	MG	2A	3558	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3668	1/1	0.97	0.11	31,31,31,31	0
56	MG	1A	3916	1/1	0.97	0.05	45,45,45,45	0
56	MG	1A	3669	1/1	0.97	0.18	46,46,46,46	0
56	MG	1A	3670	1/1	0.97	0.06	38,38,38,38	0
56	MG	1E	306	1/1	0.97	0.12	42,42,42,42	0
56	MG	2A	3071	1/1	0.97	0.16	62,62,62,62	0
56	MG	1A	3393	1/1	0.97	0.18	66,66,66,66	0
56	MG	2A	3703	1/1	0.97	0.07	71,71,71,71	0
56	MG	1A	3354	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3439	1/1	0.97	0.24	46,46,46,46	0
56	MG	1A	3543	1/1	0.97	0.19	40,40,40,40	0
56	MG	1A	3923	1/1	0.97	0.07	27,27,27,27	0
56	MG	1A	3116	1/1	0.97	0.14	34,34,34,34	0
56	MG	1a	1801	1/1	0.97	0.19	64,64,64,64	0
56	MG	1A	3755	1/1	0.97	0.22	64,64,64,64	0
56	MG	1A	3098	1/1	0.97	0.15	27,27,27,27	0
56	MG	1A	3284	1/1	0.97	0.12	47,47,47,47	0
56	MG	1A	3606	1/1	0.97	0.04	27,27,27,27	0
56	MG	1E	317	1/1	0.97	0.11	60,60,60,60	0
56	MG	1F	301	1/1	0.97	0.11	44,44,44,44	0
56	MG	1A	3760	1/1	0.97	0.04	45,45,45,45	0
56	MG	1A	3159	1/1	0.97	0.19	38,38,38,38	0
56	MG	1A	3214	1/1	0.97	0.09	56,56,56,56	0
56	MG	1A	3015	1/1	0.97	0.11	40,40,40,40	0
56	MG	1F	306	1/1	0.97	0.19	39,39,39,39	0
56	MG	1A	3019	1/1	0.97	0.32	55,55,55,55	0
56	MG	2A	3584	1/1	0.97	0.12	66,66,66,66	0
56	MG	2A	3451	1/1	0.97	0.11	68,68,68,68	0
56	MG	2a	1761	1/1	0.97	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3452	1/1	0.97	0.15	46,46,46,46	0
56	MG	1A	3612	1/1	0.97	0.13	36,36,36,36	0
56	MG	1A	3289	1/1	0.97	0.18	32,32,32,32	0
56	MG	1A	3120	1/1	0.97	0.18	41,41,41,41	0
56	MG	2A	3456	1/1	0.97	0.07	37,37,37,37	0
56	MG	1F	311	1/1	0.97	0.08	47,47,47,47	0
56	MG	1A	3405	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3689	1/1	0.97	0.05	22,22,22,22	0
56	MG	1A	3054	1/1	0.97	0.15	42,42,42,42	0
56	MG	1a	1709	1/1	0.97	0.13	44,44,44,44	0
56	MG	2A	3099	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3849	1/1	0.97	0.09	56,56,56,56	0
56	MG	1w	101	1/1	0.97	0.09	57,57,57,57	0
56	MG	1A	3555	1/1	0.97	0.13	38,38,38,38	0
56	MG	2A	3741	1/1	0.97	0.06	27,27,27,27	0
56	MG	1A	4041	1/1	0.97	0.07	39,39,39,39	0
56	MG	1A	3063	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3852	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	3557	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3031	1/1	0.97	0.17	27,27,27,27	0
56	MG	1N	204	1/1	0.97	0.07	48,48,48,48	0
56	MG	1a	1610	1/1	0.97	0.10	29,29,29,29	0
56	MG	2A	3473	1/1	0.97	0.07	46,46,46,46	0
56	MG	2A	3110	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	3778	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3078	1/1	0.97	0.15	35,35,35,35	0
56	MG	2A	3477	1/1	0.97	0.10	51,51,51,51	0
56	MG	1A	3329	1/1	0.97	0.07	51,51,51,51	0
56	MG	1A	3145	1/1	0.97	0.21	37,37,37,37	0
56	MG	1A	3331	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	4051	1/1	0.97	0.11	71,71,71,71	0
56	MG	2a	1793	1/1	0.97	0.10	67,67,67,67	0
56	MG	1A	3033	1/1	0.97	0.41	30,30,30,30	0
56	MG	1a	1618	1/1	0.97	0.05	61,61,61,61	0
56	MG	1P	201	1/1	0.97	0.28	40,40,40,40	0
56	MG	1a	1728	1/1	0.97	0.09	41,41,41,41	0
56	MG	2A	3487	1/1	0.97	0.10	39,39,39,39	0
56	MG	1P	202	1/1	0.97	0.24	42,42,42,42	0
56	MG	1A	3863	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3007	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3785	1/1	0.97	0.08	61,61,61,61	0
56	MG	1A	3565	1/1	0.97	0.20	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	3702	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	3460	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3705	1/1	0.97	0.06	20,20,20,20	0
56	MG	1A	3107	1/1	0.97	0.23	41,41,41,41	0
56	MG	1B	202	1/1	0.97	0.31	64,64,64,64	0
56	MG	1A	3108	1/1	0.97	0.30	42,42,42,42	0
56	MG	1A	3632	1/1	0.97	0.10	56,56,56,56	0
56	MG	2A	3370	1/1	0.97	0.17	46,46,46,46	0
56	MG	1R	203	1/1	0.97	0.22	46,46,46,46	0
56	MG	2A	3503	1/1	0.97	0.10	41,41,41,41	0
56	MG	2A	3504	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3093	1/1	0.97	0.13	29,29,29,29	0
56	MG	1A	3418	1/1	0.97	0.26	43,43,43,43	0
56	MG	1A	3013	1/1	0.97	0.21	31,31,31,31	0
56	MG	1A	3880	1/1	0.97	0.09	52,52,52,52	0
56	MG	1A	3466	1/1	0.97	0.17	38,38,38,38	0
56	MG	1A	3199	1/1	0.97	0.19	28,28,28,28	0
56	MG	1A	3152	1/1	0.97	0.09	40,40,40,40	0
56	MG	1A	3422	1/1	0.97	0.21	43,43,43,43	0
56	MG	1A	3023	1/1	0.97	0.08	20,20,20,20	0
56	MG	2A	3382	1/1	0.97	0.23	47,47,47,47	0
56	MG	1A	3203	1/1	0.97	0.05	22,22,22,22	0
56	MG	1A	3204	1/1	0.97	0.04	36,36,36,36	0
56	MG	2A	3264	1/1	0.97	0.13	54,54,54,54	0
56	MG	2D	302	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3524	1/1	0.97	0.09	38,38,38,38	0
56	MG	2A	3147	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3525	1/1	0.97	0.22	45,45,45,45	0
56	MG	1U	208	1/1	0.97	0.37	43,43,43,43	0
56	MG	1A	3978	1/1	0.97	0.10	45,45,45,45	0
56	MG	2A	3151	1/1	0.97	0.08	53,53,53,53	0
56	MG	1A	3979	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3343	1/1	0.97	0.19	33,33,33,33	0
56	MG	1A	3239	1/1	0.97	0.26	32,32,32,32	0
56	MG	1V	204	1/1	0.97	0.20	39,39,39,39	0
56	MG	1A	3649	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3177	1/1	0.97	0.15	32,32,32,32	0
56	MG	1W	203	1/1	0.97	0.16	51,51,51,51	0
56	MG	1A	3178	1/1	0.97	0.15	28,28,28,28	0
56	MG	1A	3652	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3988	1/1	0.97	0.10	46,46,46,46	0
56	MG	2F	301	1/1	0.97	0.07	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	3604	1/1	0.98	0.08	26,26,26,26	0
56	MG	1D	303	1/1	0.98	0.10	27,27,27,27	0
56	MG	1A	3432	1/1	0.98	0.12	42,42,42,42	0
56	MG	2A	3717	1/1	0.98	0.12	44,44,44,44	0
56	MG	1D	305	1/1	0.98	0.14	36,36,36,36	0
56	MG	15	105	1/1	0.98	0.15	36,36,36,36	0
56	MG	1A	3112	1/1	0.98	0.14	41,41,41,41	0
56	MG	1A	3573	1/1	0.98	0.15	19,19,19,19	0
56	MG	2A	3543	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3130	1/1	0.98	0.16	44,44,44,44	0
56	MG	2A	3374	1/1	0.98	0.14	28,28,28,28	0
56	MG	1A	4040	1/1	0.98	0.04	33,33,33,33	0
56	MG	2A	3726	1/1	0.98	0.08	55,55,55,55	0
56	MG	1A	3264	1/1	0.98	0.15	45,45,45,45	0
56	MG	1A	3345	1/1	0.98	0.42	33,33,33,33	0
56	MG	1A	3645	1/1	0.98	0.09	27,27,27,27	0
56	MG	2A	3638	1/1	0.98	0.06	58,58,58,58	0
56	MG	1A	3367	1/1	0.98	0.18	29,29,29,29	0
56	MG	2A	3551	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	3984	1/1	0.98	0.07	57,57,57,57	0
56	MG	1A	3514	1/1	0.98	0.14	42,42,42,42	0
56	MG	2A	3735	1/1	0.98	0.11	46,46,46,46	0
56	MG	1A	3648	1/1	0.98	0.03	25,25,25,25	0
56	MG	1A	3515	1/1	0.98	0.21	43,43,43,43	0
56	MG	1A	3179	1/1	0.98	0.09	36,36,36,36	0
56	MG	1A	3233	1/1	0.98	0.09	66,66,66,66	0
56	MG	1U	201	1/1	0.98	0.15	35,35,35,35	0
56	MG	1a	1746	1/1	0.98	0.10	53,53,53,53	0
56	MG	1A	3234	1/1	0.98	0.26	41,41,41,41	0
56	MG	1A	3012	1/1	0.98	0.04	30,30,30,30	0
56	MG	1A	3738	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3993	1/1	0.98	0.15	30,30,30,30	0
56	MG	1U	206	1/1	0.98	0.18	44,44,44,44	0
56	MG	1a	1752	1/1	0.98	0.04	64,64,64,64	0
56	MG	1A	3654	1/1	0.98	0.04	28,28,28,28	0
56	MG	1A	3069	1/1	0.98	0.11	22,22,22,22	0
56	MG	1A	4057	1/1	0.98	0.19	61,61,61,61	0
56	MG	1A	3032	1/1	0.98	0.17	36,36,36,36	0
56	MG	1V	201	1/1	0.98	0.42	34,34,34,34	0
56	MG	1A	3889	1/1	0.98	0.04	18,18,18,18	0
56	MG	1A	3396	1/1	0.98	0.10	51,51,51,51	0
56	MG	1A	3658	1/1	0.98	0.09	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	1V	206	1/1	0.98	0.15	61,61,61,61	0
56	MG	1A	4000	1/1	0.98	0.07	26,26,26,26	0
56	MG	1A	3160	1/1	0.98	0.22	44,44,44,44	0
56	MG	1A	3010	1/1	0.98	0.05	38,38,38,38	0
56	MG	1W	204	1/1	0.98	0.17	41,41,41,41	0
56	MG	1A	3072	1/1	0.98	0.07	16,16,16,16	0
56	MG	2A	3493	1/1	0.98	0.10	41,41,41,41	0
56	MG	2A	3670	1/1	0.98	0.06	65,65,65,65	0
56	MG	1A	3747	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	3021	1/1	0.98	0.12	35,35,35,35	0
56	MG	2A	3766	1/1	0.98	0.04	51,51,51,51	0
56	MG	2A	3166	1/1	0.98	0.09	35,35,35,35	0
56	MG	1A	3625	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3153	1/1	0.98	0.14	46,46,46,46	0
56	MG	1A	3752	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3592	1/1	0.98	0.07	27,27,27,27	0
56	MG	1A	4010	1/1	0.98	0.09	55,55,55,55	0
56	MG	1A	3276	1/1	0.98	0.12	30,30,30,30	0
56	MG	1A	3475	1/1	0.98	0.20	45,45,45,45	0
56	MG	2A	3014	1/1	0.98	0.08	53,53,53,53	0
56	MG	1A	3450	1/1	0.98	0.12	61,61,61,61	0
56	MG	1A	3227	1/1	0.98	0.15	41,41,41,41	0
56	MG	1A	3758	1/1	0.98	0.06	48,48,48,48	0
56	MG	10	101	1/1	0.98	0.10	54,54,54,54	0
56	MG	1A	4017	1/1	0.98	0.12	49,49,49,49	0
56	MG	2A	3020	1/1	0.98	0.10	29,29,29,29	0
56	MG	1a	1633	1/1	0.98	0.12	27,27,27,27	0
56	MG	1A	3144	1/1	0.98	0.11	40,40,40,40	0
56	MG	1A	3005	1/1	0.98	0.09	49,49,49,49	0
56	MG	1A	3535	1/1	0.98	0.11	42,42,42,42	0
56	MG	2A	3025	1/1	0.98	0.08	44,44,44,44	0
56	MG	1A	3762	1/1	0.98	0.08	25,25,25,25	0
56	MG	1A	3536	1/1	0.98	0.10	46,46,46,46	0
56	MG	1A	3675	1/1	0.98	0.05	29,29,29,29	0
56	MG	1A	3965	1/1	0.98	0.08	46,46,46,46	0
56	MG	2A	3697	1/1	0.98	0.20	68,68,68,68	0
56	MG	1A	3280	1/1	0.98	0.33	43,43,43,43	0
56	MG	1A	3677	1/1	0.98	0.04	18,18,18,18	0
56	MG	2A	3436	1/1	0.98	0.10	60,60,60,60	0
56	MG	1A	3860	1/1	0.98	0.07	36,36,36,36	0
56	MG	1A	3767	1/1	0.98	0.08	29,29,29,29	0
56	MG	1A	4030	1/1	0.98	0.19	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3862	1/1	0.98	0.08	54,54,54,54	0
56	MG	1a	1795	1/1	0.98	0.04	55,55,55,55	0
56	MG	1A	3971	1/1	0.98	0.04	62,62,62,62	0
56	MG	13	101	1/1	0.98	0.11	45,45,45,45	0
56	MG	1A	3281	1/1	0.98	0.31	41,41,41,41	0
56	MG	1A	3864	1/1	0.98	0.12	38,38,38,38	0
56	MG	1A	3215	1/1	0.98	0.14	46,46,46,46	0
58	WC9	1A	4061	34/34	0.98	0.06	21,28,31,33	0
58	WC9	2A	3772	34/34	0.98	0.07	36,44,47,52	0
56	MG	2A	3447	1/1	0.98	0.06	43,43,43,43	0
59	ZN	2Y	501	1/1	0.98	0.04	96,96,96,96	0
56	MG	1a	1652	1/1	0.98	0.12	54,54,54,54	0
56	MG	1P	206	1/1	0.98	0.05	43,43,43,43	0
60	SF4	2d	302	8/8	0.98	0.05	70,77,82,85	0
56	MG	1A	3882	1/1	0.99	0.04	65,65,65,65	0
56	MG	1A	3014	1/1	0.99	0.11	34,34,34,34	0
56	MG	1A	3109	1/1	0.99	0.04	42,42,42,42	0
56	MG	1A	3982	1/1	0.99	0.04	50,50,50,50	0
56	MG	1A	3140	1/1	0.99	0.07	25,25,25,25	0
56	MG	1A	3905	1/1	0.99	0.04	54,54,54,54	0
56	MG	1A	3748	1/1	0.99	0.03	48,48,48,48	0
56	MG	1A	3584	1/1	0.99	0.04	45,45,45,45	0
56	MG	1A	3084	1/1	0.99	0.12	42,42,42,42	0
56	MG	1A	3947	1/1	0.99	0.03	57,57,57,57	0
56	MG	1A	3222	1/1	0.99	0.14	45,45,45,45	0
56	MG	1A	3872	1/1	0.99	0.02	26,26,26,26	0
56	MG	2A	3480	1/1	0.99	0.07	38,38,38,38	0
56	MG	1A	3873	1/1	0.99	0.03	31,31,31,31	0
56	MG	1V	205	1/1	0.99	0.21	56,56,56,56	0
56	MG	1A	3566	1/1	0.99	0.25	39,39,39,39	0
56	MG	1A	3610	1/1	0.99	0.03	20,20,20,20	0
56	MG	1A	3768	1/1	0.99	0.07	24,24,24,24	0
56	MG	1A	3068	1/1	0.99	0.12	30,30,30,30	0
56	MG	1A	4018	1/1	0.99	0.08	34,34,34,34	0
59	ZN	1Y	203	1/1	0.99	0.02	67,67,67,67	0
56	MG	1A	3047	1/1	0.99	0.07	41,41,41,41	0
59	ZN	1n	102	1/1	0.99	0.03	65,65,65,65	0
56	MG	2A	3008	1/1	0.99	0.04	45,45,45,45	0
56	MG	1A	3661	1/1	0.99	0.03	27,27,27,27	0
59	ZN	26	501	1/1	0.99	0.03	68,68,68,68	0
59	ZN	29	501	1/1	0.99	0.03	78,78,78,78	0
56	MG	1A	3200	1/1	0.99	0.05	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	SF4	1d	302	8/8	0.99	0.04	62,72,73,73	0
56	MG	1A	3009	1/1	0.99	0.03	30,30,30,30	0
59	ZN	16	102	1/1	1.00	0.03	48,48,48,48	0
59	ZN	19	102	1/1	1.00	0.06	52,52,52,52	0
56	MG	1A	4013	1/1	1.00	0.07	36,36,36,36	0
56	MG	2A	3630	1/1	1.00	0.03	35,35,35,35	0
56	MG	1A	3704	1/1	1.00	0.07	28,28,28,28	0
59	ZN	25	102	1/1	1.00	0.03	59,59,59,59	0
56	MG	1A	3727	1/1	1.00	0.03	28,28,28,28	0
56	MG	1A	3734	1/1	1.00	0.04	42,42,42,42	0
56	MG	1A	3867	1/1	1.00	0.09	45,45,45,45	0
56	MG	1A	3892	1/1	1.00	0.03	34,34,34,34	0
59	ZN	15	108	1/1	1.00	0.02	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.