wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2026 – 04:31 AM EDT

PDB ID	:	8UD8 / pdb_00008ud8
Title	:	Crystal structure of the A2503-C2,C8-dimethylated 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
Authors	:	Aleksandrova, E.V.; Syroegin, E.A.; Wu, K.J.Y.; Tresco, B.I.C.; Ramkissoon, A.; See, D.N.Y.; Liow, P.; Dittemore, G.A.; Yu, M.; Testolin, G.; Mitcheltree, M.J.; Liu, R.Y.; Svetlov, M.S.; Myers, A.G.; Polikanov, Y.S.
Deposited on	:	2023-09-28
Resolution	:	2.60 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:

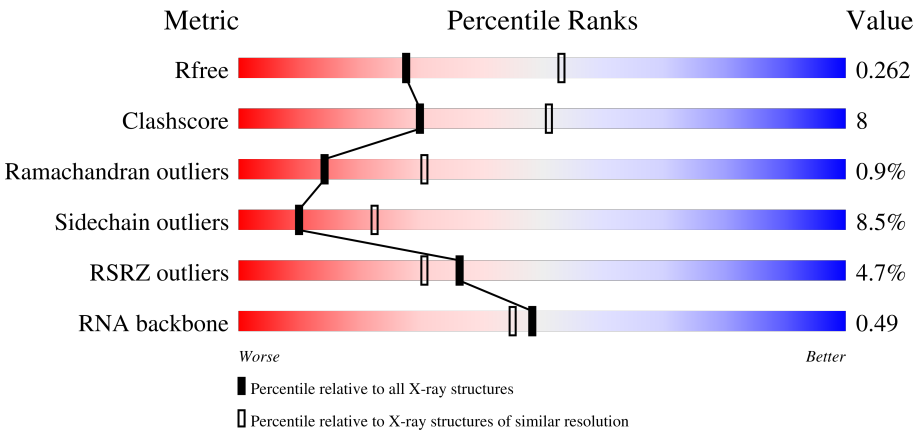
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12

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 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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% 63% 29% 6% •

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Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
1	2A	2915	4% 57% 33% 7% •
2	1B	121	74% 24% • •
2	2B	121	% 52% 38% 9% •
3	1D	276	% 77% 21% •
3	2D	276	% 82% 17% •
4	1E	206	79% 17% • •
4	2E	206	3% 72% 25% • •
5	1F	210	71% 23% • •
5	2F	210	% 65% 28% • • •
6	1G	182	3% 69% 29% • •
6	2G	182	4% 55% 38% 5% • •
7	1H	180	2% 68% 27% • •
7	2H	180	20% 69% 26% • •
8	1I	148	3% 64% 30% 5% •
8	2I	148	7% 69% 23% 7% •
9	1N	140	% 77% 21% •
9	2N	140	4% 78% 21% •
10	1O	122	76% 24%
10	2O	122	% 59% 35% 6%
11	1P	150	71% 25% • • •
11	2P	150	% 71% 25% • • •
12	1Q	141	% 79% 20% •
12	2Q	141	4% 75% 24% •
13	1R	118	78% 20% •
13	2R	118	% 76% 19% •

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Mol	Chain	Length	Quality of chain
14	1S	112	73% 23%
14	2S	112	5% 63% 28% 7%
15	1T	146	2% 71% 18% 10%
15	2T	146	% 62% 25% 10%
16	1U	118	81% 15%
16	2U	118	3% 76% 21%
17	1V	101	82% 16%
17	2V	101	% 76% 22%
18	1W	113	% 82% 15%
18	2W	113	76% 21%
19	1X	96	73% 24%
19	2X	96	3% 70% 25%
20	1Y	110	2% 70% 21% 6%
20	2Y	110	11% 67% 29%
21	1Z	206	3% 49% 22% 25%
21	2Z	206	10% 45% 28% 22%
22	10	85	4% 82% 15%
22	20	85	9% 79% 16%
23	11	98	3% 85% 10%
23	21	98	% 72% 23%
24	12	72	3% 82% 15%
24	22	72	3% 64% 29%
25	13	60	3% 58% 37%
25	23	60	2% 63% 32%
26	14	71	14% 37% 48% 11%

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Mol	Chain	Length	Quality of chain
26	24	71	10% 41% 44% 13%
27	15	60	90% 8%
27	25	60	5% 77% 20%
28	16	54	74% 20%
28	26	54	85% 13%
29	17	49	6% 73% 20%
29	27	49	6% 69% 24%
30	18	65	68% 31%
30	28	65	2% 75% 23%
31	19	37	86% 14%
31	29	37	8% 70% 30%
32	1a	1521	3% 58% 35% 6%
32	2a	1521	4% 52% 39% 8%
33	1b	256	16% 46% 37% 7% 10%
33	2b	256	16% 46% 36% 7% 10%
34	1c	239	3% 58% 24% 14%
34	2c	239	10% 50% 32% 14%
35	1d	209	6% 65% 29% 6%
35	2d	209	% 67% 29%
36	1e	162	2% 51% 37% 9%
36	2e	162	2% 46% 40% 6% 9%
37	1f	101	58% 41%
37	2f	101	2% 68% 27%
38	1g	156	5% 71% 27%
38	2g	156	6% 76% 19%

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Mol	Chain	Length	Quality of chain
39	1h	138	%, 64%, 30%
39	2h	138	2%, 69%, 27%
40	1i	128	16%, 60%, 36%
40	2i	128	23%, 57%, 38%, 5%
41	1j	105	12%, 61%, 26%, 6%, 8%
41	2j	105	40%, 52%, 33%, 6%, 9%
42	1k	129	3%, 64%, 21%, 12%
42	2k	129	3%, 57%, 28%, 12%
43	1l	132	2%, 74%, 17%, 8%
43	2l	132	3%, 68%, 23%, 8%
44	1m	126	6%, 67%, 25%, 6%
44	2m	126	17%, 52%, 40%, 5%
45	1n	61	11%, 70%, 28%
45	2n	61	34%, 70%, 28%
46	1o	89	%, 72%, 24%
46	2o	89	2%, 69%, 27%
47	1p	88	2%, 61%, 26%, 6%, 7%
47	2p	88	6%, 56%, 35%, 7%
48	1q	105	3%, 68%, 26%, 6%
48	2q	105	5%, 71%, 23%, 6%
49	1r	88	%, 61%, 15%, 23%
49	2r	88	%, 53%, 23%, 23%
50	1s	93	3%, 56%, 29%, 11%
50	2s	93	15%, 45%, 40%, 11%
51	1t	106	7%, 60%, 25%, 9%

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Mol	Chain	Length	Quality of chain
51	2t	106	2% 65% 23% 9%
52	1u	27	15% 59% 26% 15%
52	2u	27	15% 63% 22% 15%
53	1v	24	4% 38% 17% 46%
53	2v	24	12% 46% 46%
54	1w	76	17% 32% 47% 18%
54	1y	76	3% 30% 43% 20%
54	2w	76	18% 36% 50% 9% 5%
54	2y	76	12% 30% 45% 20%
55	1x	77	3% 70% 25%
55	2x	77	4% 61% 35%

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	-
60	SF4	1d	302	-	-	X	-

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 299649 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	61853	27532	11572	19878	2871	0	0	0
1	2A	2800	60323	26849	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	74	1592	713	285	518	74	2	0	0	0
54	1y	74	1585	707	285	518	74	1	0	0	0
54	2w	72	1544	690	278	502	72	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	1096	1096	1096	0	0
56	1B	36	36	36	0	0
56	1D	14	14	14	0	0
56	1E	15	15	15	0	0
56	1F	15	15	15	0	0
56	1G	5	5	5	0	0
56	1H	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1I	1	1	1	0	0
56	1N	6	6	6	0	0
56	1O	5	5	5	0	0
56	1P	5	5	5	0	0
56	1Q	6	6	6	0	0
56	1R	6	6	6	0	0
56	1S	3	3	3	0	0
56	1T	2	2	2	0	0
56	1U	9	9	9	0	0
56	1V	6	6	6	0	0
56	1W	7	7	7	0	0
56	1X	7	7	7	0	0
56	1Y	5	5	5	0	0
56	1Z	4	4	4	0	0
56	10	8	8	8	0	0
56	11	6	6	6	0	0
56	12	2	2	2	0	0
56	13	3	3	3	0	0
56	14	1	1	1	0	0
56	15	10	10	10	0	0
56	16	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	17	6	6	6	0	0
56	18	6	6	6	0	0
56	19	1	1	1	0	0
56	1a	210	210	210	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	2	2	2	0	0
56	1k	1	1	1	0	0
56	1l	2	2	2	0	0
56	1m	1	1	1	0	0
56	1n	2	2	2	0	0
56	1p	1	1	1	0	0
56	1t	1	1	1	0	0
56	1w	8	8	8	0	0
56	1x	15	15	15	0	0
56	1y	1	1	1	0	0
56	2A	844	844	844	0	0
56	2B	19	19	19	0	0
56	2D	8	8	8	0	0
56	2E	9	9	9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	2F	8	8	8	0	0
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	4	4	4	0	0
56	2R	4	4	4	0	0
56	2T	3	3	3	0	0
56	2U	2	2	2	0	0
56	2V	2	2	2	0	0
56	2W	3	3	3	0	0
56	2X	2	2	2	0	0
56	2Z	1	1	1	0	0
56	20	4	4	4	0	0
56	21	1	1	1	0	0
56	23	2	2	2	0	0
56	25	6	6	6	0	0
56	26	1	1	1	0	0
56	27	3	3	3	0	0
56	28	3	3	3	0	0
56	2a	225	225	225	0	0

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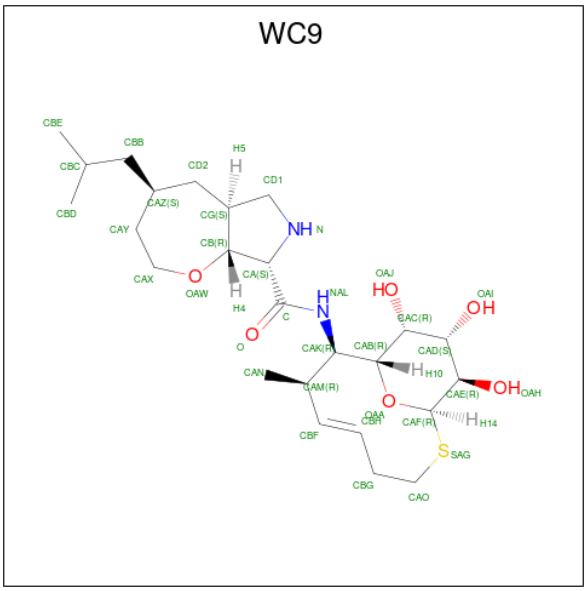
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2d	2	Total Mg 2 2	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	2	Total Mg 2 2	0	0
56	2g	1	Total Mg 1 1	0	0
56	2j	1	Total Mg 1 1	0	0
56	2l	5	Total Mg 5 5	0	0
56	2m	1	Total Mg 1 1	0	0
56	2q	3	Total Mg 3 3	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	3	Total Mg 3 3	0	0
56	2w	6	Total Mg 6 6	0	0
56	2x	7	Total Mg 7 7	0	0
56	2y	7	Total Mg 7 7	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	2A	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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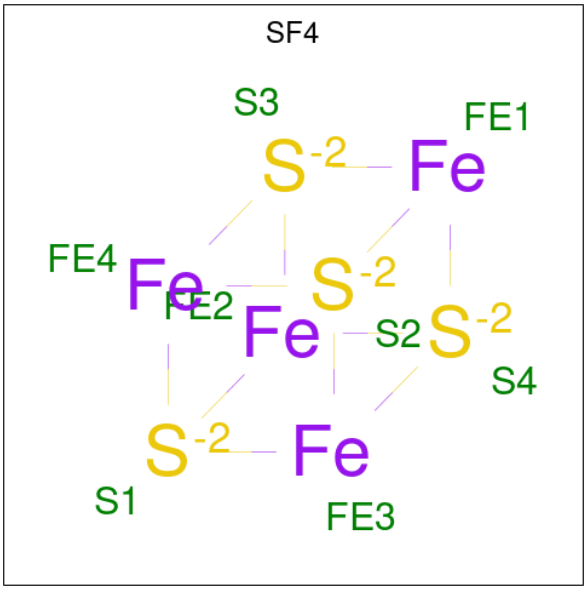
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- 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	1907	Total O 1907 1907	0	0
61	1B	59	Total O 59 59	0	0
61	1D	26	Total O 26 26	0	0
61	1E	28	Total O 28 28	0	0
61	1F	17	Total O 17 17	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	2	Total O 2 2	0	0
61	1H	2	Total O 2 2	0	0
61	1N	4	Total O 4 4	0	0
61	1O	4	Total O 4 4	0	0
61	1P	23	Total O 23 23	0	0
61	1Q	5	Total O 5 5	0	0
61	1R	10	Total O 10 10	0	0
61	1S	3	Total O 3 3	0	0
61	1T	8	Total O 8 8	0	0
61	1U	14	Total O 14 14	0	0
61	1V	7	Total O 7 7	0	0
61	1W	7	Total O 7 7	0	0
61	1X	6	Total O 6 6	0	0
61	1Y	2	Total O 2 2	0	0
61	1Z	1	Total O 1 1	0	0
61	10	11	Total O 11 11	0	0
61	11	9	Total O 9 9	0	0
61	12	3	Total O 3 3	0	0
61	13	5	Total O 5 5	0	0
61	14	1	Total O 1 1	0	0
61	15	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	16	3	Total O 3 3	0	0
61	17	8	Total O 8 8	0	0
61	18	7	Total O 7 7	0	0
61	1a	267	Total O 267 267	0	0
61	1b	1	Total O 1 1	0	0
61	1e	1	Total O 1 1	0	0
61	1j	1	Total O 1 1	0	0
61	1l	3	Total O 3 3	0	0
61	1n	1	Total O 1 1	0	0
61	1q	2	Total O 2 2	0	0
61	1v	4	Total O 4 4	0	0
61	1w	15	Total O 15 15	0	0
61	1x	10	Total O 10 10	0	0
61	1y	2	Total O 2 2	0	0
61	2A	1000	Total O 1000 1000	0	0
61	2B	18	Total O 18 18	0	0
61	2D	17	Total O 17 17	0	0
61	2E	10	Total O 10 10	0	0
61	2F	12	Total O 12 12	0	0
61	2O	2	Total O 2 2	0	0
61	2P	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2Q	2	Total O 2 2	0	0
61	2R	2	Total O 2 2	0	0
61	2T	4	Total O 4 4	0	0
61	2U	2	Total O 2 2	0	0
61	2V	1	Total O 1 1	0	0
61	2W	3	Total O 3 3	0	0
61	2X	1	Total O 1 1	0	0
61	2Y	2	Total O 2 2	0	0
61	20	3	Total O 3 3	0	0
61	21	8	Total O 8 8	0	0
61	23	1	Total O 1 1	0	0
61	27	4	Total O 4 4	0	0
61	28	3	Total O 3 3	0	0
61	29	1	Total O 1 1	0	0
61	2a	172	Total O 172 172	0	0
61	2d	2	Total O 2 2	0	0
61	2e	1	Total O 1 1	0	0
61	2i	1	Total O 1 1	0	0
61	2j	2	Total O 2 2	0	0
61	2l	4	Total O 4 4	0	0
61	2p	1	Total O 1 1	0	0

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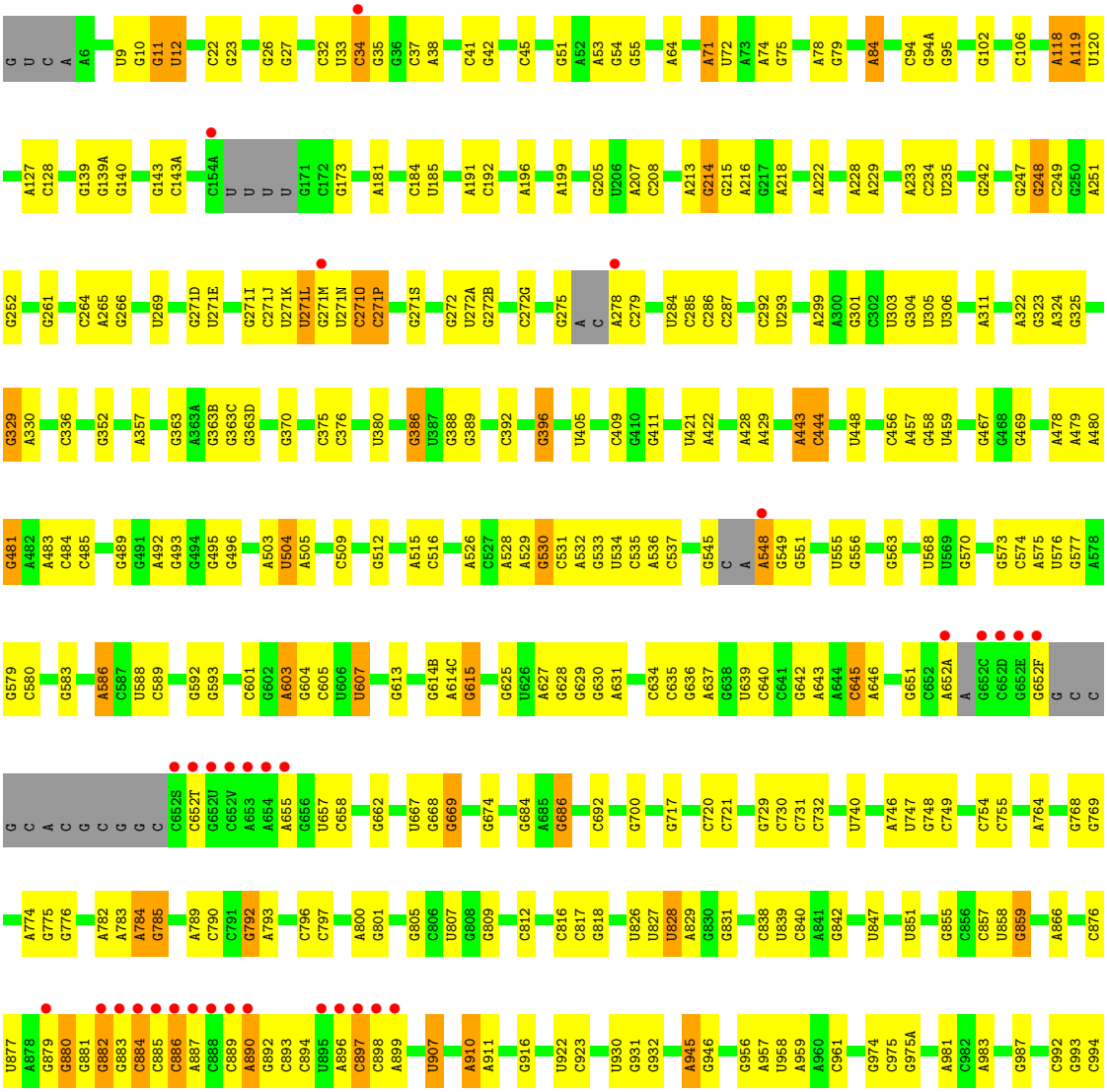
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2q	1	Total O 1 1	0	0
61	2r	1	Total O 1 1	0	0
61	2t	2	Total O 2 2	0	0
61	2v	3	Total O 3 3	0	0
61	2w	3	Total O 3 3	0	0
61	2x	4	Total O 4 4	0	0
61	2y	4	Total O 4 4	0	0

3 Residue-property plots (i)

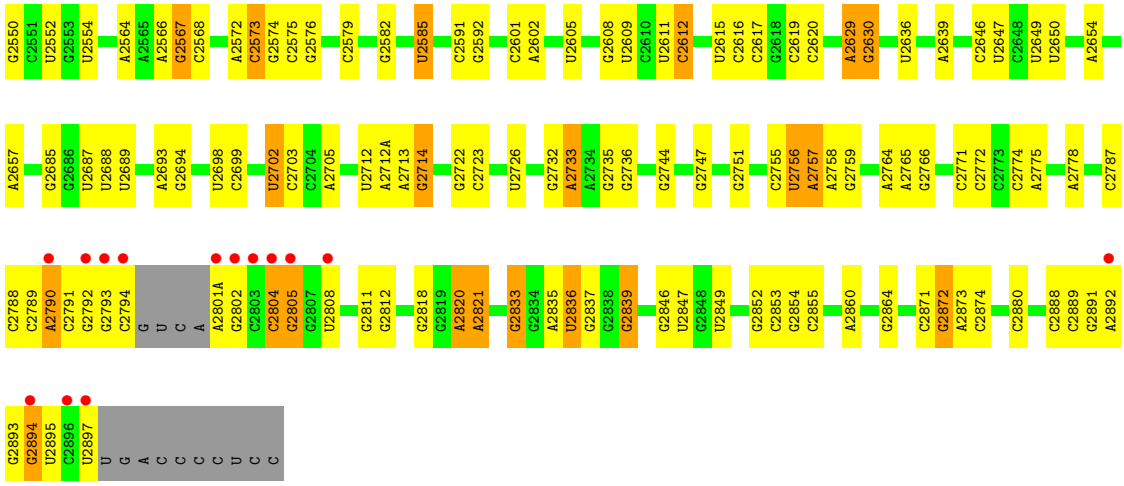
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:

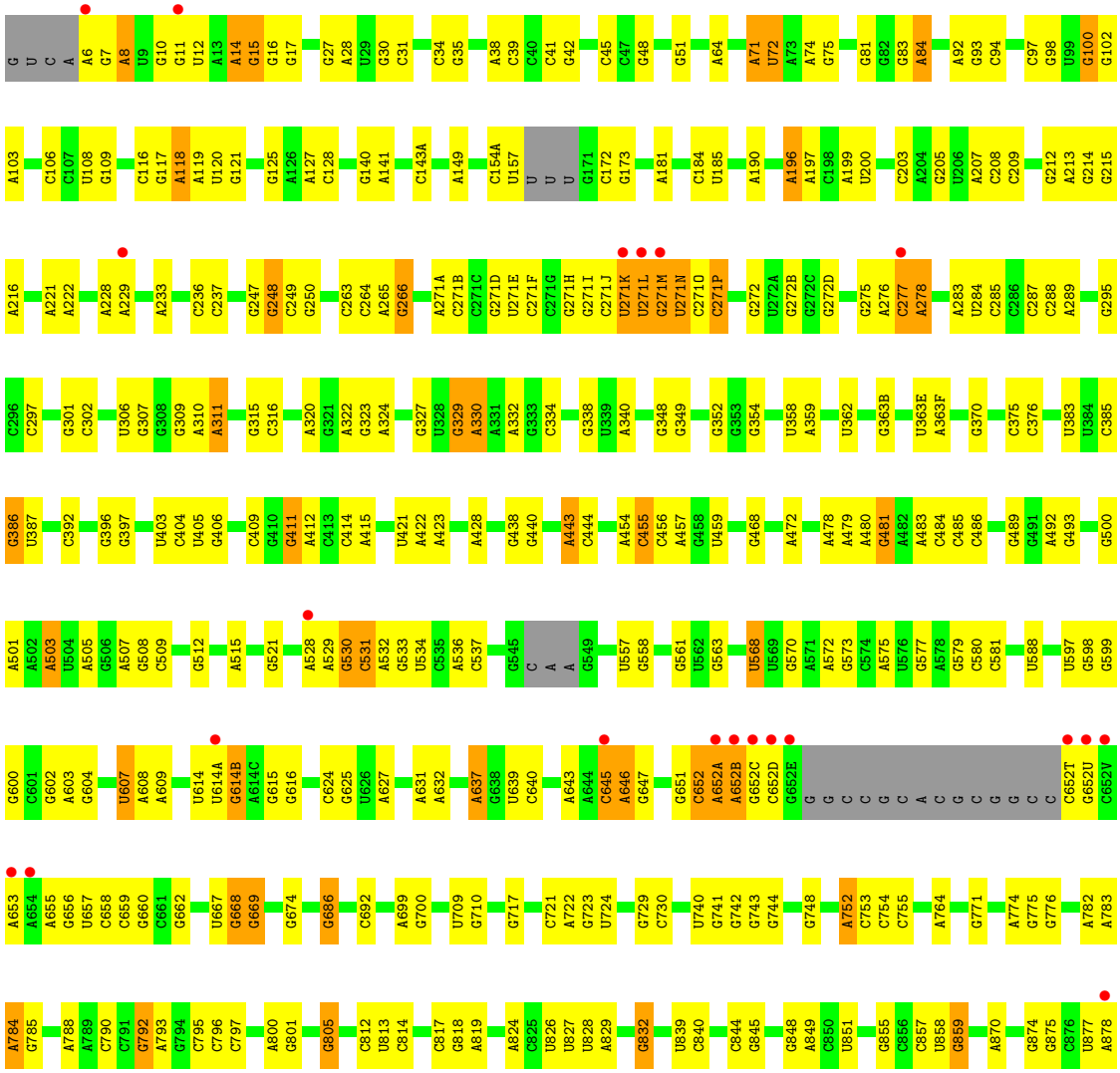


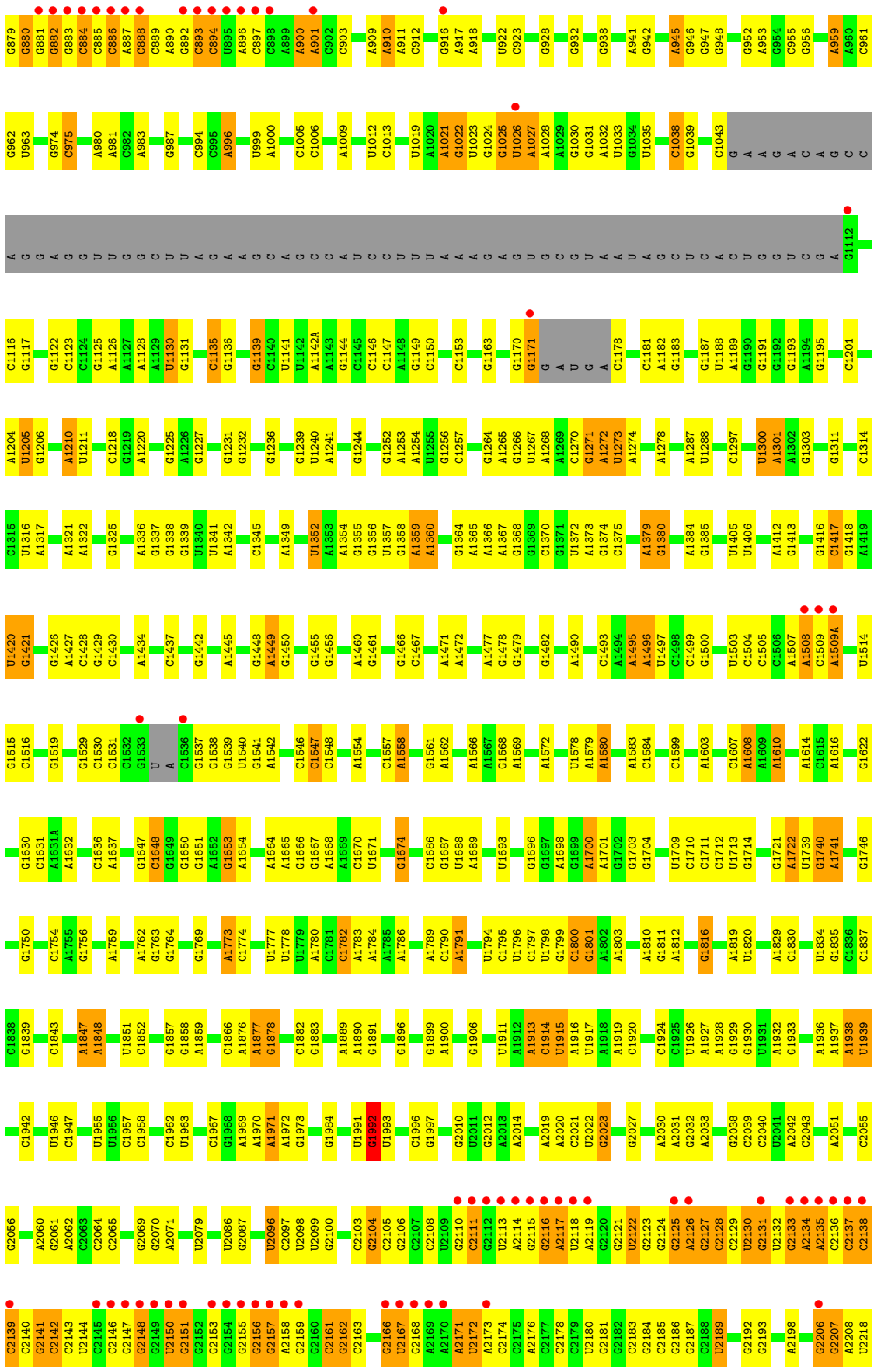
C995 A996 A1000 G1003 C1004 C1005 C1006 A1009 A1010 G1011 U1012 C1013 U1014 U1019 G1022 U1023 G1024 G1025 U1026 A1027 A1028 U1033 G1034 U1035 C1038 G1039 C1040 C1041 G1044 A1045 A1046 G1047 A1048 G1051 C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U G1062 G1063 C1064 U1065 U1066 A1067 G1068
A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1125 A1126 C1135 G1136 G1137 G1138 G1139 C1140 U1141
C1152 A1155 A1156 U1165 C1166 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 G1187 U1188 C1201 G1209 C1218 G1219 A1220 G1223 A1226 G1243 A1247 A1253 G1256 C1257 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 G1283 A1286 U1292
C1293 C1297 U1300 A1301 A1302 G1303 G1310 G1311 U1312 C1315 U1316 A1317 C1320 U1323 G1324 G1332 U1341 U1352 G1356 A1359 A1360 A1365 G1368 G1369 C1370 G1371 U1372 A1379 A1384 G1385 U1396 U1405 U1406 C1407 G1416 C1417 G1418 A1419 U1420 G1421 G1424
G1425 G1426 A1427 C1428 G1429 C1430 U1431 A1445 G1448 A1449 G1450 U1453 G1455 G1456 C1467 A1471 A1472 G1478 G1482 C1493 A1494 A1495 A1496 C1506 A1507 A1508 C1509 A1509A A1528 C1532 G U A C G1537 U1540 G1541 A1542 C1543 C1557 A1558 G1559 A1569 A1570 A1571 A1572
U1578 A1579 A1580 G1581 C1584 A1586 A1587 C1588 C1589 G1593 G1594 U1602 C1607 A1608 A1609 A1610 A1614 G1622 A1632 G1633 A1634 G1647 C1648 C1658 C1663 A1664 A1669 C1670 U1671 C1672 U1673 G1674 C1686 G1687 U1688 U1693 C1694 G1695 G1696 G1697 A1698 G1699 A1700 A1701 G1702 G1703
G1704 G1705 U1706 U1709 C1710 C1711 C1712 U1713 G1721 A1722 U1739 G1740 A1741 C1744 C1745 C1745A G1746 G1750 G1756 U1757 G1758 A1762 G1763 G1764 G1769 A1773 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 C1790 A1791 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 A1810
G1811 G1814 A1815 G1816 G1817 U1818 C1827 G1828 A1829 G1840 G1846 A1847 U1851 C1852 G1865 C1866 A1876 A1877 G1878 C1881 C1882 A1889 G1899 A1900 G1903 G1906 U1911 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 G1929 G1930 A1936 A1937 A1938 U1939 C1942
U1943 A1952 U1955 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1974 G1975 G1992 U1993 C1996 G1997 G1998 C1999 G2000 A2001 G2002 G2012 A2013 A2014 A2020 C2021 U2022 G2023 G2027 A2030 A2031 G2032 A2033 G2037 G2038 C2039 C2040 U2041 A2042 C2043 G2046 A2051
C2055 G2056 A2057 A2060 G2061 A2062 G2067 U2068 G2069 G2070 A2071 U2074 U2075 G2090 C2097 U2098 U2099 G2100 C2101 U2102 C2103 C2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137
C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 U2180 G2181 G2182 C2183 G2184 G2187 C2188 U2189 G2190 G2191 G2192 A2198 U2203 C2205 G2206 G2207 A2208 U2218 G2219
G2222 G2223 G2224 A2225 U2233 G2234 G2235 C2236 G2237 G2238 G2239 U2243 U2244 A2247 C2248 U2249 G2250 G2251 C2254 U2262 C2263 C2264 A2268 A2269 G2270 G2271 G2276 G2277 G2280 C2283 C2284 C2285 A2286 A2287 U2291 C2292 U2296 C2297 A2298 G2299 A2305 C2306 G2307 G2308 G2315 C2316
G2319 A2320 G2325 C2326 A2327 A2328 G2329 G2330 G2331 G2334 A2335 A2336 G2341 C2342 C2343 U2344 C2347 C2350 G2353 G2354 C2355 C2359 A2360 A2361 A2369 A2376 A2377 A2378 G2379 C2380 G2383 G2384 C2385 C2386 U2387 U2390 G2391 G2400 G2405 U2406 G2407 A2422 U2423 C2424 A2425
A2426 C2427 G2428 G2429 A2430 U2431 A2435 A2439 C2440 C2441 G2445 G2446 G2447 A2448 U2449 A2450 G2454 C2466 C2467 G2468 A2469 G2470 C2474 C2475 A2476 C2477 A2478 G2485 G2490 U2491 U2492 U2493 A2497 C2498 C2499 G2502 8AH2503 U2504 G2505 U2506 C2512 G2513 A2518 U2537 C2538 G2549



- Molecule 1: 23S Ribosomal RNA

Chain 2A:

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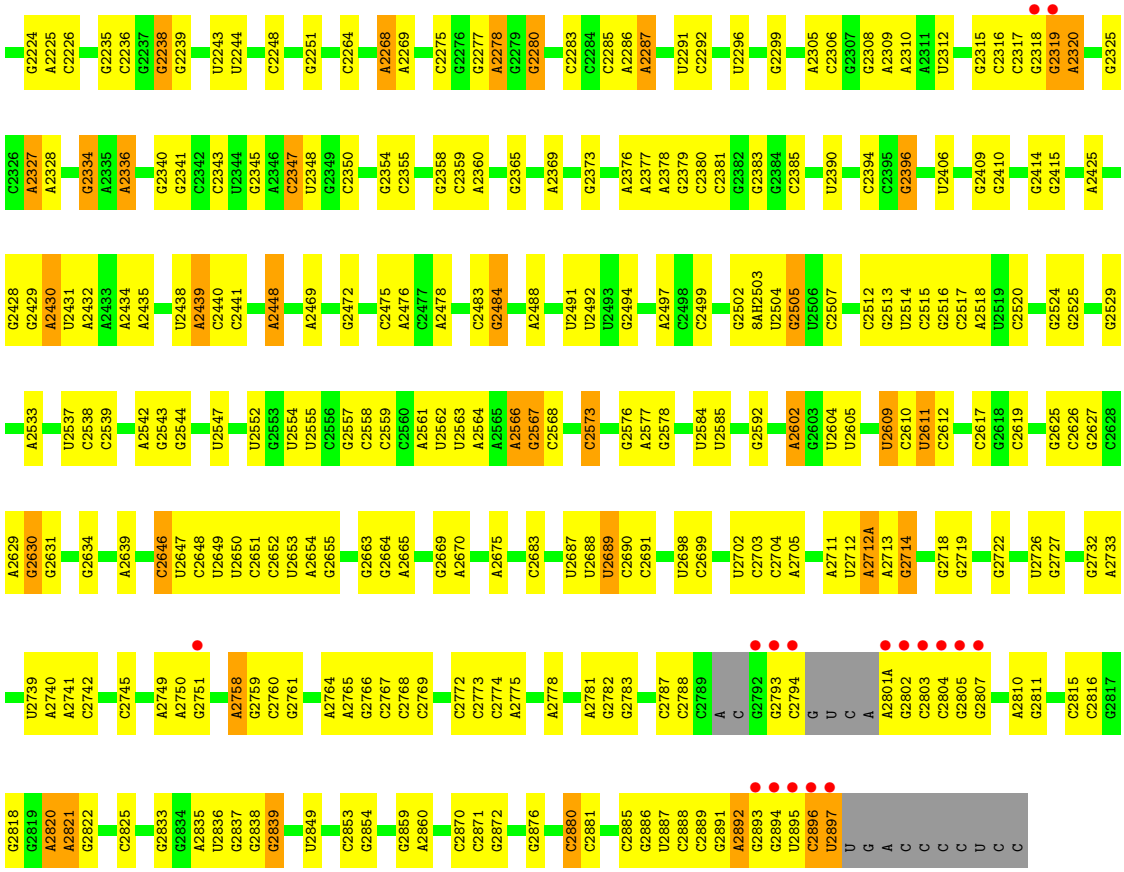
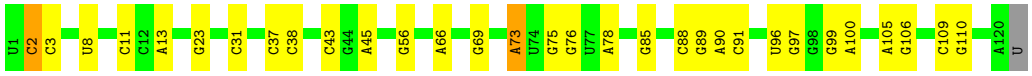


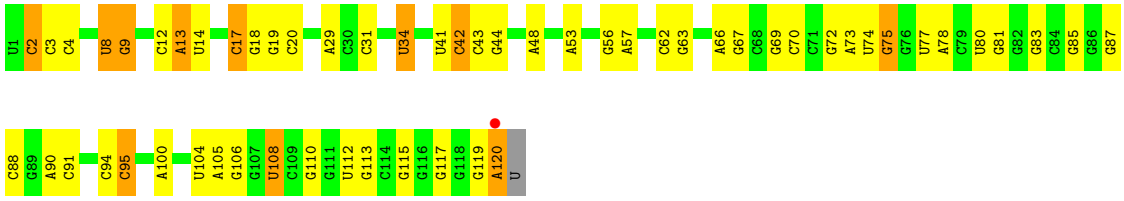
- Molecule 2: 5S Ribosomal RNA

Chain 1B:



- Molecule 2: 5S Ribosomal RNA

Chain 2B:

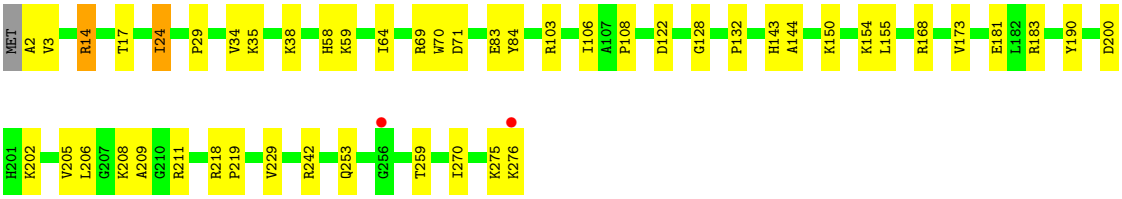


- Molecule 3: 50S ribosomal protein L2

Chain 1D:

• Molecule 3: 50S ribosomal protein L2

Chain 2D:

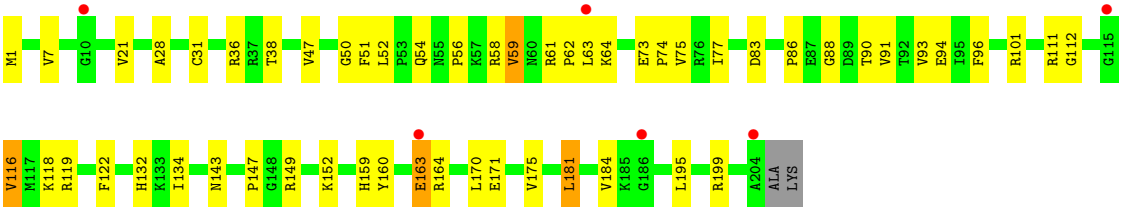


• Molecule 4: 50S ribosomal protein L3

Chain 1E:

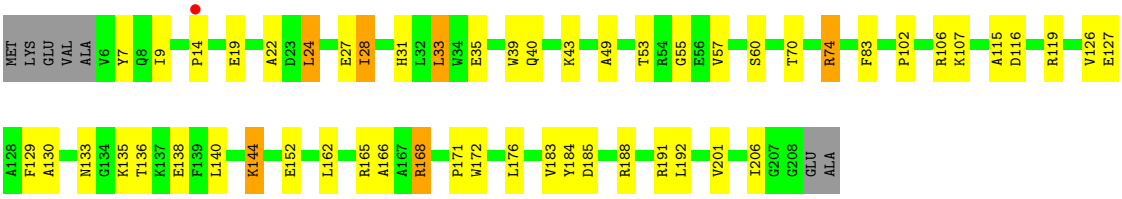
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



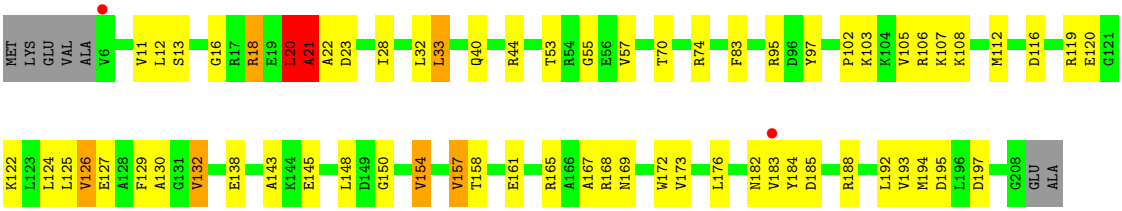
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



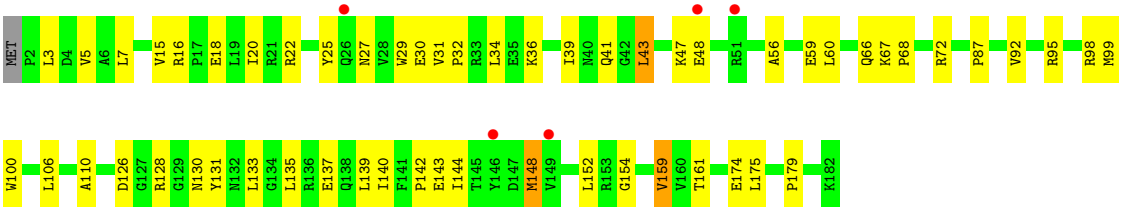
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



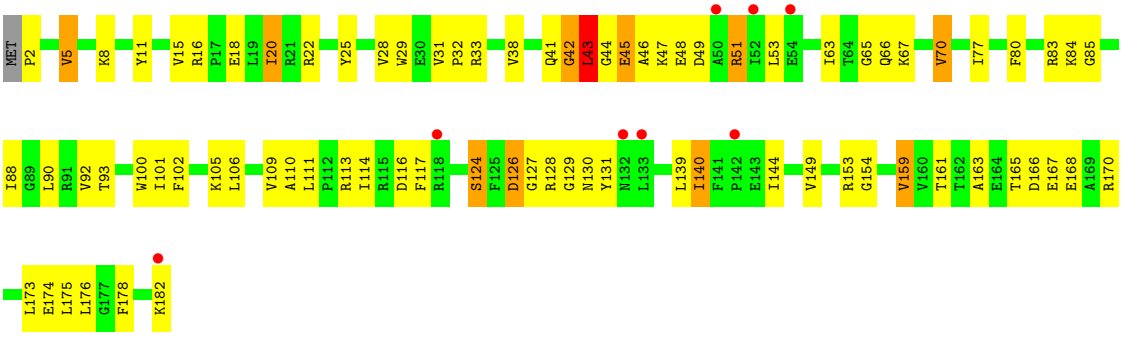
- Molecule 6: 50S ribosomal protein L5

Chain 1G:



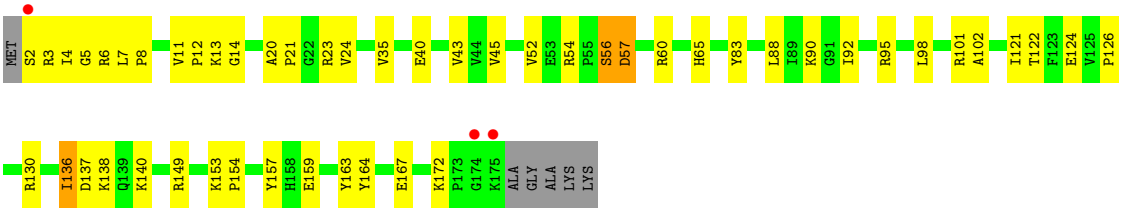
- Molecule 6: 50S ribosomal protein L5

Chain 2G:



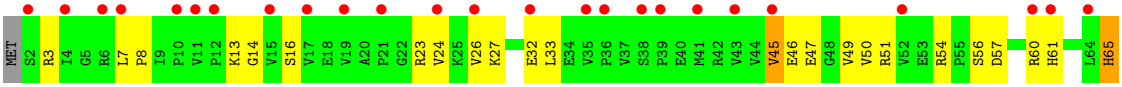
- Molecule 7: 50S ribosomal protein L6

Chain 1H:



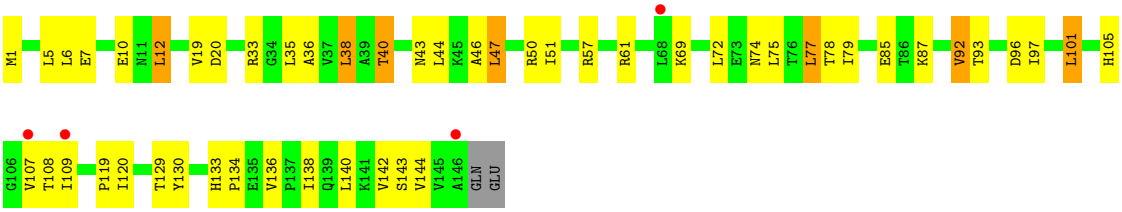
- Molecule 7: 50S ribosomal protein L6

Chain 2H:



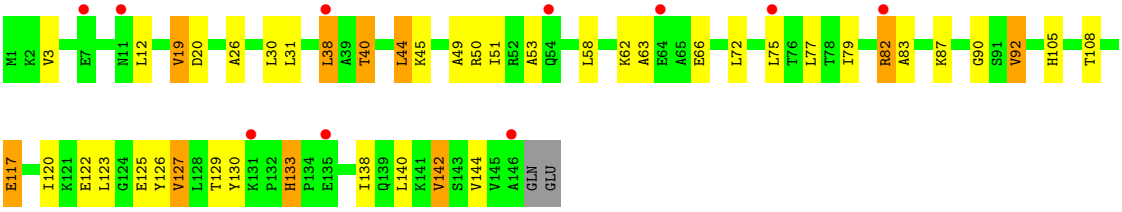
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



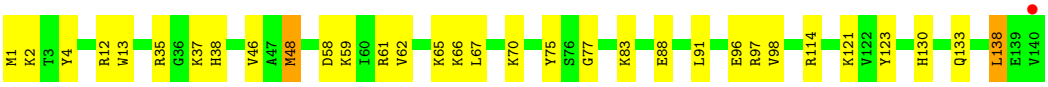
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



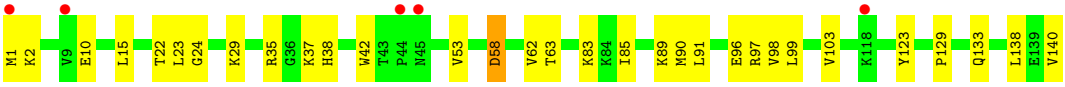
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



• Molecule 9: 50S ribosomal protein L13

Chain 2N:

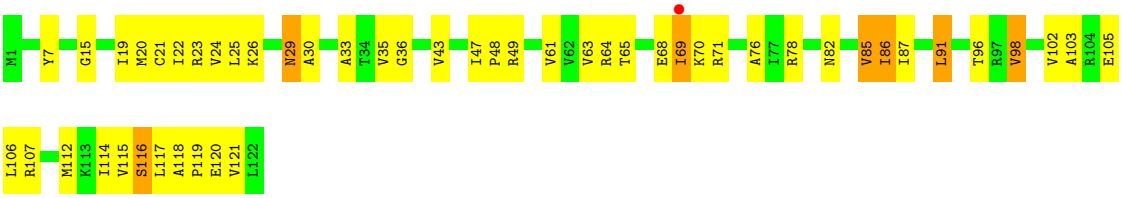


• Molecule 10: 50S ribosomal protein L14

Chain 1O:

• Molecule 10: 50S ribosomal protein L14

Chain 2O:

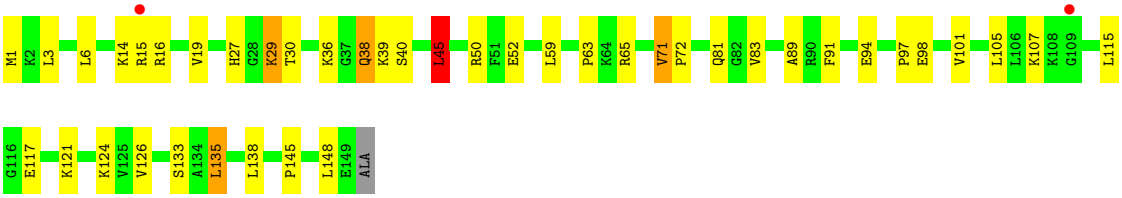


• Molecule 11: 50S ribosomal protein L15

Chain 1P:

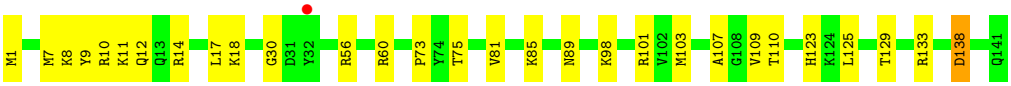
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



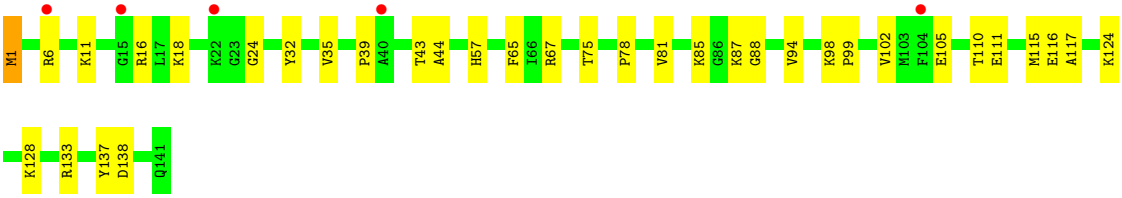
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



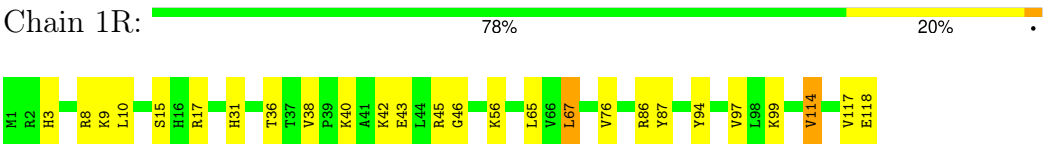
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



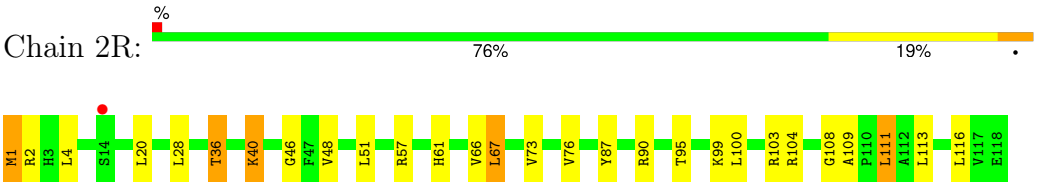
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



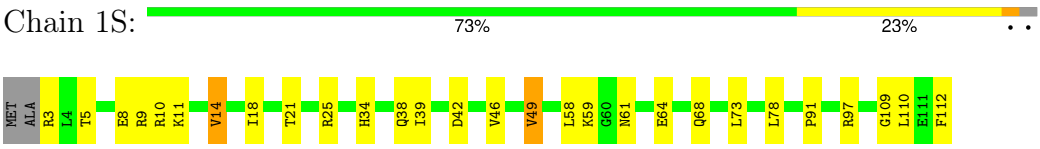
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



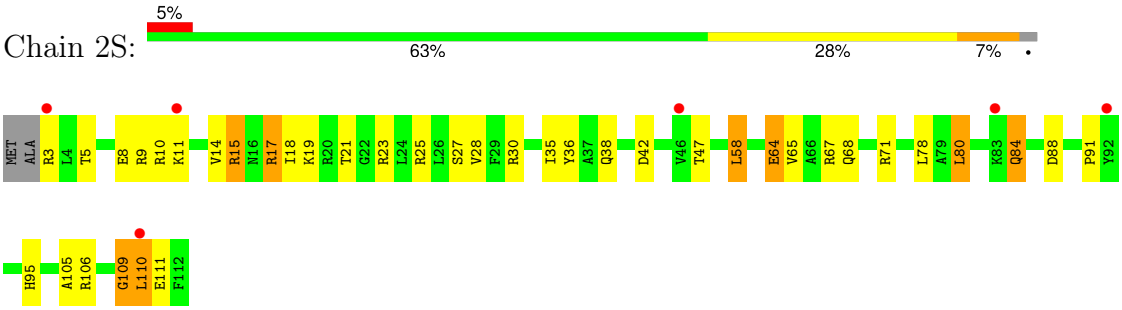
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



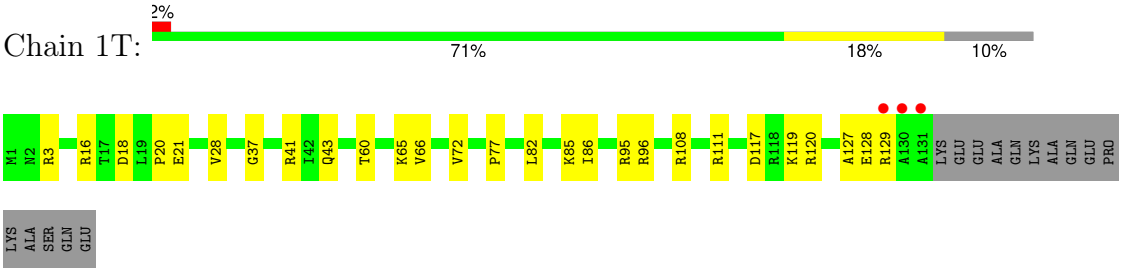
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



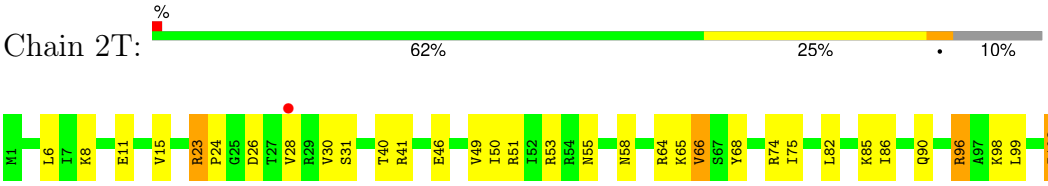
• Molecule 15: 50S ribosomal protein L19

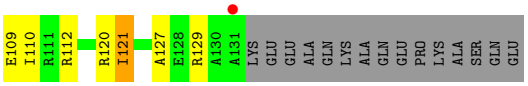
Chain 1T:



• Molecule 15: 50S ribosomal protein L19

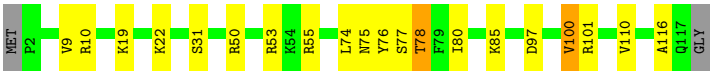
Chain 2T:





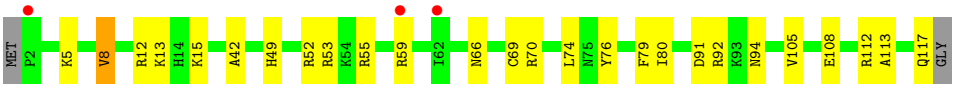
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



• Molecule 16: 50S ribosomal protein L20

Chain 2U:

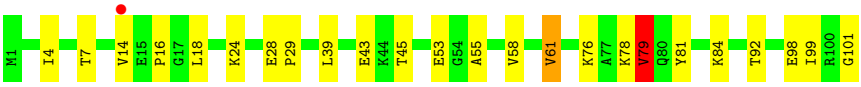


• Molecule 17: 50S ribosomal protein L21

Chain 1V:

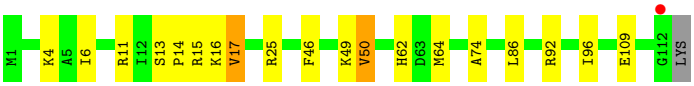
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



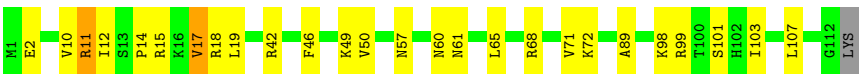
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



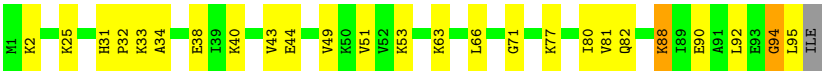
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



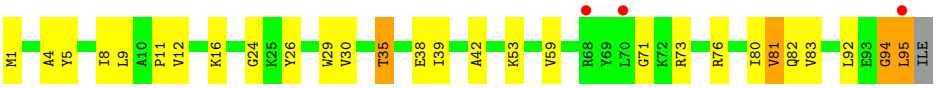
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



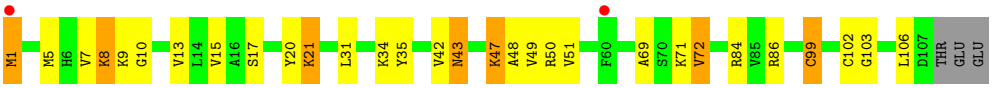
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



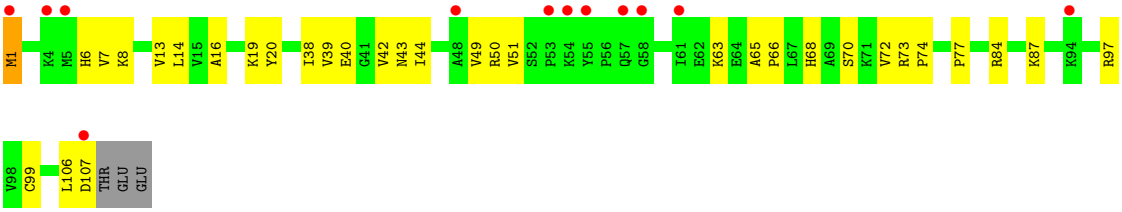
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



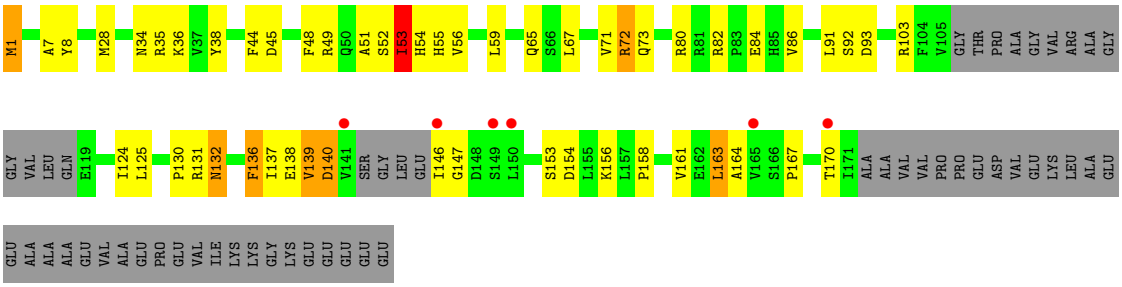
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



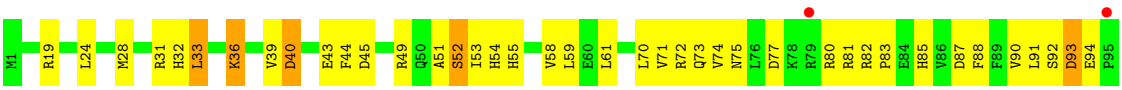
• Molecule 21: 50S ribosomal protein L25

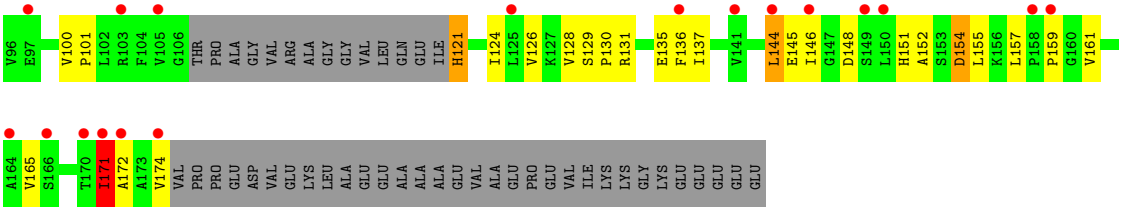
Chain 1Z:



• Molecule 21: 50S ribosomal protein L25

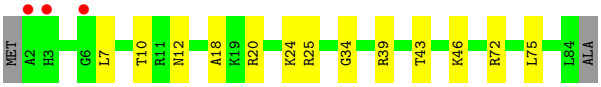
Chain 2Z:





- Molecule 22: 50S ribosomal protein L27

Chain 10:



- Molecule 22: 50S ribosomal protein L27

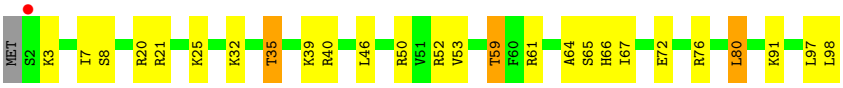
Chain 20:

- Molecule 23: 50S ribosomal protein L28

Chain 11:

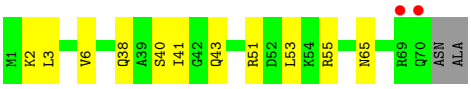
- Molecule 23: 50S ribosomal protein L28

Chain 21:



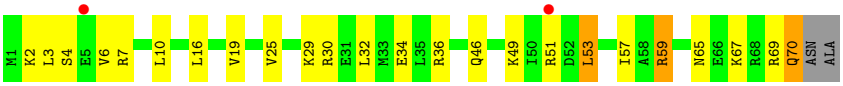
- Molecule 24: 50S ribosomal protein L29

Chain 12:



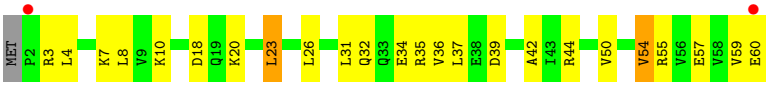
- Molecule 24: 50S ribosomal protein L29

Chain 22:



• Molecule 25: 50S ribosomal protein L30

Chain 13:

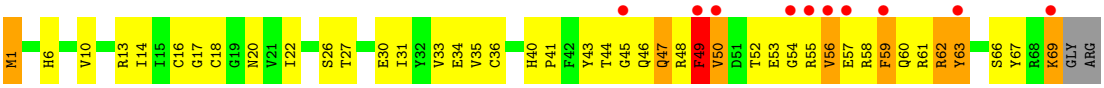


• Molecule 25: 50S ribosomal protein L30

Chain 23:

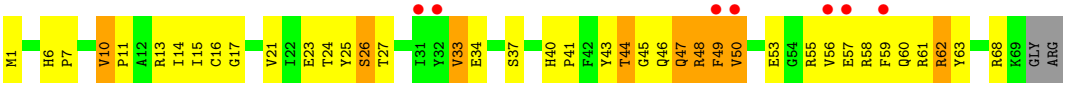
• Molecule 26: 50S ribosomal protein L31

Chain 14:



• Molecule 26: 50S ribosomal protein L31

Chain 24:



• Molecule 27: 50S ribosomal protein L32

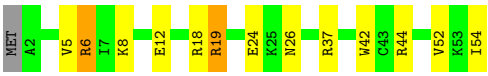
Chain 15:

• Molecule 27: 50S ribosomal protein L32

Chain 25:

• Molecule 28: 50S ribosomal protein L33

Chain 16: 74% 20%

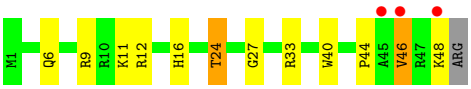


• Molecule 28: 50S ribosomal protein L33

Chain 26: 85% 13%

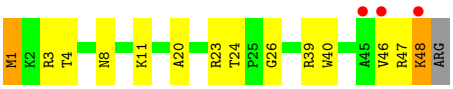
• Molecule 29: 50S ribosomal protein L34

Chain 17: 6% 73% 20%



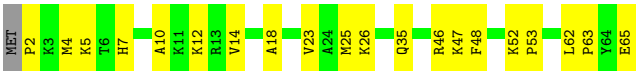
• Molecule 29: 50S ribosomal protein L34

Chain 27: 6% 69% 24%



• Molecule 30: 50S ribosomal protein L35

Chain 18: 68% 31%

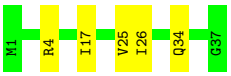


• Molecule 30: 50S ribosomal protein L35

Chain 28: 2% 75% 23%

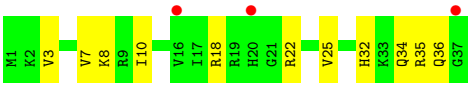
• Molecule 31: 50S ribosomal protein L36

Chain 19: 86% 14%



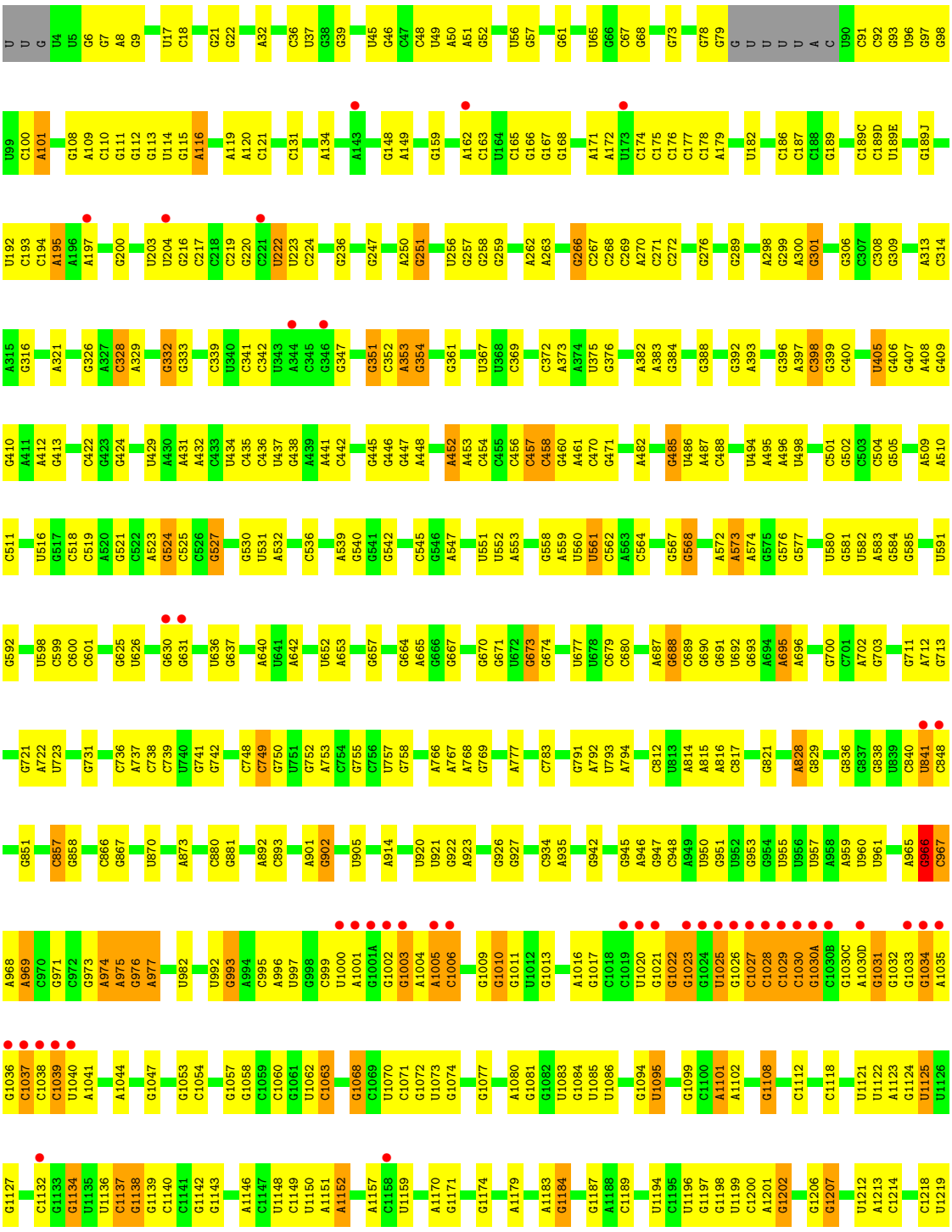
• Molecule 31: 50S ribosomal protein L36

Chain 29:



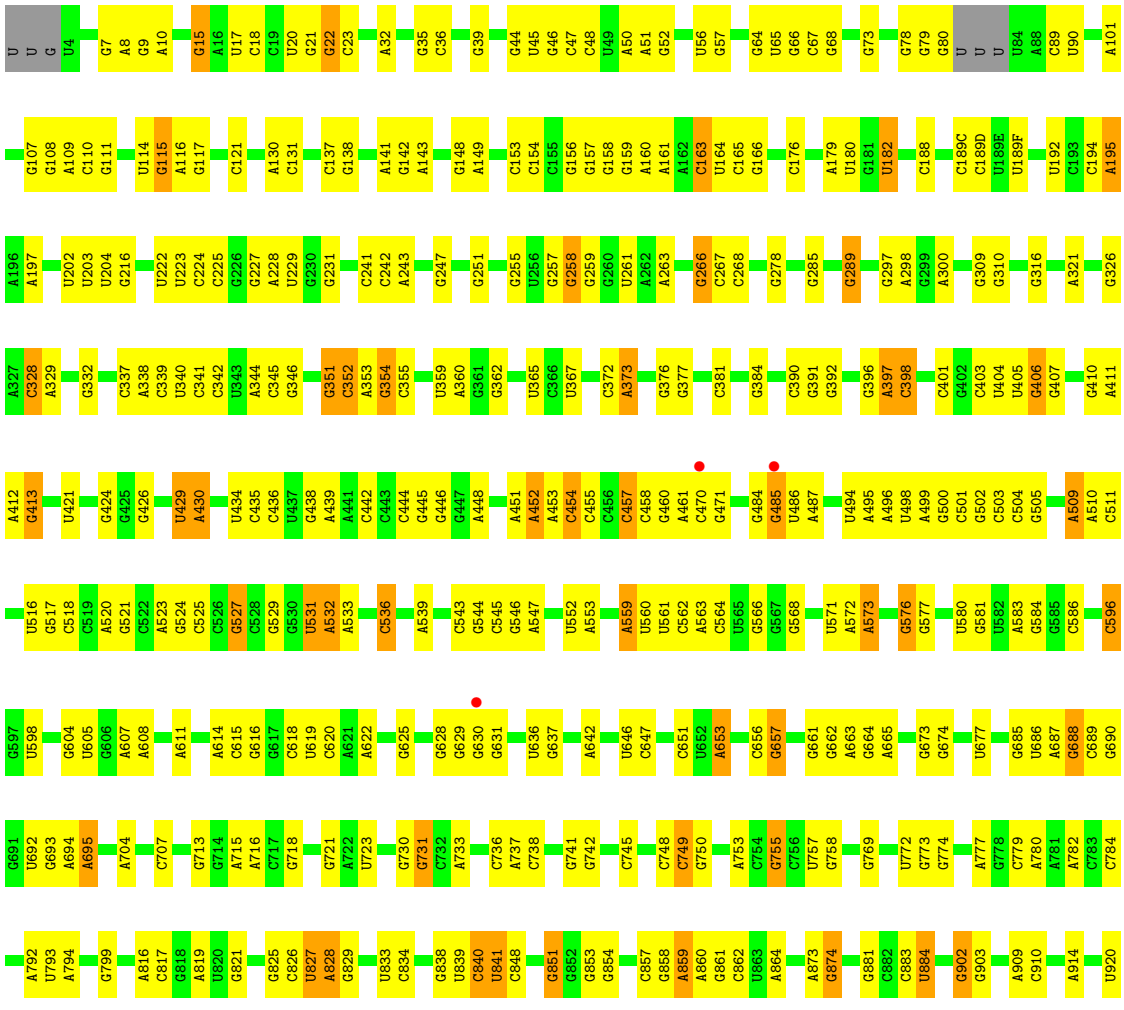
• Molecule 32: 16S Ribosomal RNA

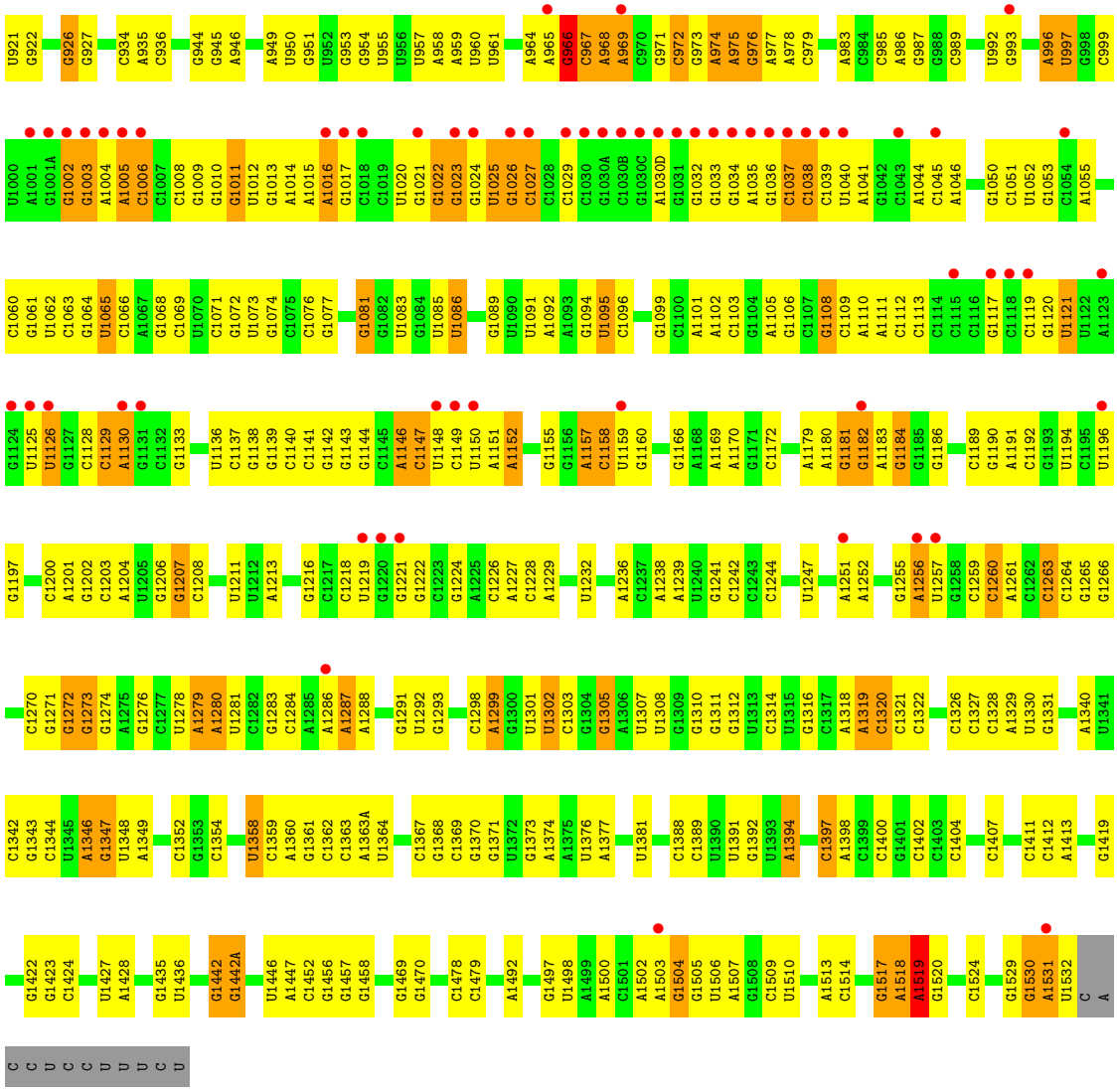
Chain 1a:



- Molecule 32: 16S Ribosomal RNA

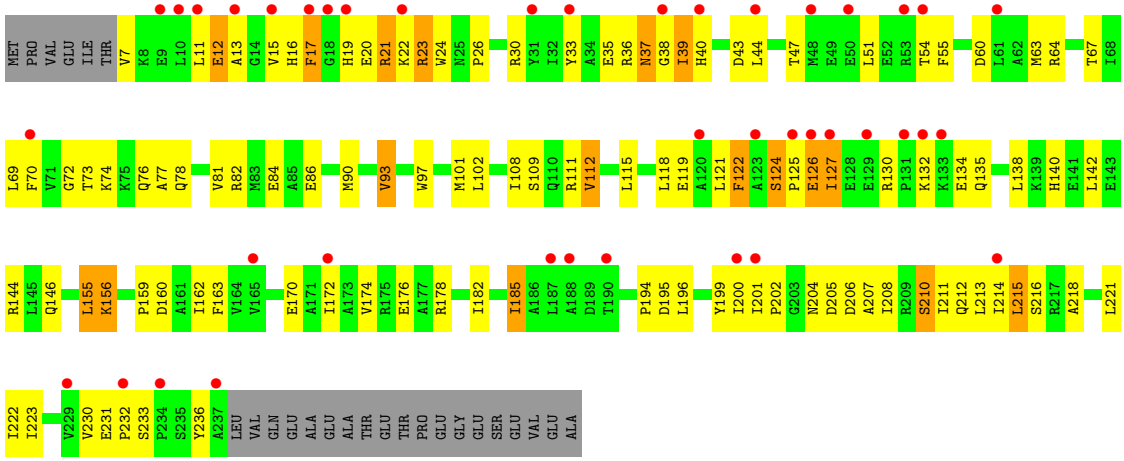
Chain 2a:





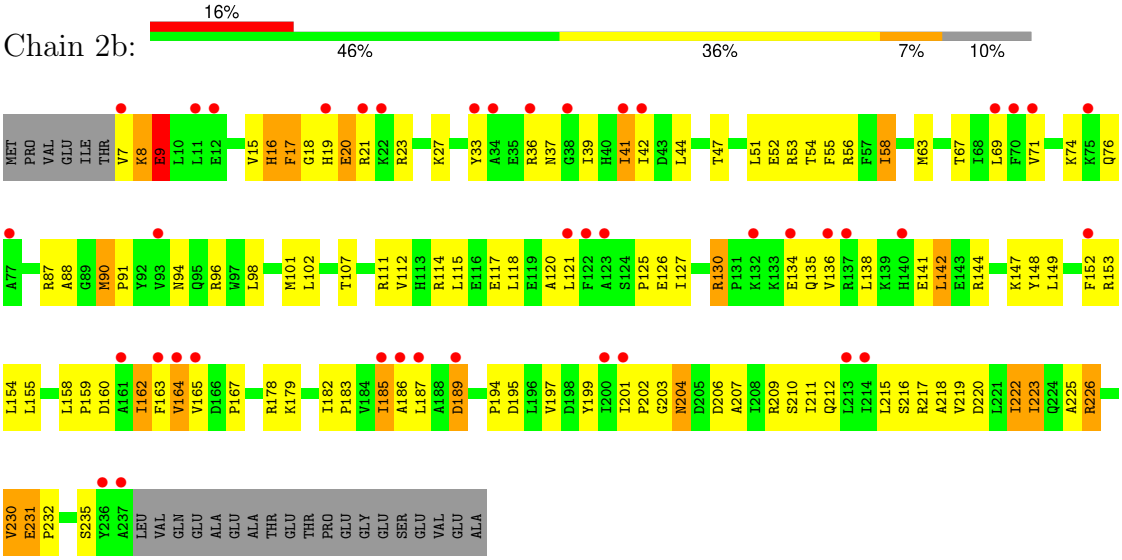
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



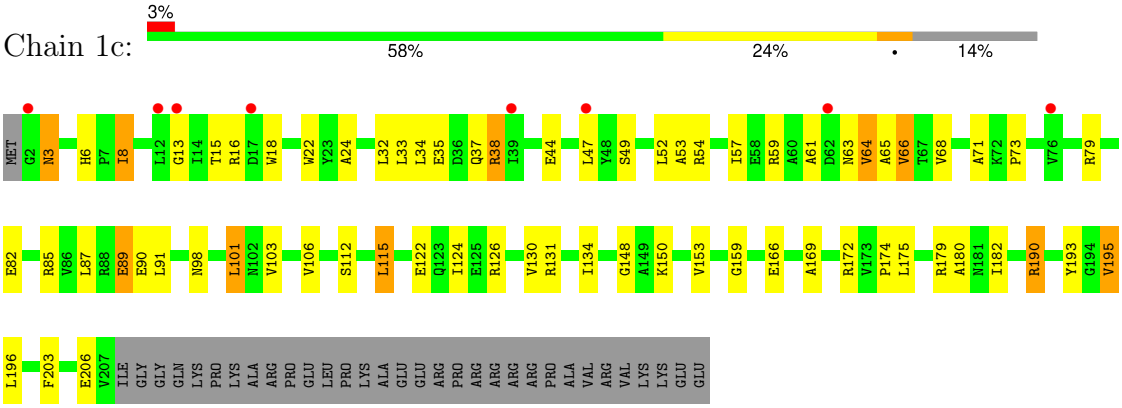
- Molecule 33: 30S ribosomal protein S2

Chain 2b:



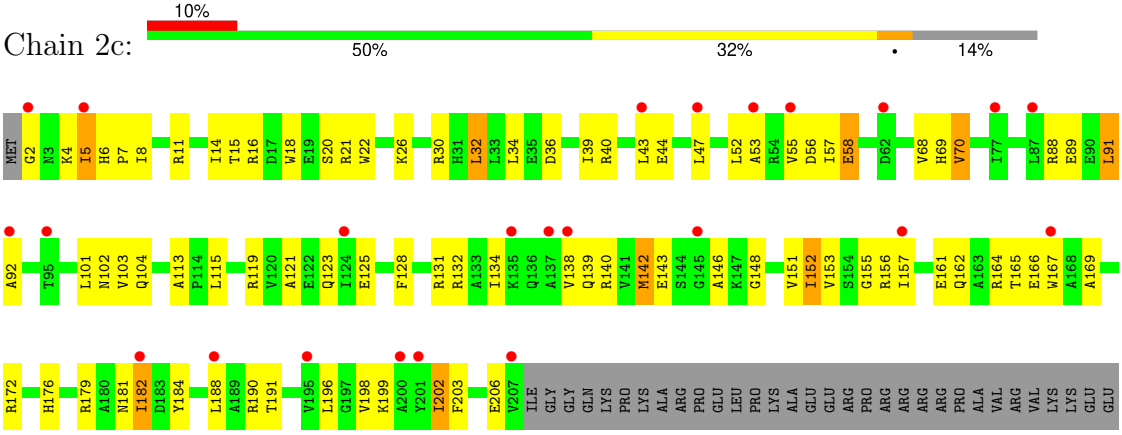
- Molecule 34: 30S ribosomal protein S3

Chain 1c:



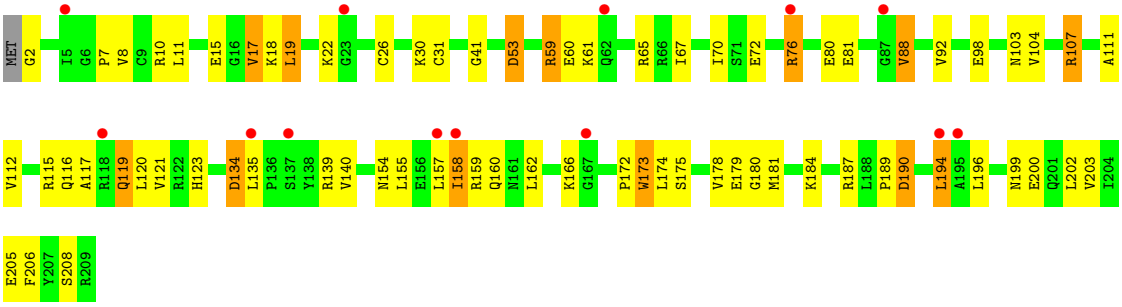
- Molecule 34: 30S ribosomal protein S3

Chain 2c:



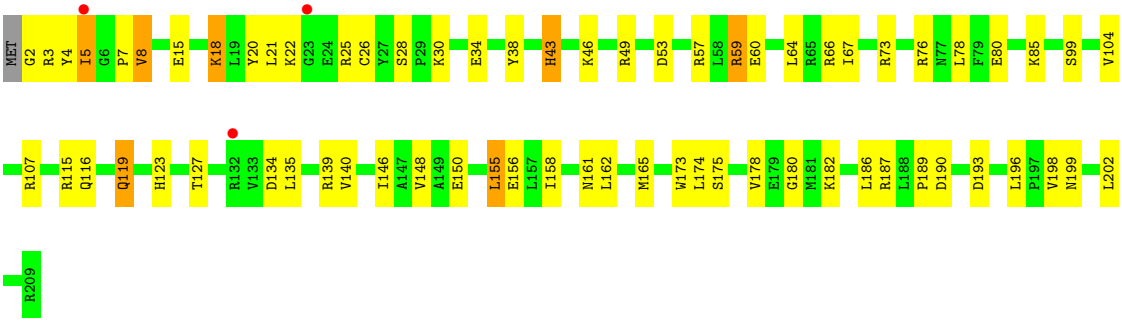
- Molecule 35: 30S ribosomal protein S4

Chain 1d:



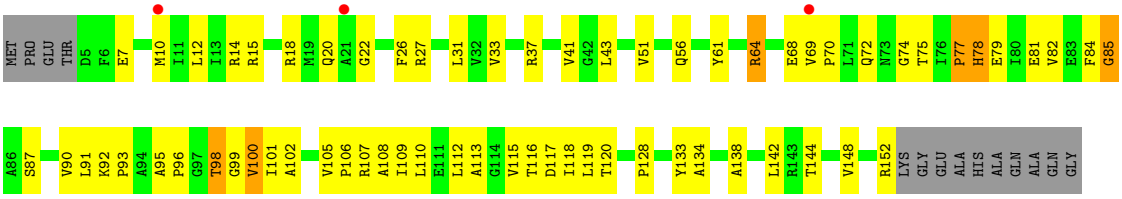
- Molecule 35: 30S ribosomal protein S4

Chain 2d:



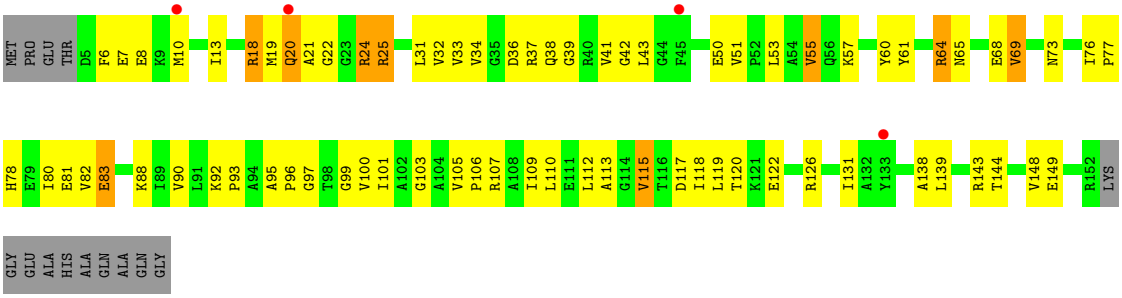
- Molecule 36: 30S ribosomal protein S5

Chain 1e:



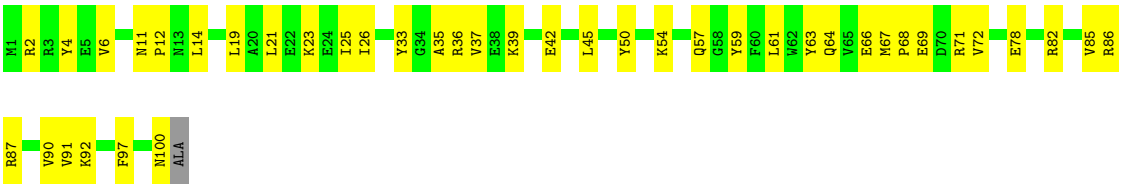
- Molecule 36: 30S ribosomal protein S5

Chain 2e:



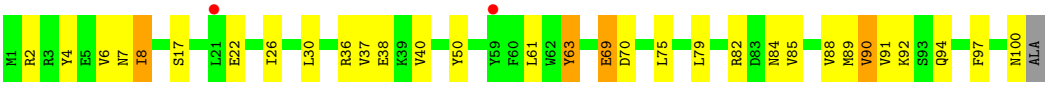
- Molecule 37: 30S ribosomal protein S6

Chain 1f:



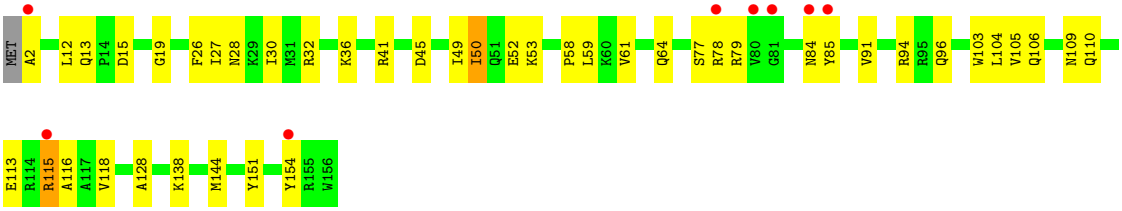
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



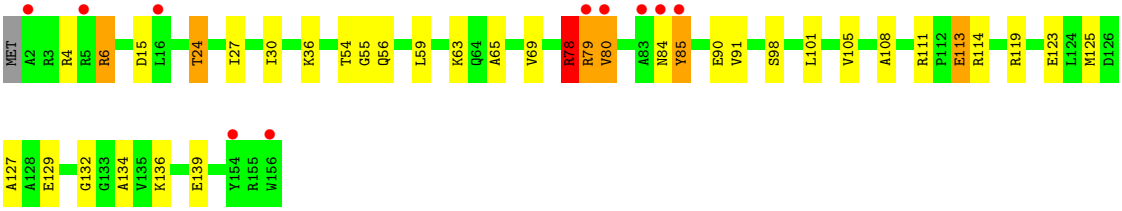
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



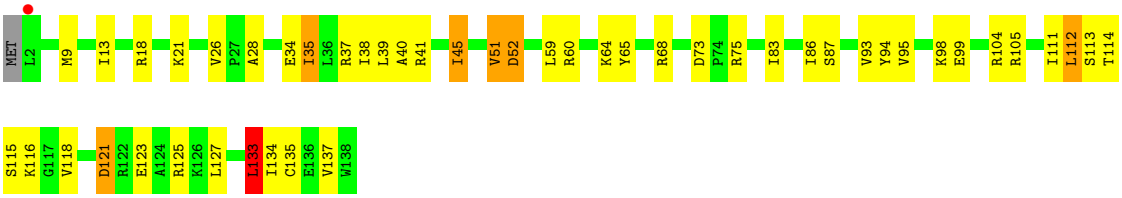
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



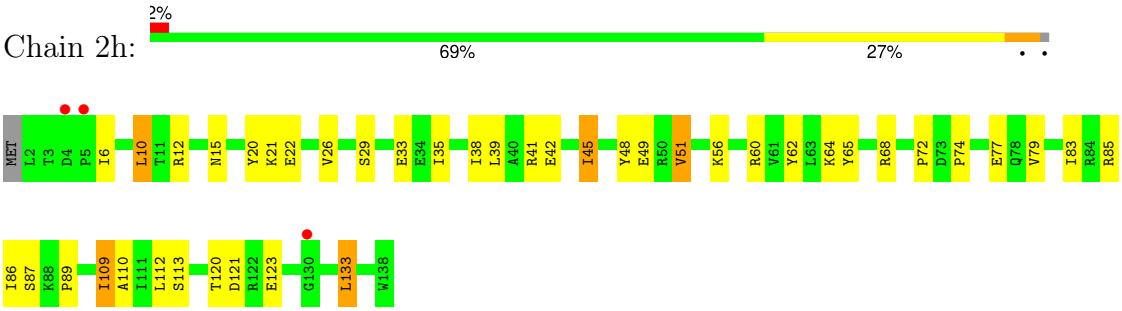
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



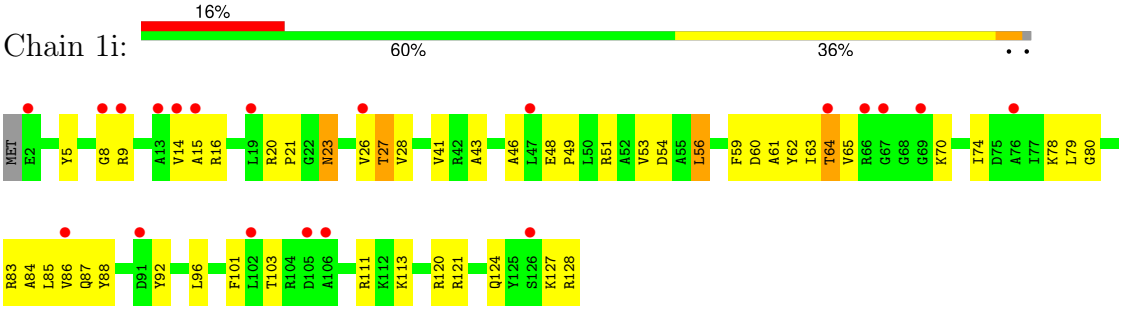
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



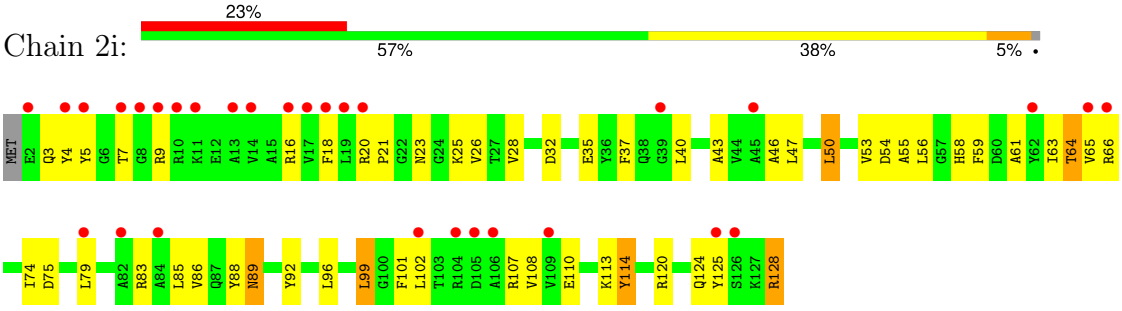
- Molecule 40: 30S ribosomal protein S9

Chain 1i:



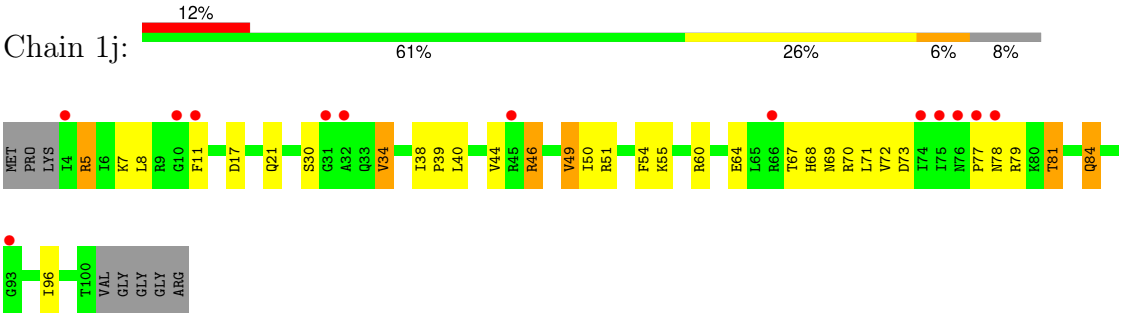
- Molecule 40: 30S ribosomal protein S9

Chain 2i:



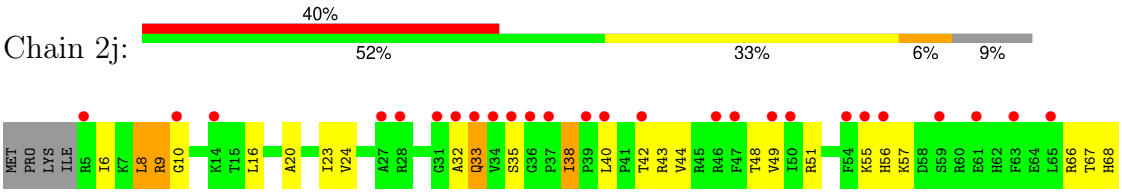
- Molecule 41: 30S ribosomal protein S10

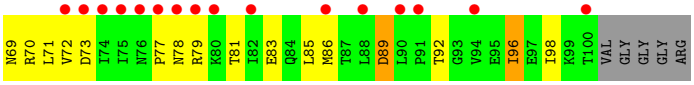
Chain 1j:



- Molecule 41: 30S ribosomal protein S10

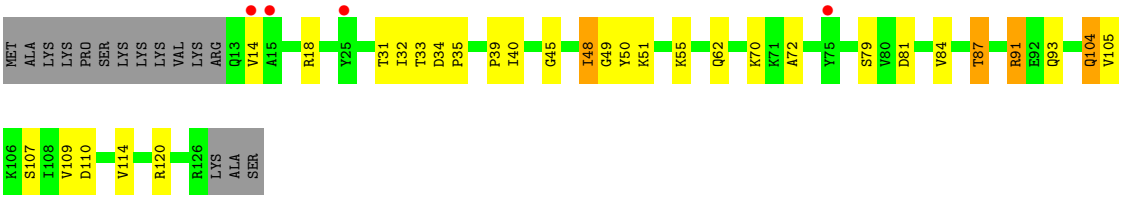
Chain 2j:





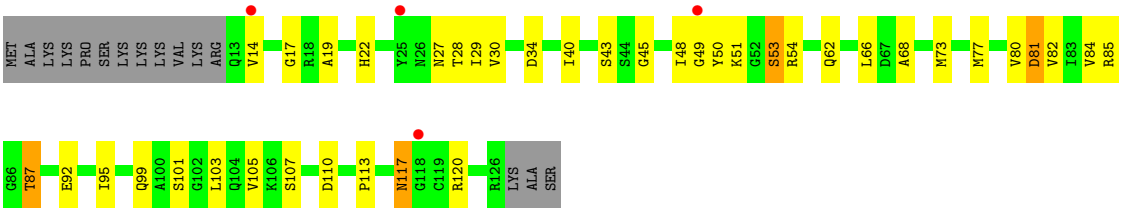
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



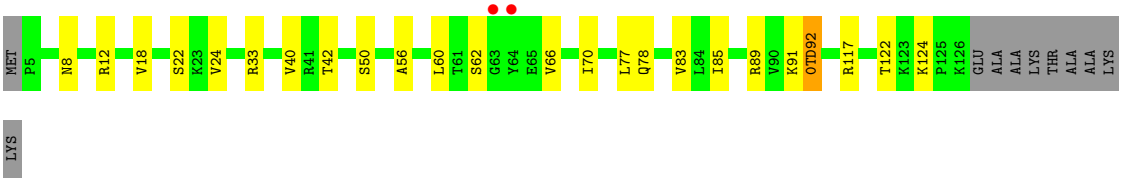
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



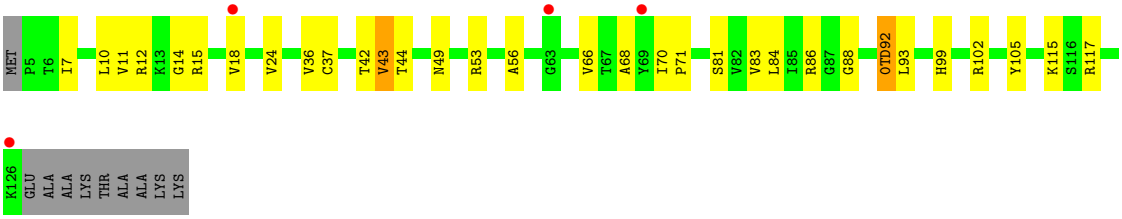
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



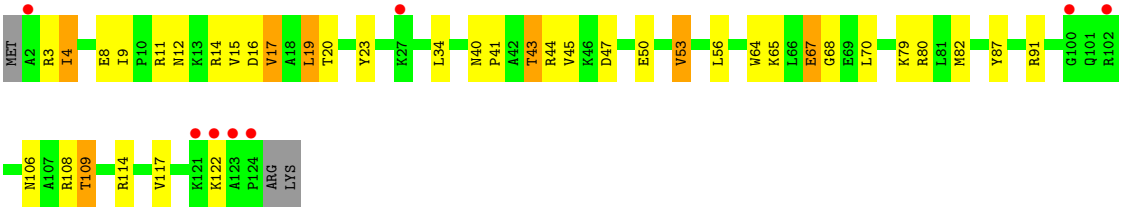
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



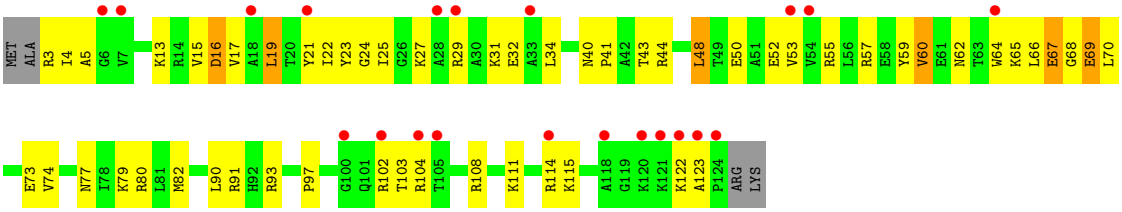
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



• Molecule 44: 30S ribosomal protein S13

Chain 2m:

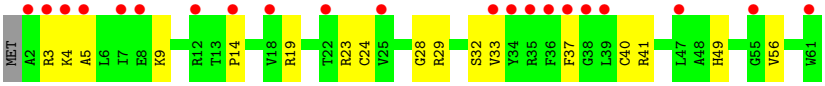


• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:

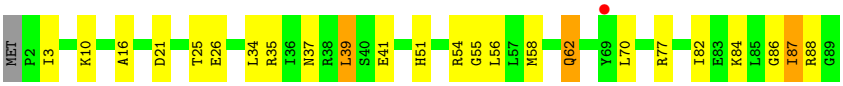
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



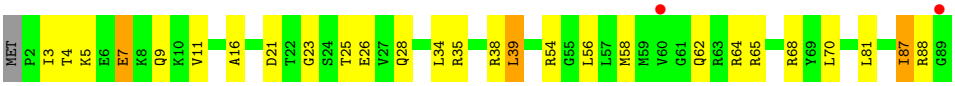
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



• Molecule 46: 30S ribosomal protein S15

Chain 2o:



• Molecule 47: 30S ribosomal protein S16

Chain 1p: 2% 61% 26% 6% 7%

M1 R5 S11 P15 H16 V20 R25 R26 K27 R28 D29 Y39 D40 P41 R42 K43 T44 W48 L49 K50 V53 A56 R57 L60 S61 V62 T67 D68 T69 A70 R71 R72 L73 L74 R75 V79 Q82 GLU ALA ARG GLU GLY ALA

• Molecule 47: 30S ribosomal protein S16

Chain 2p: 6% 56% 35% • 7%

M1 V2 K3 I4 R5 R8 F9 P15 H16 Y17 R18 I19 V20 V21 T22 D23 A24 R25 R26 K27 R28 D29 K35 P41 R42 K43 T44 T45 W48 V53 R57 Y58 W59 L60 S61 D68 L73 L74 R75 Q76 V79 Q82 GLU ALA ARG GLU GLY ALA

• Molecule 48: 30S ribosomal protein S17

Chain 1q: 3% 68% 26% • 6%

MET P2 L6 T7 M15 T18 L22 V23 E24 R25 Q26 F27 P28 K37 R38 S39 Y42 L43 A44 H45 D46 P47 L53 E58 I59 I60 R63 S66 K67 R68 K69 R70 V73 L74 E78 M82 V85 R91 L98 S99 K100 ARG GLY GLY LYS ALA

• Molecule 48: 30S ribosomal protein S17

Chain 2q: 5% 71% 23% 6%

MET P2 L6 T7 D13 K14 M15 Q16 K17 T18 F27 I36 K40 K41 Y42 L43 A44 H45 D46 P47 K52 L53 E58 I59 I60 R63 R72 R75 L76 V77 E78 R81 L84 Y95 L98 S99 K100 ARG GLY GLY LYS ALA

• Molecule 49: 30S ribosomal protein S18

Chain 1r: % 61% 15% • 23%

MET SER THR LYS ASN ALA LYS PRO LYS LYS GLU ALA GLN ARG ARG PRO SER ARG LYS A20 T25 L26 G27 E28 L31 R32 R42 E46 T47 P52 R53 R54 K61 T69 R72 E83 R87 LYS

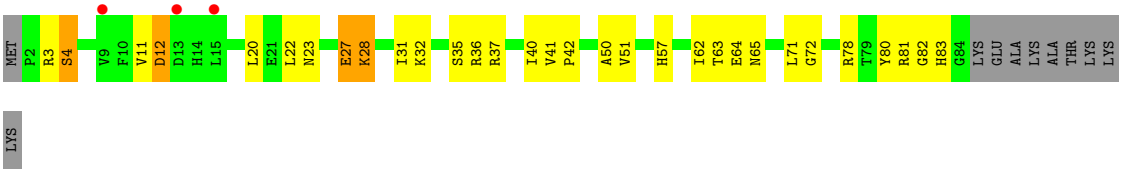
• Molecule 49: 30S ribosomal protein S18

Chain 2r: % 53% 23% • 23%

MET SER THR LYS ASN ALA LYS PRO LYS LYS GLU ALA GLN ARG ARG PRO SER ARG LYS A20 K21 V22 T25 L26 G27 E28 F29 D30 L31 R32 V37 R42 E46 T56 G57 L58 E62 Q63 L66 A67 K68 T69 R72 A73 R74 G77 L85 V86 R87 LYS

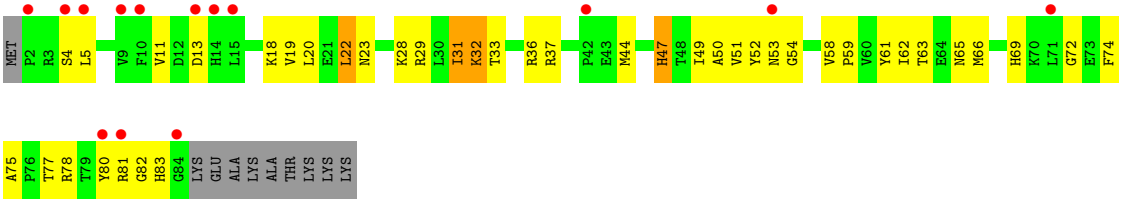
• Molecule 50: 30S ribosomal protein S19

Chain 1s: 3% 56% 29% • 11%



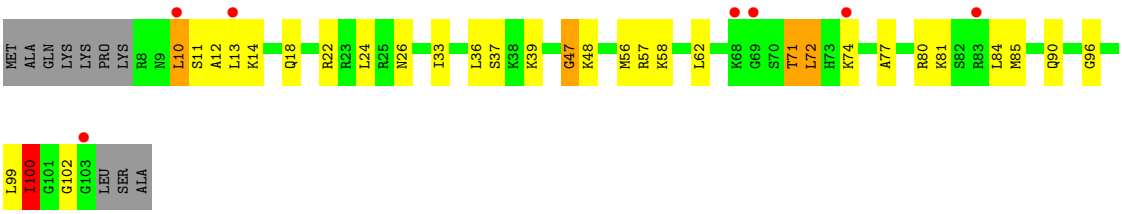
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



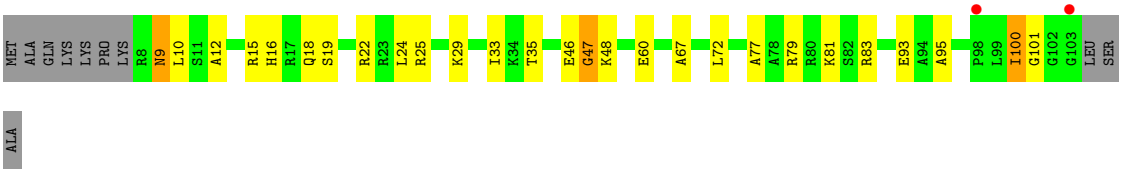
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



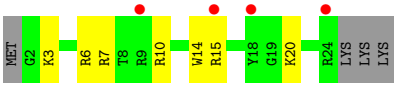
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



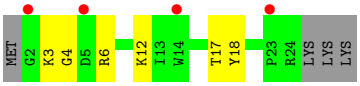
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



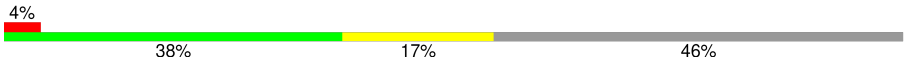
• Molecule 52: 30S ribosomal protein Thx

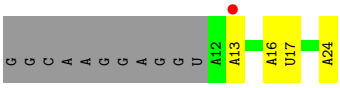
Chain 2u:



• Molecule 53: MF-mRNA

Chain 1v:



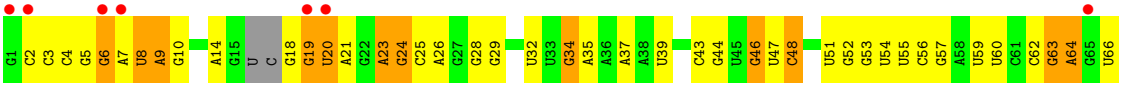


• Molecule 53: MF-mRNA

Chain 2v:

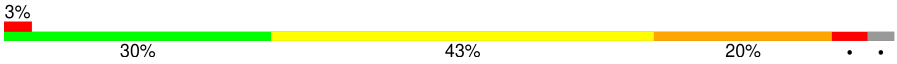
• Molecule 54: A- and E-site Deacylated tRNAphe

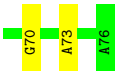
Chain 1w:



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

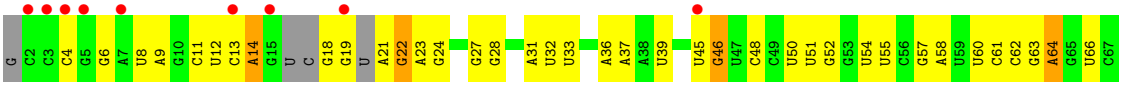
Chain 1y:

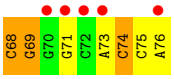




• Molecule 54: A- and E-site Deacylated tRNAphe

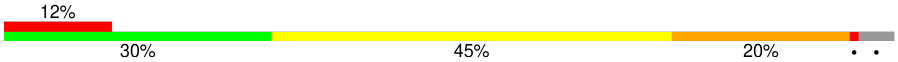
Chain 2w:

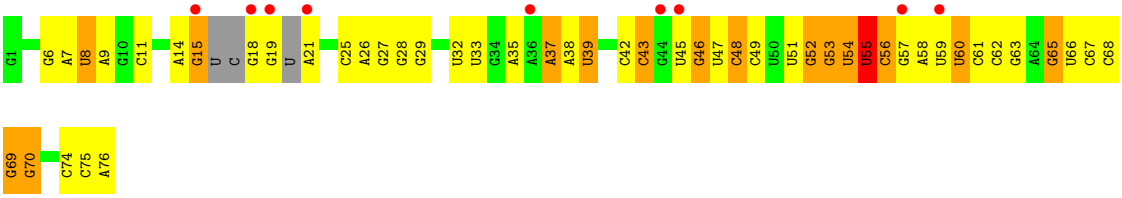




- Molecule 54: A- and E-site Deacylated tRNAphe

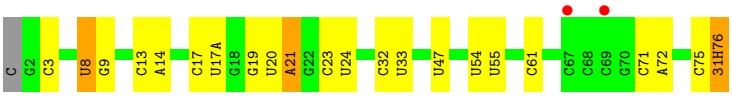
Chain 2y:





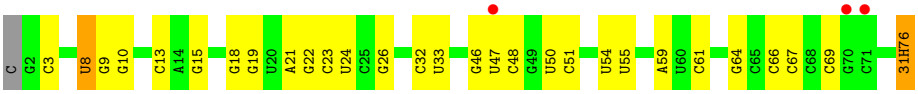
- Molecule 55: P-site Aminoacyl-tRNA fMet-tRNAmet

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	210.01Å 449.04Å 621.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.89 – 2.60 121.89 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (121.89-2.60) 97.0 (121.89-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.216 , 0.261 0.218 , 0.262	Depositor DCC
R_{free} test set	86389 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	299649	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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: OMU, K, MA6, ZN, G7M, 5MC, PSU, 5MU, MIA, M2G, 8AH, 0TD, UR3, 4SU, 4OC, SF4, 2MG, 31H, WC9, MG, OMG, OMC

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	0.28	0/69011	0.45	1/107720 (0.0%)
1	2A	0.21	1/67295 (0.0%)	0.40	1/105042 (0.0%)
2	1B	0.22	0/2882	0.39	0/4494
2	2B	0.18	0/2879	0.36	0/4487
3	1D	0.26	0/2186	0.49	0/2944
3	2D	0.22	0/2186	0.43	0/2944
4	1E	0.27	0/1592	0.51	0/2149
4	2E	0.22	0/1592	0.47	0/2149
5	1F	0.25	0/1619	0.48	0/2193
5	2F	0.21	0/1615	0.47	2/2188 (0.1%)
6	1G	0.21	0/1448	0.43	0/1957
6	2G	0.22	0/1453	0.42	0/1963
7	1H	0.22	0/1356	0.43	0/1834
7	2H	0.19	0/1356	0.37	0/1834
8	1I	0.24	0/1112	0.42	0/1514
8	2I	0.20	0/1079	0.43	0/1475
9	1N	0.25	0/1144	0.47	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.25	0/943	0.46	0/1269
10	2O	0.20	0/943	0.43	0/1269
11	1P	0.25	0/1152	0.52	0/1533
11	2P	0.21	0/1152	0.45	0/1533
12	1Q	0.28	0/1143	0.48	0/1527
12	2Q	0.19	0/1143	0.40	0/1527
13	1R	0.27	0/982	0.50	0/1312
13	2R	0.22	0/982	0.48	0/1312
14	1S	0.22	0/883	0.46	0/1176
14	2S	0.19	0/880	0.44	0/1172
15	1T	0.24	0/1105	0.46	0/1477
15	2T	0.20	0/1097	0.42	0/1468
16	1U	0.29	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.19	0/977	0.39	0/1301
17	1V	0.26	0/782	0.47	0/1049
17	2V	0.19	0/782	0.39	0/1049
18	1W	0.27	0/897	0.46	0/1205
18	2W	0.22	0/897	0.40	0/1205
19	1X	0.26	0/764	0.50	0/1025
19	2X	0.22	0/764	0.49	2/1025 (0.2%)
20	1Y	0.23	0/819	0.48	0/1095
20	2Y	0.20	0/819	0.49	0/1095
21	1Z	0.21	0/1267	0.47	0/1717
21	2Z	0.22	0/1299	0.45	0/1763
22	10	0.26	0/662	0.49	0/881
22	20	0.21	0/662	0.43	0/881
23	11	0.23	0/762	0.40	0/1014
23	21	0.22	0/762	0.42	0/1014
24	12	0.24	0/590	0.42	0/781
24	22	0.18	0/590	0.38	0/781
25	13	0.25	0/474	0.46	0/635
25	23	0.18	0/469	0.43	0/630
26	14	0.26	0/565	0.57	0/761
26	24	0.24	0/545	0.55	0/737
27	15	0.29	0/469	0.50	0/635
27	25	0.22	0/469	0.48	0/635
28	16	0.25	0/460	0.44	0/613
28	26	0.23	0/456	0.45	0/608
29	17	0.29	0/426	0.52	0/561
29	27	0.24	0/426	0.50	0/561
30	18	0.26	0/525	0.48	0/691
30	28	0.22	0/525	0.40	0/691
31	19	0.28	0/310	0.52	0/407
31	29	0.19	0/310	0.42	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.20	0/35886	0.38	4/56005 (0.0%)
33	1b	0.21	0/1881	0.52	0/2542
33	2b	0.22	0/1860	0.47	0/2518
34	1c	0.20	0/1572	0.45	0/2126
34	2c	0.25	0/1566	0.41	0/2119
35	1d	0.18	0/1685	0.42	0/2262
35	2d	0.20	0/1704	0.43	0/2284
36	1e	0.21	0/1145	0.46	0/1543
36	2e	0.27	0/1149	0.47	0/1548
37	1f	0.19	0/823	0.40	0/1115
37	2f	0.20	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.19	0/1250	0.39	0/1679
38	2g	0.18	0/1254	0.40	0/1683
39	1h	0.19	0/1108	0.42	0/1494
39	2h	0.19	0/1108	0.41	0/1494
40	1i	0.20	0/1002	0.47	0/1346
40	2i	0.22	0/997	0.52	0/1343
41	1j	0.26	0/722	0.46	0/982
41	2j	0.23	0/727	0.51	0/988
42	1k	0.18	0/844	0.42	0/1145
42	2k	0.18	0/848	0.40	0/1149
43	1l	0.22	0/937	0.44	0/1260
43	2l	0.18	0/937	0.40	0/1260
44	1m	0.20	0/969	0.48	1/1302 (0.1%)
44	2m	0.20	0/961	0.45	0/1291
45	1n	0.20	0/501	0.44	0/664
45	2n	0.20	0/501	0.42	0/664
46	1o	0.20	0/739	0.38	0/985
46	2o	0.17	0/739	0.38	0/985
47	1p	0.19	0/697	0.44	0/939
47	2p	0.20	0/693	0.46	0/935
48	1q	0.19	0/836	0.39	0/1117
48	2q	0.18	0/836	0.38	0/1117
49	1r	0.20	0/560	0.40	0/746
49	2r	0.18	0/560	0.39	0/746
50	1s	0.19	0/667	0.49	0/900
50	2s	0.24	0/661	0.55	0/893
51	1t	0.20	0/730	0.51	0/965
51	2t	0.21	0/729	0.46	0/965
52	1u	0.20	0/203	0.46	0/266
52	2u	0.27	0/203	0.56	0/266
53	1v	0.21	0/310	0.33	0/480
53	2v	0.19	0/310	0.34	0/480
54	1w	0.28	1/1606 (0.1%)	0.40	0/2497
54	1y	0.28	2/1606 (0.1%)	0.38	0/2497
54	2w	0.31	2/1556 (0.1%)	0.41	0/2418
54	2y	0.28	2/1583 (0.1%)	0.40	0/2459
55	1x	0.27	0/1700	0.40	0/2650
55	2x	0.25	0/1700	0.39	0/2650
All	All	0.23	8/316640 (0.0%)	0.42	11/474051 (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
33	1b	0	2
38	2g	0	1
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	O3'-P	5.62	1.61	1.56
54	2w	46	G7M	O3'-P	5.57	1.61	1.56
54	1y	8	4SU	O3'-P	5.36	1.61	1.56
54	2w	8	4SU	O3'-P	5.30	1.61	1.56
54	2y	46	G7M	O3'-P	5.30	1.61	1.56

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1992	G	C2'-C3'-O3'	6.70	119.54	109.50
32	2a	1272	G	N1-C2-N2	-5.92	98.45	116.20
32	2a	1263	C	N1-C2-O2	5.49	135.36	118.90
5	2F	21	ALA	CA-C-N	5.37	131.36	121.70
5	2F	21	ALA	C-N-CA	5.37	131.36	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	122	PHE	Peptide
33	1b	124	SER	Peptide
5	2F	20	LEU	Peptide
38	2g	78	ARG	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	61853	0	31183	617	0
1	2A	60323	0	30413	682	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	33	0
3	1D	2136	0	2217	56	0
3	2D	2136	0	2218	33	0
4	1E	1559	0	1618	31	0
4	2E	1559	0	1618	34	0
5	1F	1584	0	1625	33	0
5	2F	1580	0	1619	38	0
6	1G	1423	0	1436	37	0
6	2G	1428	0	1438	57	0
7	1H	1330	0	1407	31	0
7	2H	1330	0	1407	26	0
8	1I	1097	0	1140	34	0
8	2I	1064	0	1082	27	0
9	1N	1117	0	1184	22	0
9	2N	1117	0	1184	16	0
10	1O	933	0	996	21	0
10	2O	933	0	996	35	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	32	0
12	1Q	1122	0	1179	16	0
12	2Q	1122	0	1179	25	0
13	1R	968	0	1033	17	0
13	2R	968	0	1033	23	0
14	1S	873	0	927	16	0
14	2S	870	0	923	30	0
15	1T	1091	0	1151	13	0
15	2T	1083	0	1136	28	0
16	1U	959	0	1019	13	0
16	2U	959	0	1019	17	0
17	1V	771	0	830	14	0
17	2V	771	0	830	16	0
18	1W	886	0	940	12	0
18	2W	886	0	940	19	0
19	1X	750	0	814	21	0
19	2X	750	0	814	22	0
20	1Y	806	0	881	23	0
20	2Y	806	0	881	17	0
21	1Z	1240	0	1240	37	0
21	2Z	1271	0	1273	43	0
22	10	653	0	674	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	653	0	674	11	0
23	11	755	0	826	7	0
23	21	755	0	826	18	0
24	12	588	0	643	5	0
24	22	588	0	643	18	0
25	13	469	0	518	12	0
25	23	464	0	514	12	0
26	14	552	0	533	36	0
26	24	532	0	503	29	0
27	15	455	0	465	4	0
27	25	455	0	465	9	0
28	16	453	0	473	9	0
28	26	449	0	469	3	0
29	17	418	0	467	9	0
29	27	418	0	467	11	0
30	18	517	0	582	16	0
30	28	517	0	582	12	0
31	19	307	0	335	2	0
31	29	307	0	335	7	0
32	1a	32246	0	16295	374	0
32	2a	32327	0	16338	457	0
33	1b	1846	0	1867	72	0
33	2b	1825	0	1828	83	0
34	1c	1548	0	1535	42	0
34	2c	1542	0	1517	54	0
35	1d	1655	0	1672	57	0
35	2d	1674	0	1714	43	0
36	1e	1129	0	1185	38	0
36	2e	1133	0	1191	49	0
37	1f	810	0	804	24	0
37	2f	816	0	808	16	0
38	1g	1231	0	1238	20	0
38	2g	1235	0	1249	23	0
39	1h	1088	0	1126	32	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	32	0
40	2i	978	0	966	38	0
41	1j	709	0	650	24	0
41	2j	714	0	672	37	0
42	1k	829	0	825	15	0
42	2k	833	0	836	23	0
43	1l	932	0	981	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	20	0
44	1m	958	0	1002	28	0
44	2m	950	0	988	43	0
45	1n	492	0	528	12	0
45	2n	492	0	529	14	0
46	1o	728	0	760	16	0
46	2o	728	0	760	20	0
47	1p	681	0	697	19	0
47	2p	677	0	686	22	0
48	1q	823	0	891	13	0
48	2q	823	0	891	14	0
49	1r	555	0	618	9	0
49	2r	555	0	618	11	0
50	1s	652	0	662	27	0
50	2s	646	0	644	34	0
51	1t	728	0	798	21	0
51	2t	727	0	796	20	0
52	1u	199	0	208	5	0
52	2u	199	0	208	6	0
53	1v	277	0	140	1	0
53	2v	277	0	140	2	0
54	1w	1592	0	818	31	0
54	1y	1585	0	803	25	0
54	2w	1544	0	787	20	0
54	2y	1565	0	794	37	0
55	1x	1635	0	839	7	0
55	2x	1635	0	839	12	0
56	10	8	0	0	0	0
56	11	6	0	0	0	0
56	12	2	0	0	0	0
56	13	3	0	0	0	0
56	14	1	0	0	0	0
56	15	10	0	0	0	0
56	16	1	0	0	0	0
56	17	6	0	0	0	0
56	18	6	0	0	0	0
56	19	1	0	0	0	0
56	1A	1096	0	0	0	0
56	1B	36	0	0	0	0
56	1D	14	0	0	0	0
56	1E	15	0	0	0	0
56	1F	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1G	5	0	0	0	0
56	1H	1	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	5	0	0	0	0
56	1P	5	0	0	0	0
56	1Q	6	0	0	0	0
56	1R	6	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	9	0	0	0	0
56	1V	6	0	0	0	0
56	1W	7	0	0	0	0
56	1X	7	0	0	0	0
56	1Y	5	0	0	0	0
56	1Z	4	0	0	0	0
56	1a	210	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	2	0	0	0	0
56	1k	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	0	0	0	0
56	1p	1	0	0	0	0
56	1t	1	0	0	0	0
56	1w	8	0	0	0	0
56	1x	15	0	0	0	0
56	1y	1	0	0	0	0
56	20	4	0	0	0	0
56	21	1	0	0	0	0
56	23	2	0	0	0	0
56	25	6	0	0	0	0
56	26	1	0	0	0	0
56	27	3	0	0	0	0
56	28	3	0	0	0	0
56	2A	844	0	0	0	0
56	2B	19	0	0	0	0
56	2D	8	0	0	0	0
56	2E	9	0	0	0	0
56	2F	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	0	0	0	0
56	2R	4	0	0	0	0
56	2T	3	0	0	0	0
56	2U	2	0	0	0	0
56	2V	2	0	0	0	0
56	2W	3	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	225	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2j	1	0	0	0	0
56	2l	5	0	0	0	0
56	2m	1	0	0	0	0
56	2q	3	0	0	0	0
56	2t	1	0	0	0	0
56	2v	3	0	0	0	0
56	2w	6	0	0	0	0
56	2x	7	0	0	0	0
56	2y	7	0	0	0	0
57	1A	1	0	0	0	0
57	2A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1d	8	0	0	2	0
60	2d	8	0	0	0	0
61	10	11	0	0	0	0
61	11	9	0	0	0	0
61	12	3	0	0	0	0
61	13	5	0	0	0	0
61	14	1	0	0	0	0
61	15	5	0	0	0	0
61	16	3	0	0	0	0
61	17	8	0	0	0	0
61	18	7	0	0	0	0
61	1A	1907	0	0	82	0
61	1B	59	0	0	3	0
61	1D	26	0	0	0	0
61	1E	28	0	0	2	0
61	1F	17	0	0	0	0
61	1G	2	0	0	0	0
61	1H	2	0	0	1	0
61	1N	4	0	0	0	0
61	1O	4	0	0	1	0
61	1P	23	0	0	1	0
61	1Q	5	0	0	0	0
61	1R	10	0	0	2	0
61	1S	3	0	0	1	0
61	1T	8	0	0	0	0
61	1U	14	0	0	0	0
61	1V	7	0	0	0	0
61	1W	7	0	0	2	0
61	1X	6	0	0	0	0
61	1Y	2	0	0	1	0
61	1Z	1	0	0	0	0
61	1a	267	0	0	18	0
61	1b	1	0	0	0	0
61	1e	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	3	0	0	0	0
61	1n	1	0	0	0	0
61	1q	2	0	0	0	0
61	1v	4	0	0	0	0
61	1w	15	0	0	0	0
61	1x	10	0	0	0	0
61	1y	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	20	3	0	0	0	0
61	21	8	0	0	1	0
61	23	1	0	0	0	0
61	27	4	0	0	0	0
61	28	3	0	0	0	0
61	29	1	0	0	0	0
61	2A	1000	0	0	74	0
61	2B	18	0	0	0	0
61	2D	17	0	0	0	0
61	2E	10	0	0	0	0
61	2F	12	0	0	0	0
61	2O	2	0	0	0	0
61	2P	8	0	0	0	0
61	2Q	2	0	0	0	0
61	2R	2	0	0	0	0
61	2T	4	0	0	0	0
61	2U	2	0	0	0	0
61	2V	1	0	0	0	0
61	2W	3	0	0	0	0
61	2X	1	0	0	0	0
61	2Y	2	0	0	0	0
61	2a	172	0	0	13	0
61	2d	2	0	0	0	0
61	2e	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	2	0	0	0	0
61	2l	4	0	0	1	0
61	2p	1	0	0	0	0
61	2q	1	0	0	0	0
61	2r	1	0	0	0	0
61	2t	2	0	0	1	0
61	2v	3	0	0	0	0
61	2w	3	0	0	0	0
61	2x	4	0	0	1	0
61	2y	4	0	0	0	0
All	All	299649	0	196683	4079	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 8.

The worst 5 of 4079 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	1.32	1.26
1:1A:1082:U:O4	1:1A:1086:A:N1	1.99	0.95
54:2y:55:PSU:HN1	54:2y:57:G:H5"	1.32	0.93
1:1A:1062:G:H1	1:1A:1077:A:H61	1.02	0.93
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.49	0.93

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%)	255 (93%)	18 (7%)	0	100 100
3	2D	273/276 (99%)	257 (94%)	16 (6%)	0	100 100
4	1E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24 46
4	2E	202/206 (98%)	187 (93%)	14 (7%)	1 (0%)	24 46
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	24 46
5	2F	201/210 (96%)	196 (98%)	1 (0%)	4 (2%)	6 12
6	1G	179/182 (98%)	167 (93%)	12 (7%)	0	100 100
6	2G	179/182 (98%)	153 (86%)	23 (13%)	3 (2%)	7 15
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21 42
7	2H	172/180 (96%)	152 (88%)	20 (12%)	0	100 100
8	1I	144/148 (97%)	124 (86%)	20 (14%)	0	100 100
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	18 38
9	1N	138/140 (99%)	134 (97%)	3 (2%)	1 (1%)	18 38
9	2N	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	9 19
10	1O	120/122 (98%)	115 (96%)	5 (4%)	0	100 100
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	128 (87%)	15 (10%)	4 (3%)	4	7
11	2P	147/150 (98%)	132 (90%)	11 (8%)	4 (3%)	4	7
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	6	13
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	34
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	12
17	2V	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6	12
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	25
19	2X	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	9	19
21	2Z	156/206 (76%)	128 (82%)	23 (15%)	5 (3%)	3	5
22	10	81/85 (95%)	81 (100%)	0	0	100	100
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
23	11	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	11	25
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
26	14	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	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%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	200 (87%)	22 (10%)	7 (3%)	3	5
33	2b	229/256 (90%)	182 (80%)	39 (17%)	8 (4%)	3	4
34	1c	204/239 (85%)	182 (89%)	22 (11%)	0	100	100
34	2c	204/239 (85%)	170 (83%)	30 (15%)	4 (2%)	6	12
35	1d	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	12	28
35	2d	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	12	28
36	1e	146/162 (90%)	129 (88%)	14 (10%)	3 (2%)	5	11
36	2e	146/162 (90%)	131 (90%)	12 (8%)	3 (2%)	5	11
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	146 (95%)	6 (4%)	1 (1%)	18	38
38	2g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	9	21
39	1h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	18	38
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	16	34
40	2i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
41	1j	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	3	5
41	2j	94/105 (90%)	79 (84%)	11 (12%)	4 (4%)	2	2
42	1k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	6	14
42	2k	112/129 (87%)	99 (88%)	11 (10%)	2 (2%)	6	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	107 (90%)	12 (10%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	121/126 (96%)	109 (90%)	11 (9%)	1 (1%)	16	34
44	2m	120/126 (95%)	104 (87%)	15 (12%)	1 (1%)	16	34
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	15
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
47	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
48	2q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
49	1r	66/88 (75%)	58 (88%)	8 (12%)	0	100	100
49	2r	66/88 (75%)	59 (89%)	7 (11%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	4	8
50	2s	81/93 (87%)	68 (84%)	13 (16%)	0	100	100
51	1t	94/106 (89%)	84 (89%)	6 (6%)	4 (4%)	2	2
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5	11
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11370/12128 (94%)	10431 (92%)	836 (7%)	103 (1%)	14	30

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	36	LYS
21	1Z	53	ILE
26	14	62	ARG
33	1b	17	PHE
33	1b	125	PRO

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	207 (96%)	8 (4%)	30	57
3	2D	215/218 (99%)	207 (96%)	8 (4%)	30	57
4	1E	164/166 (99%)	157 (96%)	7 (4%)	26	51
4	2E	164/166 (99%)	154 (94%)	10 (6%)	17	37
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5	12
5	2F	159/166 (96%)	141 (89%)	18 (11%)	5	12
6	1G	143/156 (92%)	133 (93%)	10 (7%)	14	31
6	2G	143/156 (92%)	128 (90%)	15 (10%)	6	14
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12	27
7	2H	144/148 (97%)	134 (93%)	10 (7%)	14	32
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3	5
8	2I	105/124 (85%)	88 (84%)	17 (16%)	2	4
9	1N	118/119 (99%)	113 (96%)	5 (4%)	26	52
9	2N	118/119 (99%)	111 (94%)	7 (6%)	18	38
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	64
10	2O	100/100 (100%)	90 (90%)	10 (10%)	7	16
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8	17
11	2P	115/116 (99%)	110 (96%)	5 (4%)	26	51
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11	24
12	2Q	111/111 (100%)	108 (97%)	3 (3%)	39	67
13	1R	101/101 (100%)	96 (95%)	5 (5%)	22	46
13	2R	101/101 (100%)	95 (94%)	6 (6%)	18	38
14	1S	86/88 (98%)	78 (91%)	8 (9%)	8	18
14	2S	85/88 (97%)	76 (89%)	9 (11%)	6	14
15	1T	115/127 (91%)	110 (96%)	5 (4%)	26	51
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20	43
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15	35
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26	51
17	1V	80/82 (98%)	76 (95%)	4 (5%)	22	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	2V	80/82 (98%)	76 (95%)	4 (5%)	22	46
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33	61
18	2W	90/92 (98%)	88 (98%)	2 (2%)	45	72
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61	82
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	55
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5	10
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6	14
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	24
21	2Z	137/179 (76%)	117 (85%)	20 (15%)	3	6
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	36
23	11	80/83 (96%)	74 (92%)	6 (8%)	12	28
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	28
24	12	65/67 (97%)	61 (94%)	4 (6%)	16	36
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	19
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	7
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	25
26	14	59/63 (94%)	48 (81%)	11 (19%)	1	3
26	24	53/63 (84%)	41 (77%)	12 (23%)	1	1
27	15	50/52 (96%)	49 (98%)	1 (2%)	48	74
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	25
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	26
28	26	50/52 (96%)	47 (94%)	3 (6%)	17	37
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	47
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	17
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	57
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	57
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	38
33	1b	192/220 (87%)	162 (84%)	30 (16%)	2	4
33	2b	187/220 (85%)	161 (86%)	26 (14%)	3	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6	14
34	2c	140/188 (74%)	117 (84%)	23 (16%)	2	4
35	1d	169/181 (93%)	149 (88%)	20 (12%)	5	10
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8	19
36	1e	113/123 (92%)	102 (90%)	11 (10%)	8	17
36	2e	114/123 (93%)	98 (86%)	16 (14%)	3	6
37	1f	84/90 (93%)	81 (96%)	3 (4%)	31	58
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	14
38	1g	119/127 (94%)	108 (91%)	11 (9%)	8	19
38	2g	120/127 (94%)	108 (90%)	12 (10%)	7	16
39	1h	114/119 (96%)	104 (91%)	10 (9%)	9	21
39	2h	114/119 (96%)	105 (92%)	9 (8%)	11	26
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	12
40	2i	89/99 (90%)	75 (84%)	14 (16%)	2	4
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	5
41	2j	69/92 (75%)	63 (91%)	6 (9%)	9	21
42	1k	82/99 (83%)	71 (87%)	11 (13%)	4	7
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	13
43	1l	96/108 (89%)	88 (92%)	8 (8%)	10	23
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	29
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	13
44	2m	92/101 (91%)	80 (87%)	12 (13%)	4	8
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	10
45	2n	49/50 (98%)	48 (98%)	1 (2%)	48	74
46	1o	78/80 (98%)	75 (96%)	3 (4%)	29	56
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	45
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	8
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	8
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13	29
48	2q	94/97 (97%)	90 (96%)	4 (4%)	26	51
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5 10
50	1s	69/80 (86%)	65 (94%)	4 (6%)	18 39
50	2s	67/80 (84%)	63 (94%)	4 (6%)	17 37
51	1t	70/82 (85%)	62 (89%)	8 (11%)	5 11
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10 22
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19 40
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19 40
All	All	9303/10064 (92%)	8516 (92%)	787 (8%)	10 22

5 of 787 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	2N	138	LEU
26	24	59	PHE
11	2P	71	VAL
9	2N	83	LYS
20	2Y	50	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 144 such sidechains are listed below:

Mol	Chain	Res	Type
38	2g	13	GLN
51	2t	75	ASN
38	2g	109	ASN
43	2l	80	HIS
41	1j	56	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	436 (15%)	24 (0%)
1	2A	2791/2915 (95%)	476 (17%)	25 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	27 (22%)	0
32	1a	1497/1521 (98%)	241 (16%)	0
32	2a	1501/1521 (98%)	273 (18%)	0
53	1v	12/24 (50%)	2 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	2v	12/24 (50%)	1 (8%)	0
54	1w	72/76 (94%)	26 (36%)	0
54	1y	72/76 (94%)	29 (40%)	0
54	2w	69/76 (90%)	18 (26%)	0
54	2y	70/76 (92%)	19 (27%)	0
55	1x	74/77 (96%)	9 (12%)	0
55	2x	74/77 (96%)	10 (13%)	0
All	All	9345/9620 (97%)	1574 (16%)	49 (0%)

5 of 1574 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	11	G
1	1A	12	U
1	1A	34	C
1	1A	45	C

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	271(K)	U
1	2A	1026	U
1	2A	271(M)	G
1	2A	752	A
1	2A	1379	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	$\#\|Z\| > 2$
1	8AH	2A	2503	56,1	22,26,27	1.68	5 (22%)	29,39,42	2.19	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	4SU	1y	8	54	18,21,22	1.84	5 (27%)	25,30,33	1.88	4 (16%)
55	4SU	2x	8	55	18,21,22	2.02	5 (27%)	25,30,33	1.29	4 (16%)
1	5MU	2A	1939	56,1	19,22,23	1.45	6 (31%)	27,32,35	2.20	6 (22%)
54	PSU	2y	32	54	18,21,22	1.33	2 (11%)	21,30,33	1.95	3 (14%)
55	31H	1x	76	55,56	31,34,35	1.21	3 (9%)	35,47,50	2.37	11 (31%)
54	PSU	1y	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.03	5 (23%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	21,30,33	1.97	4 (19%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.98	4 (19%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.91	1 (4%)
32	PSU	1a	516	32,56	18,21,22	1.42	2 (11%)	21,30,33	2.06	5 (23%)
1	PSU	2A	2605	1	18,21,22	1.34	3 (16%)	21,30,33	2.12	5 (23%)
32	5MC	1a	967	32	19,22,23	1.75	3 (15%)	26,32,35	1.15	2 (7%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.88	1 (4%)
1	5MC	2A	1962	56,1	19,22,23	1.67	3 (15%)	26,32,35	1.18	2 (7%)
55	5MC	2x	32	55	19,22,23	1.59	3 (15%)	26,32,35	1.31	4 (15%)
54	MIA	2y	37	54	21,24,32	1.59	3 (14%)	30,35,47	2.00	7 (23%)
32	UR3	2a	1498	32	19,22,23	1.04	1 (5%)	26,32,35	1.82	3 (11%)
43	0TD	2l	92	43	8,9,10	4.62	1 (12%)	6,11,13	2.31	3 (50%)
54	G7M	1y	46	54	23,26,27	1.58	3 (13%)	34,39,42	1.70	4 (11%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.01	3 (14%)
32	2MG	1a	1207	32,56	23,26,27	1.24	2 (8%)	33,38,41	2.25	8 (24%)
55	PSU	1x	55	55,56	18,21,22	1.35	2 (11%)	21,30,33	2.05	4 (19%)
54	PSU	1y	39	54	18,21,22	1.39	2 (11%)	21,30,33	1.84	3 (14%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.03	9 (27%)
32	M2G	1a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.84	6 (18%)
54	PSU	1y	32	54	18,21,22	1.35	2 (11%)	21,30,33	1.90	3 (14%)
1	5MC	1A	1962	56,1	19,22,23	1.81	3 (15%)	26,32,35	1.13	4 (15%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.16	9 (27%)
54	5MU	2w	54	54	19,22,23	1.39	5 (26%)	27,32,35	1.72	6 (22%)
32	5MC	2a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.11	2 (7%)
54	G7M	2y	46	54	23,26,27	1.60	3 (13%)	34,39,42	1.89	5 (14%)
32	5MC	1a	1404	32	19,22,23	1.78	3 (15%)	26,32,35	1.27	3 (11%)
54	5MU	1w	54	54	19,22,23	1.40	5 (26%)	27,32,35	1.86	6 (22%)
55	4SU	1x	8	55	18,21,22	2.43	5 (27%)	25,30,33	1.83	6 (24%)
55	5MU	2x	54	55	19,22,23	1.44	5 (26%)	27,32,35	1.94	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	5MC	2a	967	32	19,22,23	1.68	3 (15%)	26,32,35	1.06	2 (7%)
54	PSU	1w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.03	4 (19%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.87	6 (18%)
32	UR3	1a	1498	32	19,22,23	1.01	2 (10%)	26,32,35	1.79	4 (15%)
55	5MC	1x	32	55	19,22,23	1.69	3 (15%)	26,32,35	1.20	3 (11%)
1	5MC	1A	1942	56,1	19,22,23	1.60	3 (15%)	26,32,35	1.26	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.99	3 (14%)
54	MIA	1y	37	54	21,24,32	1.65	4 (19%)	30,35,47	2.01	7 (23%)
54	4SU	1w	8	54	18,21,22	1.85	5 (27%)	25,30,33	1.97	4 (16%)
54	PSU	1w	32	54,56	18,21,22	1.33	2 (11%)	21,30,33	1.90	3 (14%)
54	4SU	2y	8	54	18,21,22	1.69	4 (22%)	25,30,33	2.26	5 (20%)
54	PSU	2y	39	54	18,21,22	1.41	2 (11%)	21,30,33	1.69	3 (14%)
54	5MU	1y	54	54	19,22,23	1.48	5 (26%)	27,32,35	1.77	5 (18%)
1	OMU	1A	2552	56,1	19,22,23	1.29	4 (21%)	25,31,34	1.82	5 (20%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.06	9 (27%)
54	4SU	2w	8	54	18,21,22	1.73	5 (27%)	25,30,33	2.11	5 (20%)
32	G7M	1a	527	32,56	23,26,27	1.52	4 (17%)	34,39,42	1.62	5 (14%)
32	5MC	2a	1400	32	19,22,23	1.61	3 (15%)	26,32,35	1.22	3 (11%)
54	PSU	2w	55	54	18,21,22	1.42	2 (11%)	21,30,33	1.97	3 (14%)
54	5MU	2y	54	54	19,22,23	1.46	5 (26%)	27,32,35	1.90	6 (22%)
54	G7M	1w	46	54	23,26,27	1.59	3 (13%)	34,39,42	1.74	4 (11%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	2.03	9 (27%)
54	PSU	1w	39	54	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
1	8AH	1A	2503	56,1	22,26,27	1.61	5 (22%)	29,39,42	2.14	5 (17%)
1	5MU	2A	1915	56,1	19,22,23	1.46	5 (26%)	27,32,35	2.09	6 (22%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	0.97	1 (4%)
1	OMG	1A	2251	55,56,1	23,26,27	1.24	3 (13%)	32,38,41	1.89	5 (15%)
54	PSU	2w	39	54	18,21,22	1.36	2 (11%)	21,30,33	2.07	3 (14%)
32	2MG	2a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.25	8 (24%)
1	5MU	1A	1915	1	19,22,23	1.41	5 (26%)	27,32,35	2.18	7 (25%)
54	MIA	1w	37	54	28,31,32	2.33	6 (21%)	38,44,47	2.78	12 (31%)
54	PSU	2w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.93	4 (19%)
55	5MU	1x	54	55,56	19,22,23	1.48	6 (31%)	27,32,35	1.87	8 (29%)
54	MIA	2w	37	54	24,27,32	2.00	6 (25%)	32,39,47	2.62	10 (31%)
1	OMU	2A	2552	56,1	19,22,23	1.20	3 (15%)	25,31,34	1.76	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	2A	1917	56,1	18,21,22	1.32	2 (11%)	21,30,33	1.95	4 (19%)
32	5MC	2a	1407	32,56	19,22,23	1.54	3 (15%)	26,32,35	1.16	3 (11%)
55	31H	2x	76	55,56,57,1	31,34,35	1.21	3 (9%)	35,47,50	1.95	9 (25%)
32	5MC	1a	1407	32	19,22,23	1.65	3 (15%)	26,32,35	1.15	2 (7%)
32	5MC	1a	1400	32	19,22,23	1.53	3 (15%)	26,32,35	1.10	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.77	0	25,32,35	0.95	1 (4%)
32	G7M	2a	527	32,56	23,26,27	1.52	4 (17%)	34,39,42	1.70	5 (14%)
1	PSU	1A	2605	56,1	18,21,22	1.40	3 (16%)	21,30,33	2.09	4 (19%)
54	PSU	2y	55	54	18,21,22	1.44	3 (16%)	21,30,33	1.95	5 (23%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)
54	G7M	2w	46	54	23,26,27	1.53	4 (17%)	34,39,42	1.59	4 (11%)
1	5MC	2A	1942	1	19,22,23	1.59	3 (15%)	26,32,35	1.12	2 (7%)
43	0TD	1l	92	43	8,9,10	4.53	1 (12%)	6,11,13	1.79	2 (33%)
1	OMG	2A	2251	55,56,1	23,26,27	1.22	3 (13%)	32,38,41	2.05	7 (21%)
1	5MU	1A	1939	56,1	19,22,23	1.43	6 (31%)	27,32,35	2.20	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	8AH	2A	2503	56,1	-	0/7/25/26	0/3/3/3
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
55	31H	1x	76	55,56	-	5/22/40/41	0/3/3/3
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
1	5MC	2A	1962	56,1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/7/25/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
54	G7M	1y	46	54	-	1/7/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32,56	-	2/9/27/28	0/3/3/3
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
54	G7M	2y	46	54	-	2/7/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	56,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	1/7/25/34	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54,56	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
1	OMU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,56	-	3/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	8AH	1A	2503	56,1	-	1/7/25/26	0/3/3/3
1	5MU	2A	1915	56,1	-	1/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	OMG	1A	2251	55,56,1	-	0/9/27/28	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/11/29/34	0/3/3/3
1	OMU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
1	PSU	2A	1917	56,1	-	1/7/25/26	0/2/2/2
32	5MC	2a	1407	32,56	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,56,57,1	-	6/22/40/41	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
32	G7M	2a	527	32,56	-	3/7/25/26	0/3/3/3
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	OMG	2A	2251	55,56,1	-	0/9/27/28	0/3/3/3
1	5MU	1A	1939	56,1	-	0/7/25/26	0/2/2/2

The worst 5 of 258 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.64	1.69	1.82
43	1l	92	0TD	CB-SB	-12.37	1.69	1.82
54	1w	37	MIA	C2-S10	-7.07	1.69	1.75
1	1A	1962	5MC	C5-C4	6.82	1.49	1.44
54	1w	37	MIA	C13-C14	6.78	1.52	1.32

The worst 5 of 404 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	C12-C13-C14	-9.44	110.07	127.01
54	2w	37	MIA	C5-C4-N3	-9.22	117.47	127.18
1	2A	2503	8AH	C5-C4-N3	-8.19	118.56	127.18
54	1w	37	MIA	C5-C4-N3	-7.94	118.81	127.18
1	1A	2503	8AH	C5-C4-N3	-7.67	119.10	127.18

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C12-C13-C14-C16
55	1x	76	31H	CB-CA-N-CN

There are no ring outliers.

33 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	1y	8	4SU	1	0
55	2x	8	4SU	2	0
1	2A	1939	5MU	2	0
55	1x	76	31H	1	0
54	1y	55	PSU	1	0
32	1a	967	5MC	1	0
54	2y	37	MIA	1	0
43	2l	92	0TD	1	0
54	1y	46	G7M	1	0
32	1a	1207	2MG	1	0
32	2a	1518	MA6	1	0
32	1a	966	M2G	2	0
32	1a	1519	MA6	1	0
54	2y	46	G7M	2	0
55	1x	8	4SU	2	0
32	2a	967	5MC	2	0
32	2a	966	M2G	1	0
1	1A	1942	5MC	1	0
54	1y	37	MIA	3	0
54	2y	8	4SU	3	0
54	2y	39	PSU	1	0
54	1y	54	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1519	MA6	1	0
54	2y	54	5MU	1	0
32	1a	1518	MA6	1	0
1	2A	1915	5MU	1	0
1	1A	1920	OMC	1	0
32	2a	1207	2MG	1	0
55	2x	76	31H	1	0
32	1a	1402	4OC	1	0
54	2y	55	PSU	7	0
43	1l	92	0TD	1	0
1	1A	1939	5MU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2763 ligands modelled in this entry, 2759 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	3846	-	34,37,37	1.32	4 (11%)	31,53,53	1.01	2 (6%)
60	SF4	1d	302	35	0,12,12	-	-	-		
58	WC9	1A	4098	1	34,37,37	1.68	6 (17%)	31,53,53	1.10	2 (6%)
60	SF4	2d	303	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	WC9	2A	3846	-	-	0/28/71/71	0/3/4/4
60	SF4	1d	302	35	-	-	0/6/5/5
58	WC9	1A	4098	1	-	2/28/71/71	0/3/4/4
60	SF4	2d	303	35	-	-	0/6/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4098	WC9	CAM-CBF	-4.79	1.39	1.51
58	1A	4098	WC9	OAW-CB	4.63	1.47	1.42
58	2A	3846	WC9	CAM-CBF	-4.48	1.40	1.51
58	1A	4098	WC9	OAW-CAX	3.41	1.48	1.43
58	2A	3846	WC9	OAW-CB	3.04	1.45	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	2A	3846	WC9	CBC-CBB-CAZ	-3.13	110.61	116.68
58	1A	4098	WC9	CBC-CBB-CAZ	-2.91	111.02	116.68
58	1A	4098	WC9	CD2-CAZ-CAY	-2.59	109.91	113.78
58	2A	3846	WC9	CAF-OAA-CAB	-2.46	110.94	114.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	4098	WC9	CAB-CAK-NAL-C
58	1A	4098	WC9	CAM-CAK-NAL-C

There are no ring outliers.

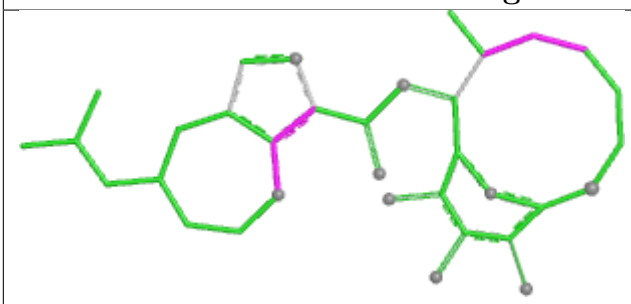
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	2A	3846	WC9	1	0
60	1d	302	SF4	2	0
58	1A	4098	WC9	1	0

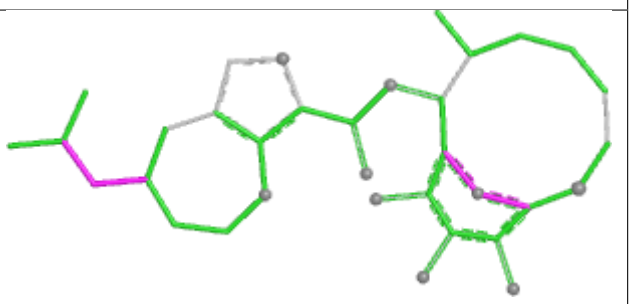
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

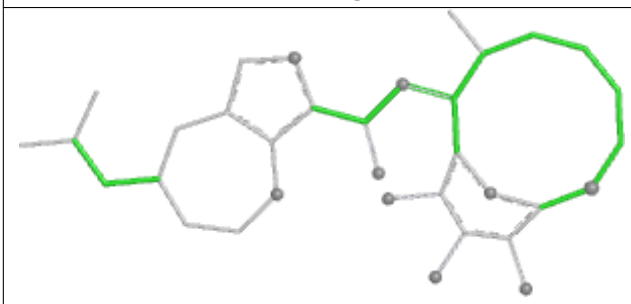
Ligand WC9 2A 3846



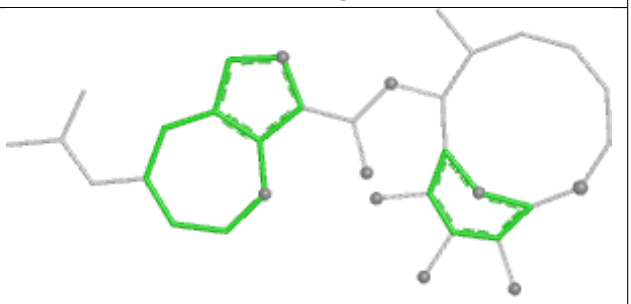
Bond lengths



Bond angles

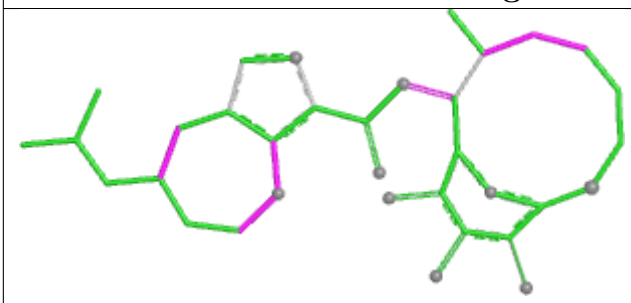


Torsions

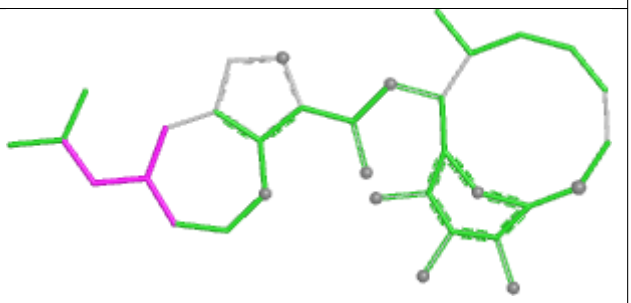


Rings

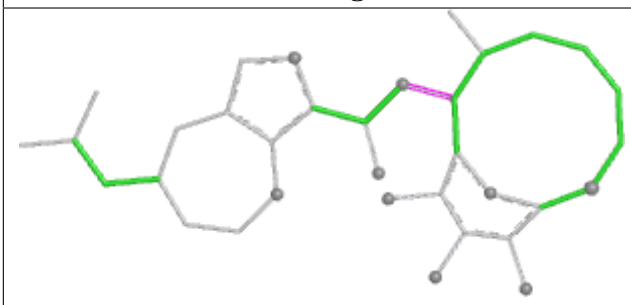
Ligand WC9 1A 4098



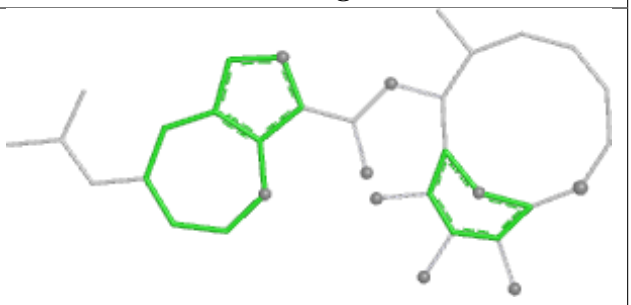
Bond lengths



Bond angles



Torsions



Rings

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%)	-0.52	120 (4%)	40	35	21, 38, 95, 108	0
1	2A	2789/2915 (95%)	-0.05	104 (3%)	45	39	34, 57, 93, 107	0
2	1B	120/121 (99%)	-0.33	0	100	100	33, 52, 67, 88	0
2	2B	120/121 (99%)	0.39	1 (0%)	82	80	61, 73, 82, 93	0
3	1D	275/276 (99%)	-0.25	2 (0%)	84	82	21, 39, 52, 79	0
3	2D	275/276 (99%)	0.10	2 (0%)	84	82	30, 50, 62, 82	0
4	1E	204/206 (99%)	-0.27	0	100	100	21, 39, 61, 72	0
4	2E	204/206 (99%)	0.39	6 (2%)	53	48	39, 60, 72, 83	0
5	1F	203/210 (96%)	-0.07	1 (0%)	87	85	22, 45, 68, 84	0
5	2F	203/210 (96%)	0.38	2 (0%)	79	76	36, 64, 76, 84	0
6	1G	181/182 (99%)	0.30	5 (2%)	55	49	46, 60, 74, 83	0
6	2G	181/182 (99%)	0.73	8 (4%)	39	33	62, 74, 82, 86	0
7	1H	174/180 (96%)	0.08	3 (1%)	69	64	39, 54, 66, 73	0
7	2H	174/180 (96%)	1.31	36 (20%)	2	2	71, 84, 91, 95	0
8	1I	146/148 (98%)	0.67	4 (2%)	56	50	49, 72, 81, 84	0
8	2I	146/148 (98%)	0.81	10 (6%)	23	19	50, 71, 82, 88	0
9	1N	140/140 (100%)	-0.24	1 (0%)	84	82	25, 38, 62, 75	0
9	2N	140/140 (100%)	0.55	5 (3%)	46	40	48, 66, 79, 84	0
10	1O	122/122 (100%)	-0.23	0	100	100	29, 41, 59, 63	0
10	2O	122/122 (100%)	0.35	1 (0%)	82	80	50, 61, 71, 76	0
11	1P	149/150 (99%)	0.02	0	100	100	23, 50, 70, 75	0
11	2P	149/150 (99%)	0.40	2 (1%)	75	71	41, 63, 80, 87	0
12	1Q	141/141 (100%)	-0.06	1 (0%)	84	82	28, 43, 61, 77	0
12	2Q	141/141 (100%)	0.64	5 (3%)	47	41	52, 67, 76, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.33	0 100 100	27, 36, 47, 59	0
13	2R	118/118 (100%)	0.28	1 (0%) 82 80	44, 54, 65, 73	0
14	1S	110/112 (98%)	0.10	0 100 100	41, 52, 64, 70	0
14	2S	110/112 (98%)	0.80	6 (5%) 30 25	58, 68, 77, 80	0
15	1T	131/146 (89%)	0.14	3 (2%) 61 55	36, 48, 73, 81	0
15	2T	131/146 (89%)	0.50	2 (1%) 72 68	53, 65, 75, 81	0
16	1U	116/118 (98%)	-0.47	0 100 100	20, 30, 46, 66	0
16	2U	116/118 (98%)	0.47	3 (2%) 57 51	41, 63, 75, 81	0
17	1V	101/101 (100%)	-0.39	0 100 100	23, 38, 57, 65	0
17	2V	101/101 (100%)	0.44	1 (0%) 79 76	44, 71, 79, 82	0
18	1W	112/113 (99%)	-0.41	1 (0%) 81 78	23, 32, 51, 77	0
18	2W	112/113 (99%)	0.19	0 100 100	42, 51, 67, 83	0
19	1X	95/96 (98%)	-0.23	0 100 100	29, 39, 61, 72	0
19	2X	95/96 (98%)	0.35	3 (3%) 50 44	45, 58, 74, 86	0
20	1Y	107/110 (97%)	0.24	2 (1%) 66 61	37, 52, 69, 78	0
20	2Y	107/110 (97%)	0.96	12 (11%) 10 8	56, 69, 81, 87	0
21	1Z	154/206 (74%)	0.60	6 (3%) 43 38	38, 66, 84, 91	0
21	2Z	160/206 (77%)	1.12	20 (12%) 8 6	69, 80, 89, 92	0
22	10	83/85 (97%)	0.03	3 (3%) 46 40	30, 40, 60, 76	0
22	20	83/85 (97%)	0.79	8 (9%) 13 10	45, 62, 74, 83	0
23	11	97/98 (98%)	0.20	3 (3%) 51 45	31, 46, 72, 77	0
23	21	97/98 (98%)	0.22	1 (1%) 79 76	38, 53, 72, 81	0
24	12	70/72 (97%)	-0.00	2 (2%) 53 48	38, 50, 59, 71	0
24	22	70/72 (97%)	0.50	2 (2%) 53 48	57, 67, 75, 76	0
25	13	59/60 (98%)	-0.24	2 (3%) 48 42	26, 38, 61, 82	0
25	23	59/60 (98%)	0.38	1 (1%) 69 64	54, 65, 78, 81	0
26	14	69/71 (97%)	0.96	10 (14%) 6 4	56, 76, 87, 90	0
26	24	69/71 (97%)	1.06	7 (10%) 12 9	71, 83, 92, 101	0
27	15	59/60 (98%)	-0.48	0 100 100	20, 33, 52, 59	0
27	25	59/60 (98%)	0.32	3 (5%) 33 28	39, 54, 69, 76	0
28	16	53/54 (98%)	-0.24	0 100 100	35, 47, 60, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.40	0 100 100	47, 59, 66, 75	0
29	17	48/49 (97%)	-0.18	3 (6%) 26 20	23, 29, 59, 69	0
29	27	48/49 (97%)	0.04	3 (6%) 26 20	35, 42, 68, 73	0
30	18	64/65 (98%)	-0.25	0 100 100	28, 38, 44, 58	0
30	28	64/65 (98%)	0.26	1 (1%) 70 66	46, 53, 60, 68	0
31	19	37/37 (100%)	-0.19	0 100 100	34, 42, 55, 66	0
31	29	37/37 (100%)	1.04	3 (8%) 18 14	63, 69, 78, 84	0
32	1a	1488/1521 (97%)	0.19	49 (3%) 49 43	36, 66, 93, 109	0
32	2a	1491/1521 (98%)	0.41	65 (4%) 39 33	45, 73, 93, 106	0
33	1b	231/256 (90%)	1.11	41 (17%) 4 3	64, 78, 87, 93	0
33	2b	231/256 (90%)	1.23	41 (17%) 4 3	68, 82, 88, 93	0
34	1c	206/239 (86%)	0.68	8 (3%) 43 38	60, 72, 82, 91	0
34	2c	206/239 (86%)	1.17	24 (11%) 9 7	71, 79, 86, 90	0
35	1d	208/209 (99%)	0.77	13 (6%) 26 20	56, 69, 78, 85	0
35	2d	208/209 (99%)	0.51	3 (1%) 73 69	54, 66, 74, 79	0
36	1e	148/162 (91%)	0.42	3 (2%) 65 60	51, 64, 74, 85	0
36	2e	148/162 (91%)	0.74	4 (2%) 56 50	57, 71, 79, 88	0
37	1f	100/101 (99%)	0.48	0 100 100	56, 68, 74, 77	0
37	2f	100/101 (99%)	0.51	2 (2%) 65 60	55, 67, 75, 77	0
38	1g	155/156 (99%)	0.58	8 (5%) 33 27	59, 70, 80, 88	0
38	2g	155/156 (99%)	0.70	10 (6%) 25 19	67, 74, 81, 88	0
39	1h	137/138 (99%)	0.39	1 (0%) 84 82	55, 67, 73, 78	0
39	2h	137/138 (99%)	0.83	3 (2%) 62 57	65, 73, 78, 82	0
40	1i	127/128 (99%)	1.21	20 (15%) 5 4	56, 77, 83, 88	0
40	2i	127/128 (99%)	1.42	30 (23%) 2 1	64, 81, 87, 90	0
41	1j	97/105 (92%)	1.12	13 (13%) 7 5	58, 77, 87, 92	0
41	2j	96/105 (91%)	1.89	42 (43%) 0 0	71, 82, 90, 91	0
42	1k	114/129 (88%)	0.53	4 (3%) 47 41	43, 64, 76, 81	0
42	2k	114/129 (88%)	0.57	4 (3%) 47 41	53, 70, 79, 81	0
43	1l	121/132 (91%)	0.13	2 (1%) 69 64	44, 53, 67, 74	0
43	2l	121/132 (91%)	0.51	4 (3%) 49 43	55, 63, 74, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.77	8 (6%) 25 19	52, 70, 78, 90	0
44	2m	122/126 (96%)	1.38	21 (17%) 4 3	66, 79, 85, 90	0
45	1n	60/61 (98%)	1.03	7 (11%) 9 7	60, 68, 77, 81	0
45	2n	60/61 (98%)	1.85	21 (35%) 1 1	73, 80, 85, 89	0
46	1o	88/89 (98%)	0.55	1 (1%) 78 74	50, 65, 75, 82	0
46	2o	88/89 (98%)	0.61	2 (2%) 61 55	57, 68, 79, 81	0
47	1p	82/88 (93%)	0.90	2 (2%) 59 54	55, 69, 77, 85	0
47	2p	82/88 (93%)	0.85	5 (6%) 27 22	57, 67, 75, 79	0
48	1q	99/105 (94%)	0.72	3 (3%) 52 47	53, 66, 74, 77	0
48	2q	99/105 (94%)	0.71	5 (5%) 33 28	61, 70, 77, 80	0
49	1r	68/88 (77%)	0.36	1 (1%) 72 68	53, 66, 76, 78	0
49	2r	68/88 (77%)	0.45	1 (1%) 72 68	57, 68, 75, 80	0
50	1s	83/93 (89%)	0.67	3 (3%) 46 40	62, 74, 79, 82	0
50	2s	83/93 (89%)	1.31	14 (16%) 4 3	74, 82, 87, 93	0
51	1t	96/106 (90%)	0.81	7 (7%) 21 17	58, 70, 80, 83	0
51	2t	96/106 (90%)	0.65	2 (2%) 63 58	57, 68, 80, 86	0
52	1u	23/27 (85%)	1.05	4 (17%) 4 3	63, 68, 71, 79	0
52	2u	23/27 (85%)	1.32	4 (17%) 4 3	69, 76, 79, 85	0
53	1v	13/24 (54%)	0.22	1 (7%) 19 15	48, 58, 84, 92	0
53	2v	13/24 (54%)	0.79	3 (23%) 2 1	62, 72, 87, 98	0
54	1w	67/76 (88%)	1.09	13 (19%) 3 2	49, 86, 99, 101	0
54	1y	67/76 (88%)	0.83	2 (2%) 52 47	38, 90, 97, 101	0
54	2w	65/76 (85%)	1.37	14 (21%) 2 2	69, 94, 102, 108	0
54	2y	66/76 (86%)	1.06	9 (13%) 7 5	50, 92, 98, 102	0
55	1x	71/77 (92%)	0.21	2 (2%) 55 49	33, 63, 80, 86	0
55	2x	71/77 (92%)	0.42	3 (4%) 40 35	46, 75, 86, 97	0
All	All	20873/21748 (95%)	0.25	983 (4%) 36 30	20, 63, 88, 109	0

The worst 5 of 983 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	652(V)	C	10.6
1	1A	653	A	10.6

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Mol	Chain	Res	Type	RSRZ
1	2A	652(V)	C	10.5
1	2A	652(U)	G	10.5
1	1A	652(U)	G	9.6

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	0.60	0.15	91,95,108,119	0
54	4SU	2y	8	20/21	0.68	0.16	85,95,101,110	0
54	4SU	2w	8	20/21	0.70	0.15	91,95,111,121	0
54	PSU	1y	55	20/21	0.71	0.13	93,96,110,114	0
54	G7M	2w	46	24/25	0.72	0.15	84,94,106,115	0
54	G7M	2y	46	24/25	0.74	0.15	86,94,102,115	0
54	G7M	1w	46	24/25	0.74	0.15	81,90,102,115	0
54	MIA	2y	37	22/30	0.75	0.14	83,90,101,107	0
54	G7M	1y	46	24/25	0.76	0.16	84,92,106,114	0
54	5MU	1y	54	21/22	0.76	0.16	81,92,102,108	0
54	4SU	1y	8	20/21	0.76	0.12	88,92,100,101	0
54	5MU	2y	54	21/22	0.78	0.15	85,93,105,118	0
54	PSU	2y	32	20/21	0.80	0.12	84,90,96,103	0
54	MIA	1y	37	22/30	0.81	0.12	77,84,90,93	0
54	PSU	2w	55	20/21	0.81	0.10	82,87,96,99	0
54	PSU	1w	55	20/21	0.83	0.11	65,80,88,89	0
54	PSU	1y	39	20/21	0.84	0.11	77,82,86,92	0
54	4SU	1w	8	20/21	0.86	0.12	78,86,98,98	0
54	PSU	1y	32	20/21	0.86	0.10	78,84,89,90	0
54	PSU	2y	39	20/21	0.87	0.10	81,89,98,99	0
55	4SU	2x	8	20/21	0.88	0.12	77,80,85,87	0
54	5MU	2w	54	21/22	0.89	0.10	77,80,85,89	0
55	5MU	2x	54	21/22	0.90	0.11	72,76,81,84	0
54	PSU	2w	32	20/21	0.90	0.13	67,77,87,91	0
54	MIA	2w	37	25/30	0.90	0.13	58,71,83,101	0
43	0TD	2l	92	10/11	0.90	0.11	59,61,67,70	0
32	PSU	2a	516	20/21	0.91	0.10	63,69,75,81	0
55	PSU	2x	55	20/21	0.91	0.09	66,74,79,86	0
32	G7M	2a	527	24/25	0.91	0.12	58,64,70,75	0
54	PSU	1w	32	20/21	0.92	0.12	59,66,73,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	5MU	1x	54	21/22	0.92	0.09	53,64,77,81	0
55	5MC	2x	32	21/22	0.92	0.12	68,71,74,81	0
55	PSU	1x	55	20/21	0.92	0.09	54,61,75,85	0
1	PSU	2A	1917	20/21	0.92	0.09	53,63,68,69	0
32	2MG	2a	1207	24/25	0.93	0.09	70,79,82,83	0
55	4SU	1x	8	20/21	0.93	0.10	54,66,73,75	0
54	5MU	1w	54	21/22	0.93	0.09	47,66,73,75	0
1	5MU	2A	1915	21/22	0.93	0.09	57,63,68,70	0
32	M2G	2a	966	25/26	0.93	0.15	58,65,77,83	0
32	5MC	2a	967	21/22	0.94	0.12	59,65,73,80	0
43	0TD	1l	92	10/11	0.94	0.09	48,54,56,71	0
32	5MC	2a	1400	21/22	0.94	0.12	65,70,73,83	0
32	5MC	2a	1404	21/22	0.94	0.10	52,56,60,65	0
54	MIA	1w	37	29/30	0.94	0.13	45,57,69,81	0
55	5MC	1x	32	21/22	0.94	0.11	56,59,62,72	0
32	4OC	2a	1402	22/23	0.95	0.10	51,60,64,65	0
32	G7M	1a	527	24/25	0.95	0.09	44,51,57,63	0
32	MA6	2a	1518	24/25	0.95	0.11	51,62,66,70	0
32	M2G	1a	966	25/26	0.95	0.11	46,53,62,64	0
32	5MC	1a	967	21/22	0.95	0.09	46,53,61,62	0
32	2MG	1a	1207	24/25	0.95	0.09	61,70,73,75	0
54	PSU	1w	39	20/21	0.95	0.09	54,64,74,76	0
1	PSU	1A	1917	20/21	0.95	0.08	47,52,56,58	0
54	PSU	2w	39	20/21	0.95	0.09	60,74,83,83	0
1	OMC	2A	1920	21/22	0.95	0.10	48,59,62,68	0
1	5MC	2A	1942	21/22	0.95	0.09	50,56,60,64	0
32	MA6	2a	1519	24/25	0.96	0.11	45,56,65,67	0
55	31H	2x	76	32/33	0.96	0.09	39,51,61,69	0
1	PSU	2A	1911	20/21	0.96	0.07	56,58,63,63	0
1	5MU	1A	1915	21/22	0.96	0.09	46,52,57,57	0
32	MA6	1a	1519	24/25	0.96	0.09	36,43,48,52	0
55	31H	1x	76	32/33	0.96	0.10	26,37,45,60	10
32	5MC	2a	1407	21/22	0.96	0.08	48,53,59,61	0
32	UR3	2a	1498	21/22	0.96	0.10	48,53,59,60	0
1	5MC	1A	1942	21/22	0.96	0.08	32,37,41,42	0
32	PSU	1a	516	20/21	0.96	0.08	44,56,61,64	0
1	OMU	2A	2552	21/22	0.96	0.09	43,47,50,62	0
32	4OC	1a	1402	22/23	0.97	0.07	42,46,53,60	0
32	5MC	1a	1404	21/22	0.97	0.07	33,38,42,44	0
32	5MC	1a	1407	21/22	0.97	0.08	36,45,46,49	0
32	UR3	1a	1498	21/22	0.97	0.08	37,40,43,55	0
1	5MU	2A	1939	21/22	0.97	0.07	34,40,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	1A	1911	20/21	0.97	0.07	36,46,54,54	0
32	MA6	1a	1518	24/25	0.97	0.09	34,43,47,49	0
1	5MC	2A	1962	21/22	0.97	0.08	36,49,53,62	0
1	8AH	2A	2503	24/25	0.97	0.08	35,41,45,50	0
32	5MC	1a	1400	21/22	0.97	0.09	46,53,57,63	0
1	PSU	1A	2605	20/21	0.97	0.06	25,29,32,33	0
1	PSU	2A	2605	20/21	0.97	0.07	33,40,46,47	0
1	OMG	2A	2251	24/25	0.98	0.07	37,43,49,57	0
1	OMC	1A	1920	21/22	0.98	0.06	38,47,50,54	0
1	OMU	1A	2552	21/22	0.98	0.06	27,30,35,37	0
1	5MC	1A	1962	21/22	0.98	0.06	28,36,41,47	0
1	5MU	1A	1939	21/22	0.98	0.06	26,32,34,39	0
1	OMG	1A	2251	24/25	0.98	0.06	22,26,30,32	0
1	8AH	1A	2503	24/25	0.99	0.06	14,24,29,30	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	2w	104	1/1	0.63	0.20	79,79,79,79	0
56	MG	2A	3083	1/1	0.64	0.15	61,61,61,61	0
56	MG	1A	3985	1/1	0.66	0.18	37,37,37,37	0
56	MG	1A	3992	1/1	0.68	0.16	70,70,70,70	0
56	MG	2v	102	1/1	0.69	0.29	82,82,82,82	0
56	MG	2W	202	1/1	0.69	0.14	76,76,76,76	0
56	MG	1a	1771	1/1	0.70	0.15	78,78,78,78	0
56	MG	2a	1748	1/1	0.70	0.19	96,96,96,96	0
56	MG	2A	3100	1/1	0.70	0.17	78,78,78,78	0
56	MG	2A	3585	1/1	0.70	0.18	73,73,73,73	0
56	MG	2A	3689	1/1	0.71	0.22	66,66,66,66	0
56	MG	1B	207	1/1	0.71	0.25	73,73,73,73	0
56	MG	2A	3217	1/1	0.71	0.18	69,69,69,69	0
56	MG	1Z	302	1/1	0.71	0.13	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3593	1/1	0.71	0.18	74,74,74,74	0
56	MG	1A	3587	1/1	0.72	0.36	54,54,54,54	0
56	MG	1A	3674	1/1	0.72	0.14	59,59,59,59	0
56	MG	2a	1720	1/1	0.72	0.28	78,78,78,78	0
56	MG	20	101	1/1	0.73	0.30	64,64,64,64	0
56	MG	1A	3966	1/1	0.73	0.14	70,70,70,70	0
56	MG	2A	3650	1/1	0.73	0.14	72,72,72,72	0
56	MG	2a	1821	1/1	0.73	0.25	81,81,81,81	0
56	MG	2A	3227	1/1	0.73	0.24	69,69,69,69	0
56	MG	1A	3724	1/1	0.73	0.14	63,63,63,63	0
56	MG	2A	3336	1/1	0.74	0.14	78,78,78,78	0
56	MG	2A	3368	1/1	0.74	0.31	83,83,83,83	0
56	MG	1A	4015	1/1	0.74	0.24	51,51,51,51	0
56	MG	1A	3459	1/1	0.74	0.13	63,63,63,63	0
56	MG	1a	1807	1/1	0.74	0.23	85,85,85,85	0
56	MG	1w	105	1/1	0.74	0.26	86,86,86,86	0
56	MG	2A	3699	1/1	0.74	0.14	62,62,62,62	0
56	MG	1A	3761	1/1	0.75	0.09	21,21,21,21	0
56	MG	1A	3823	1/1	0.75	0.14	62,62,62,62	0
56	MG	1A	3585	1/1	0.75	0.26	64,64,64,64	0
56	MG	2A	3442	1/1	0.75	0.19	72,72,72,72	0
56	MG	2A	3815	1/1	0.75	0.14	63,63,63,63	0
56	MG	1A	4087	1/1	0.75	0.21	62,62,62,62	0
56	MG	2a	1672	1/1	0.76	0.12	63,63,63,63	0
56	MG	1A	3596	1/1	0.76	0.13	36,36,36,36	0
56	MG	2A	3712	1/1	0.76	0.18	68,68,68,68	0
56	MG	2A	3006	1/1	0.76	0.14	78,78,78,78	0
56	MG	1a	1711	1/1	0.76	0.28	60,60,60,60	0
56	MG	2w	101	1/1	0.76	0.14	79,79,79,79	0
56	MG	2A	3483	1/1	0.76	0.20	62,62,62,62	0
56	MG	2w	106	1/1	0.76	0.22	77,77,77,77	0
56	MG	1A	3738	1/1	0.77	0.18	63,63,63,63	0
56	MG	1a	1797	1/1	0.77	0.17	76,76,76,76	0
56	MG	2a	1794	1/1	0.77	0.30	65,65,65,65	0
56	MG	2a	1796	1/1	0.77	0.16	70,70,70,70	0
56	MG	2a	1814	1/1	0.77	0.38	80,80,80,80	0
56	MG	1A	3715	1/1	0.77	0.21	62,62,62,62	0
56	MG	2B	201	1/1	0.77	0.38	82,82,82,82	0
56	MG	1A	3781	1/1	0.77	0.18	75,75,75,75	0
56	MG	1A	3516	1/1	0.77	0.18	79,79,79,79	0
56	MG	2A	3069	1/1	0.77	0.30	69,69,69,69	0
56	MG	2a	1730	1/1	0.78	0.23	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	4072	1/1	0.78	0.14	60,60,60,60	0
56	MG	2A	3391	1/1	0.78	0.17	65,65,65,65	0
56	MG	1Z	304	1/1	0.78	0.11	62,62,62,62	0
56	MG	1a	1660	1/1	0.78	0.20	71,71,71,71	0
56	MG	1A	3700	1/1	0.78	0.18	52,52,52,52	0
56	MG	2A	3233	1/1	0.78	0.30	61,61,61,61	0
56	MG	2a	1607	1/1	0.78	0.33	69,69,69,69	0
56	MG	2A	3299	1/1	0.78	0.15	70,70,70,70	0
56	MG	1A	3828	1/1	0.78	0.18	63,63,63,63	0
56	MG	1A	4071	1/1	0.79	0.17	69,69,69,69	0
56	MG	2a	1778	1/1	0.79	0.22	67,67,67,67	0
56	MG	2A	3833	1/1	0.79	0.17	65,65,65,65	0
56	MG	1A	3745	1/1	0.79	0.12	46,46,46,46	0
56	MG	2A	3239	1/1	0.79	0.16	57,57,57,57	0
56	MG	2A	3243	1/1	0.79	0.15	72,72,72,72	0
56	MG	1B	226	1/1	0.79	0.19	65,65,65,65	0
56	MG	1D	312	1/1	0.79	0.17	66,66,66,66	0
56	MG	2A	3184	1/1	0.79	0.22	82,82,82,82	0
56	MG	1w	107	1/1	0.79	0.20	70,70,70,70	0
56	MG	2A	3289	1/1	0.80	0.13	66,66,66,66	0
56	MG	2A	3606	1/1	0.80	0.26	70,70,70,70	0
56	MG	2A	3110	1/1	0.80	0.17	71,71,71,71	0
56	MG	2A	3319	1/1	0.80	0.19	61,61,61,61	0
56	MG	1A	3526	1/1	0.80	0.12	51,51,51,51	0
56	MG	2A	3340	1/1	0.80	0.22	76,76,76,76	0
56	MG	1x	113	1/1	0.80	0.16	71,71,71,71	0
56	MG	2A	3821	1/1	0.80	0.15	45,45,45,45	0
56	MG	1B	221	1/1	0.80	0.16	67,67,67,67	0
56	MG	1A	3532	1/1	0.80	0.24	59,59,59,59	0
56	MG	1B	229	1/1	0.80	0.22	72,72,72,72	0
56	MG	2A	3544	1/1	0.80	0.18	40,40,40,40	0
56	MG	1a	1663	1/1	0.80	0.13	57,57,57,57	0
56	MG	2x	106	1/1	0.80	0.29	71,71,71,71	0
56	MG	2A	3724	1/1	0.81	0.17	62,62,62,62	0
56	MG	2A	3043	1/1	0.81	0.19	66,66,66,66	0
56	MG	1A	3978	1/1	0.81	0.13	38,38,38,38	0
56	MG	1A	3075	1/1	0.81	0.30	65,65,65,65	0
56	MG	2A	3835	1/1	0.81	0.13	65,65,65,65	0
56	MG	1A	3529	1/1	0.81	0.28	57,57,57,57	0
56	MG	2A	3365	1/1	0.81	0.18	74,74,74,74	0
56	MG	1a	1712	1/1	0.81	0.36	58,58,58,58	0
56	MG	2a	1603	1/1	0.81	0.17	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	3112	1/1	0.81	0.26	73,73,73,73	0
56	MG	2a	1653	1/1	0.81	0.31	74,74,74,74	0
56	MG	2A	3182	1/1	0.81	0.20	76,76,76,76	0
56	MG	2A	3473	1/1	0.81	0.17	63,63,63,63	0
56	MG	2A	3480	1/1	0.81	0.14	67,67,67,67	0
56	MG	1A	3705	1/1	0.81	0.22	64,64,64,64	0
56	MG	2A	3215	1/1	0.81	0.12	65,65,65,65	0
56	MG	1A	3873	1/1	0.81	0.12	26,26,26,26	0
56	MG	1E	309	1/1	0.81	0.38	79,79,79,79	0
56	MG	1S	202	1/1	0.81	0.27	62,62,62,62	0
56	MG	2A	3234	1/1	0.81	0.19	63,63,63,63	0
56	MG	2A	3685	1/1	0.81	0.19	70,70,70,70	0
56	MG	1A	3931	1/1	0.81	0.20	37,37,37,37	0
56	MG	2A	3690	1/1	0.81	0.23	72,72,72,72	0
56	MG	1A	3095	1/1	0.81	0.12	71,71,71,71	0
56	MG	1a	1623	1/1	0.81	0.12	68,68,68,68	0
56	MG	1A	3897	1/1	0.82	0.14	52,52,52,52	0
56	MG	2A	3474	1/1	0.82	0.17	71,71,71,71	0
56	MG	2E	302	1/1	0.82	0.08	69,69,69,69	0
56	MG	1a	1714	1/1	0.82	0.23	64,64,64,64	0
56	MG	2A	3013	1/1	0.82	0.13	59,59,59,59	0
56	MG	1a	1739	1/1	0.82	0.16	53,53,53,53	0
56	MG	1a	1740	1/1	0.82	0.24	81,81,81,81	0
56	MG	2a	1641	1/1	0.82	0.22	70,70,70,70	0
56	MG	2a	1646	1/1	0.82	0.17	63,63,63,63	0
56	MG	2a	1650	1/1	0.82	0.34	79,79,79,79	0
56	MG	1A	4008	1/1	0.82	0.19	65,65,65,65	0
56	MG	2A	3600	1/1	0.82	0.13	44,44,44,44	0
56	MG	2a	1701	1/1	0.82	0.16	69,69,69,69	0
56	MG	2a	1703	1/1	0.82	0.30	61,61,61,61	0
56	MG	1a	1789	1/1	0.82	0.20	61,61,61,61	0
56	MG	2A	3648	1/1	0.82	0.17	60,60,60,60	0
56	MG	2A	3304	1/1	0.82	0.14	62,62,62,62	0
56	MG	2a	1777	1/1	0.82	0.29	78,78,78,78	0
56	MG	1a	1658	1/1	0.82	0.13	63,63,63,63	0
56	MG	1A	3704	1/1	0.82	0.13	63,63,63,63	0
56	MG	1n	101	1/1	0.82	0.37	73,73,73,73	0
56	MG	2A	3354	1/1	0.82	0.38	66,66,66,66	0
56	MG	1w	104	1/1	0.82	0.16	67,67,67,67	0
56	MG	2a	1825	1/1	0.82	0.30	72,72,72,72	0
56	MG	2l	202	1/1	0.82	0.17	65,65,65,65	0
56	MG	2A	3213	1/1	0.82	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	3744	1/1	0.82	0.15	50,50,50,50	0
56	MG	1A	4069	1/1	0.82	0.22	71,71,71,71	0
56	MG	2A	3414	1/1	0.82	0.19	58,58,58,58	0
56	MG	1A	3932	1/1	0.82	0.14	32,32,32,32	0
56	MG	2A	3292	1/1	0.83	0.41	75,75,75,75	0
56	MG	2a	1605	1/1	0.83	0.20	67,67,67,67	0
56	MG	1a	1689	1/1	0.83	0.34	56,56,56,56	0
56	MG	2a	1611	1/1	0.83	0.39	75,75,75,75	0
56	MG	2a	1618	1/1	0.83	0.19	69,69,69,69	0
56	MG	2a	1636	1/1	0.83	0.25	61,61,61,61	0
56	MG	1Y	203	1/1	0.83	0.11	73,73,73,73	0
56	MG	1A	4059	1/1	0.83	0.11	48,48,48,48	0
56	MG	2A	3142	1/1	0.83	0.22	71,71,71,71	0
56	MG	1A	3819	1/1	0.83	0.13	39,39,39,39	0
56	MG	2A	3659	1/1	0.83	0.18	58,58,58,58	0
56	MG	2a	1677	1/1	0.83	0.31	59,59,59,59	0
56	MG	2A	3669	1/1	0.83	0.17	64,64,64,64	0
56	MG	1x	104	1/1	0.83	0.14	60,60,60,60	0
56	MG	2a	1713	1/1	0.83	0.19	67,67,67,67	0
56	MG	1a	1604	1/1	0.83	0.21	64,64,64,64	0
56	MG	2A	3005	1/1	0.83	0.18	69,69,69,69	0
56	MG	1A	3230	1/1	0.83	0.15	54,54,54,54	0
56	MG	2a	1775	1/1	0.83	0.23	73,73,73,73	0
56	MG	1A	3339	1/1	0.83	0.14	48,48,48,48	0
56	MG	1A	3956	1/1	0.83	0.23	64,64,64,64	0
56	MG	2A	3470	1/1	0.83	0.16	66,66,66,66	0
56	MG	2A	3781	1/1	0.83	0.14	77,77,77,77	0
56	MG	2a	1804	1/1	0.83	0.18	60,60,60,60	0
56	MG	2A	3784	1/1	0.83	0.11	52,52,52,52	0
56	MG	2A	3045	1/1	0.83	0.14	58,58,58,58	0
56	MG	1A	3358	1/1	0.83	0.12	72,72,72,72	0
56	MG	2j	201	1/1	0.83	0.25	80,80,80,80	0
56	MG	2A	3477	1/1	0.83	0.15	63,63,63,63	0
56	MG	2v	101	1/1	0.83	0.35	73,73,73,73	0
56	MG	2A	3078	1/1	0.83	0.37	62,62,62,62	0
56	MG	1a	1668	1/1	0.83	0.17	62,62,62,62	0
56	MG	2A	3491	1/1	0.83	0.17	66,66,66,66	0
56	MG	2A	3523	1/1	0.83	0.38	76,76,76,76	0
56	MG	2A	3291	1/1	0.83	0.16	68,68,68,68	0
56	MG	2A	3315	1/1	0.84	0.26	78,78,78,78	0
56	MG	1y	4301	1/1	0.84	0.11	63,63,63,63	0
56	MG	1a	1640	1/1	0.84	0.29	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3338	1/1	0.84	0.11	67,67,67,67	0
56	MG	2A	3209	1/1	0.84	0.21	74,74,74,74	0
56	MG	1a	1764	1/1	0.84	0.26	58,58,58,58	0
56	MG	2A	3684	1/1	0.84	0.12	79,79,79,79	0
56	MG	1A	3837	1/1	0.84	0.16	67,67,67,67	0
56	MG	1W	207	1/1	0.84	0.26	43,43,43,43	0
56	MG	2A	3371	1/1	0.84	0.19	67,67,67,67	0
56	MG	2A	3697	1/1	0.84	0.17	63,63,63,63	0
56	MG	2A	3225	1/1	0.84	0.24	62,62,62,62	0
56	MG	2A	3701	1/1	0.84	0.14	58,58,58,58	0
56	MG	1A	3435	1/1	0.84	0.10	70,70,70,70	0
56	MG	2A	3718	1/1	0.84	0.17	65,65,65,65	0
56	MG	2A	3719	1/1	0.84	0.11	66,66,66,66	0
56	MG	1A	3649	1/1	0.84	0.17	57,57,57,57	0
56	MG	1a	1673	1/1	0.84	0.15	67,67,67,67	0
56	MG	2A	3778	1/1	0.84	0.28	73,73,73,73	0
56	MG	1A	3971	1/1	0.84	0.11	59,59,59,59	0
56	MG	14	101	1/1	0.84	0.16	70,70,70,70	0
56	MG	2A	3791	1/1	0.84	0.14	48,48,48,48	0
56	MG	2A	3266	1/1	0.84	0.15	72,72,72,72	0
56	MG	2a	1815	1/1	0.84	0.22	58,58,58,58	0
56	MG	2A	3267	1/1	0.84	0.16	58,58,58,58	0
56	MG	2a	1824	1/1	0.84	0.22	65,65,65,65	0
56	MG	2A	3273	1/1	0.84	0.25	72,72,72,72	0
56	MG	1a	1603	1/1	0.84	0.15	66,66,66,66	0
56	MG	2A	3111	1/1	0.84	0.22	68,68,68,68	0
56	MG	2A	3541	1/1	0.84	0.13	70,70,70,70	0
56	MG	2F	304	1/1	0.84	0.17	61,61,61,61	0
56	MG	1A	3245	1/1	0.84	0.18	56,56,56,56	0
56	MG	2A	3547	1/1	0.84	0.19	53,53,53,53	0
56	MG	1E	312	1/1	0.84	0.21	61,61,61,61	0
56	MG	2A	3176	1/1	0.84	0.34	74,74,74,74	0
56	MG	2y	102	1/1	0.84	0.18	79,79,79,79	0
56	MG	2A	3524	1/1	0.85	0.18	63,63,63,63	0
56	MG	1A	4070	1/1	0.85	0.15	70,70,70,70	0
56	MG	1A	3518	1/1	0.85	0.15	90,90,90,90	0
56	MG	1A	3313	1/1	0.85	0.21	51,51,51,51	0
56	MG	25	101	1/1	0.85	0.20	63,63,63,63	0
56	MG	1A	3447	1/1	0.85	0.09	64,64,64,64	0
56	MG	1A	3385	1/1	0.85	0.16	64,64,64,64	0
56	MG	1B	215	1/1	0.85	0.13	68,68,68,68	0
56	MG	2a	1609	1/1	0.85	0.21	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	2A	3602	1/1	0.85	0.18	52,52,52,52	0
56	MG	2a	1617	1/1	0.85	0.21	70,70,70,70	0
56	MG	1A	3494	1/1	0.85	0.21	69,69,69,69	0
56	MG	2A	3120	1/1	0.85	0.18	60,60,60,60	0
56	MG	2a	1638	1/1	0.85	0.38	72,72,72,72	0
56	MG	2A	3124	1/1	0.85	0.29	59,59,59,59	0
56	MG	2A	3331	1/1	0.85	0.14	66,66,66,66	0
56	MG	2a	1648	1/1	0.85	0.28	64,64,64,64	0
56	MG	1B	222	1/1	0.85	0.13	68,68,68,68	0
56	MG	1A	3586	1/1	0.85	0.22	60,60,60,60	0
56	MG	2a	1670	1/1	0.85	0.20	60,60,60,60	0
56	MG	1A	3506	1/1	0.85	0.17	75,75,75,75	0
56	MG	2A	3341	1/1	0.85	0.17	81,81,81,81	0
56	MG	1A	4006	1/1	0.85	0.13	47,47,47,47	0
56	MG	2a	1702	1/1	0.85	0.20	62,62,62,62	0
56	MG	2A	3363	1/1	0.85	0.18	61,61,61,61	0
56	MG	2A	3698	1/1	0.85	0.19	65,65,65,65	0
56	MG	2A	3208	1/1	0.85	0.22	59,59,59,59	0
56	MG	1A	3876	1/1	0.85	0.14	28,28,28,28	0
56	MG	2a	1738	1/1	0.85	0.14	71,71,71,71	0
56	MG	1A	3590	1/1	0.85	0.36	60,60,60,60	0
56	MG	2a	1749	1/1	0.85	0.13	69,69,69,69	0
56	MG	2A	3389	1/1	0.85	0.43	70,70,70,70	0
56	MG	2a	1776	1/1	0.85	0.15	61,61,61,61	0
56	MG	1x	115	1/1	0.85	0.29	71,71,71,71	0
56	MG	1A	4045	1/1	0.85	0.12	44,44,44,44	0
56	MG	2a	1785	1/1	0.85	0.25	62,62,62,62	0
56	MG	2A	3728	1/1	0.85	0.23	60,60,60,60	0
56	MG	2A	3422	1/1	0.85	0.29	64,64,64,64	0
56	MG	2A	3753	1/1	0.85	0.23	60,60,60,60	0
56	MG	2a	1807	1/1	0.85	0.32	74,74,74,74	0
56	MG	2A	3756	1/1	0.85	0.12	64,64,64,64	0
56	MG	2A	3222	1/1	0.85	0.39	69,69,69,69	0
56	MG	1A	3899	1/1	0.85	0.11	58,58,58,58	0
56	MG	1A	3428	1/1	0.85	0.24	58,58,58,58	0
56	MG	2A	3231	1/1	0.85	0.25	70,70,70,70	0
56	MG	2A	3805	1/1	0.85	0.13	66,66,66,66	0
56	MG	1a	1720	1/1	0.85	0.29	73,73,73,73	0
56	MG	2A	3030	1/1	0.85	0.24	61,61,61,61	0
56	MG	1a	1722	1/1	0.85	0.27	71,71,71,71	0
56	MG	1a	1737	1/1	0.85	0.14	59,59,59,59	0
56	MG	2A	3058	1/1	0.85	0.12	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	2B	206	1/1	0.85	0.26	65,65,65,65	0
56	MG	2B	210	1/1	0.85	0.17	72,72,72,72	0
56	MG	2B	211	1/1	0.85	0.22	68,68,68,68	0
56	MG	2A	3510	1/1	0.86	0.14	61,61,61,61	0
56	MG	2A	3230	1/1	0.86	0.13	63,63,63,63	0
56	MG	1A	3410	1/1	0.86	0.24	70,70,70,70	0
56	MG	1B	218	1/1	0.86	0.14	59,59,59,59	0
56	MG	2a	1604	1/1	0.86	0.21	56,56,56,56	0
56	MG	2A	3003	1/1	0.86	0.29	64,64,64,64	0
56	MG	1A	3800	1/1	0.86	0.10	33,33,33,33	0
56	MG	2A	3561	1/1	0.86	0.18	60,60,60,60	0
56	MG	1A	3813	1/1	0.86	0.13	37,37,37,37	0
56	MG	2a	1615	1/1	0.86	0.24	73,73,73,73	0
56	MG	2A	3255	1/1	0.86	0.33	56,56,56,56	0
56	MG	1a	1683	1/1	0.86	0.17	66,66,66,66	0
56	MG	2a	1620	1/1	0.86	0.12	65,65,65,65	0
56	MG	2a	1629	1/1	0.86	0.32	76,76,76,76	0
56	MG	2a	1635	1/1	0.86	0.25	69,69,69,69	0
56	MG	1A	3414	1/1	0.86	0.24	47,47,47,47	0
56	MG	2A	3272	1/1	0.86	0.20	73,73,73,73	0
56	MG	2A	3611	1/1	0.86	0.13	53,53,53,53	0
56	MG	1a	1691	1/1	0.86	0.26	62,62,62,62	0
56	MG	2A	3275	1/1	0.86	0.12	70,70,70,70	0
56	MG	2A	3280	1/1	0.86	0.14	63,63,63,63	0
56	MG	2A	3666	1/1	0.86	0.12	72,72,72,72	0
56	MG	2A	3286	1/1	0.86	0.27	65,65,65,65	0
56	MG	1A	3420	1/1	0.86	0.32	61,61,61,61	0
56	MG	1A	3091	1/1	0.86	0.23	54,54,54,54	0
56	MG	2a	1690	1/1	0.86	0.11	79,79,79,79	0
56	MG	2a	1695	1/1	0.86	0.24	57,57,57,57	0
56	MG	1D	313	1/1	0.86	0.18	44,44,44,44	0
56	MG	1A	3195	1/1	0.86	0.23	50,50,50,50	0
56	MG	1A	3360	1/1	0.86	0.33	65,65,65,65	0
56	MG	2A	3084	1/1	0.86	0.15	58,58,58,58	0
56	MG	2A	3097	1/1	0.86	0.17	61,61,61,61	0
56	MG	1a	1729	1/1	0.86	0.20	65,65,65,65	0
56	MG	1G	205	1/1	0.86	0.16	62,62,62,62	0
56	MG	2a	1740	1/1	0.86	0.25	62,62,62,62	0
56	MG	1A	4022	1/1	0.86	0.12	45,45,45,45	0
56	MG	1S	203	1/1	0.86	0.12	73,73,73,73	0
56	MG	1a	1745	1/1	0.86	0.16	62,62,62,62	0
56	MG	1a	1749	1/1	0.86	0.22	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	4023	1/1	0.86	0.10	40,40,40,40	0
56	MG	2A	3149	1/1	0.86	0.14	67,67,67,67	0
56	MG	2a	1784	1/1	0.86	0.23	71,71,71,71	0
56	MG	1A	4043	1/1	0.86	0.17	39,39,39,39	0
56	MG	2A	3768	1/1	0.86	0.26	80,80,80,80	0
56	MG	2A	3181	1/1	0.86	0.17	67,67,67,67	0
56	MG	2a	1802	1/1	0.86	0.10	62,62,62,62	0
56	MG	1a	1781	1/1	0.86	0.14	59,59,59,59	0
56	MG	1A	3544	1/1	0.86	0.13	64,64,64,64	0
56	MG	2a	1813	1/1	0.86	0.15	71,71,71,71	0
56	MG	1A	3371	1/1	0.86	0.22	50,50,50,50	0
56	MG	1A	3476	1/1	0.86	0.13	61,61,61,61	0
56	MG	2A	3436	1/1	0.86	0.30	58,58,58,58	0
56	MG	2A	3210	1/1	0.86	0.15	53,53,53,53	0
56	MG	1A	3905	1/1	0.86	0.12	23,23,23,23	0
56	MG	1A	3208	1/1	0.86	0.15	63,63,63,63	0
56	MG	1A	3500	1/1	0.86	0.17	63,63,63,63	0
56	MG	2A	3218	1/1	0.86	0.20	64,64,64,64	0
56	MG	1A	3951	1/1	0.86	0.12	56,56,56,56	0
56	MG	1a	1656	1/1	0.86	0.23	57,57,57,57	0
56	MG	2w	103	1/1	0.86	0.16	83,83,83,83	0
56	MG	2B	215	1/1	0.86	0.23	61,61,61,61	0
56	MG	2D	307	1/1	0.86	0.30	49,49,49,49	0
56	MG	2x	102	1/1	0.86	0.24	67,67,67,67	0
56	MG	2A	3485	1/1	0.86	0.23	48,48,48,48	0
56	MG	2x	107	1/1	0.86	0.14	55,55,55,55	0
56	MG	2y	101	1/1	0.86	0.15	74,74,74,74	0
56	MG	1A	3779	1/1	0.86	0.10	46,46,46,46	0
56	MG	2A	3503	1/1	0.87	0.22	59,59,59,59	0
56	MG	2A	3012	1/1	0.87	0.23	55,55,55,55	0
56	MG	1A	3187	1/1	0.87	0.12	47,47,47,47	0
56	MG	2A	3253	1/1	0.87	0.24	77,77,77,77	0
56	MG	1F	310	1/1	0.87	0.13	52,52,52,52	0
56	MG	2A	3261	1/1	0.87	0.32	63,63,63,63	0
56	MG	1A	3326	1/1	0.87	0.15	57,57,57,57	0
56	MG	2A	3548	1/1	0.87	0.14	61,61,61,61	0
56	MG	1A	3957	1/1	0.87	0.18	63,63,63,63	0
56	MG	2A	3268	1/1	0.87	0.33	78,78,78,78	0
56	MG	1A	3965	1/1	0.87	0.11	64,64,64,64	0
56	MG	1A	3592	1/1	0.87	0.31	70,70,70,70	0
56	MG	2A	3076	1/1	0.87	0.30	58,58,58,58	0
56	MG	1A	3250	1/1	0.87	0.13	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	1738	1/1	0.87	0.16	60,60,60,60	0
56	MG	2A	3630	1/1	0.87	0.18	55,55,55,55	0
56	MG	2A	3640	1/1	0.87	0.17	62,62,62,62	0
56	MG	1A	4075	1/1	0.87	0.15	61,61,61,61	0
56	MG	2A	3089	1/1	0.87	0.21	60,60,60,60	0
56	MG	1A	3613	1/1	0.87	0.11	33,33,33,33	0
56	MG	1a	1744	1/1	0.87	0.11	60,60,60,60	0
56	MG	1A	4092	1/1	0.87	0.31	45,45,45,45	0
56	MG	2A	3680	1/1	0.87	0.15	56,56,56,56	0
56	MG	18	104	1/1	0.87	0.19	53,53,53,53	0
56	MG	1A	3625	1/1	0.87	0.08	25,25,25,25	0
56	MG	2A	3320	1/1	0.87	0.17	66,66,66,66	0
56	MG	2A	3325	1/1	0.87	0.18	76,76,76,76	0
56	MG	1a	1770	1/1	0.87	0.09	71,71,71,71	0
56	MG	2A	3122	1/1	0.87	0.24	65,65,65,65	0
56	MG	2a	1707	1/1	0.87	0.19	72,72,72,72	0
56	MG	1A	3991	1/1	0.87	0.12	72,72,72,72	0
56	MG	2a	1717	1/1	0.87	0.14	76,76,76,76	0
56	MG	1a	1605	1/1	0.87	0.11	67,67,67,67	0
56	MG	1a	1788	1/1	0.87	0.13	86,86,86,86	0
56	MG	1A	3887	1/1	0.87	0.21	42,42,42,42	0
56	MG	2A	3361	1/1	0.87	0.11	66,66,66,66	0
56	MG	1A	3556	1/1	0.87	0.29	52,52,52,52	0
56	MG	1a	1798	1/1	0.87	0.18	53,53,53,53	0
56	MG	2a	1763	1/1	0.87	0.13	59,59,59,59	0
56	MG	2A	3739	1/1	0.87	0.13	61,61,61,61	0
56	MG	1a	1800	1/1	0.87	0.10	58,58,58,58	0
56	MG	2A	3206	1/1	0.87	0.25	63,63,63,63	0
56	MG	2A	3372	1/1	0.87	0.17	60,60,60,60	0
56	MG	2a	1781	1/1	0.87	0.25	71,71,71,71	0
56	MG	1A	3492	1/1	0.87	0.12	48,48,48,48	0
56	MG	1a	1808	1/1	0.87	0.10	55,55,55,55	0
56	MG	2a	1792	1/1	0.87	0.25	68,68,68,68	0
56	MG	1A	4009	1/1	0.87	0.10	75,75,75,75	0
56	MG	1A	3678	1/1	0.87	0.13	67,67,67,67	0
56	MG	1B	232	1/1	0.87	0.13	59,59,59,59	0
56	MG	2A	3801	1/1	0.87	0.16	69,69,69,69	0
56	MG	2A	3804	1/1	0.87	0.09	53,53,53,53	0
56	MG	1B	233	1/1	0.87	0.15	69,69,69,69	0
56	MG	2A	3806	1/1	0.87	0.10	66,66,66,66	0
56	MG	2A	3811	1/1	0.87	0.13	52,52,52,52	0
56	MG	2A	3444	1/1	0.87	0.24	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	3448	1/1	0.87	0.27	69,69,69,69	0
56	MG	2A	3458	1/1	0.87	0.12	62,62,62,62	0
56	MG	1w	108	1/1	0.87	0.10	71,71,71,71	0
56	MG	2A	3836	1/1	0.87	0.12	66,66,66,66	0
56	MG	1a	1672	1/1	0.87	0.19	62,62,62,62	0
56	MG	1A	3921	1/1	0.87	0.13	54,54,54,54	0
56	MG	1a	1681	1/1	0.87	0.14	62,62,62,62	0
56	MG	1A	3689	1/1	0.87	0.09	33,33,33,33	0
56	MG	2A	3481	1/1	0.87	0.12	77,77,77,77	0
56	MG	1D	314	1/1	0.87	0.22	44,44,44,44	0
56	MG	1A	3300	1/1	0.87	0.20	56,56,56,56	0
56	MG	2E	309	1/1	0.87	0.11	59,59,59,59	0
56	MG	1a	1698	1/1	0.87	0.23	66,66,66,66	0
56	MG	2V	201	1/1	0.87	0.24	60,60,60,60	0
56	MG	2A	3495	1/1	0.87	0.12	62,62,62,62	0
56	MG	2y	107	1/1	0.87	0.18	72,72,72,72	0
56	MG	28	103	1/1	0.88	0.26	54,54,54,54	0
56	MG	2A	3567	1/1	0.88	0.17	68,68,68,68	0
56	MG	2A	3308	1/1	0.88	0.29	61,61,61,61	0
56	MG	2A	3312	1/1	0.88	0.10	57,57,57,57	0
56	MG	2A	3163	1/1	0.88	0.16	67,67,67,67	0
56	MG	2A	3316	1/1	0.88	0.14	61,61,61,61	0
56	MG	2A	3164	1/1	0.88	0.18	65,65,65,65	0
56	MG	1a	1709	1/1	0.88	0.46	70,70,70,70	0
56	MG	2A	3615	1/1	0.88	0.21	42,42,42,42	0
56	MG	2A	3324	1/1	0.88	0.16	57,57,57,57	0
56	MG	2A	3638	1/1	0.88	0.24	66,66,66,66	0
56	MG	2a	1627	1/1	0.88	0.27	71,71,71,71	0
56	MG	1A	4080	1/1	0.88	0.28	43,43,43,43	0
56	MG	2A	3327	1/1	0.88	0.12	52,52,52,52	0
56	MG	1x	111	1/1	0.88	0.09	55,55,55,55	0
56	MG	1A	3732	1/1	0.88	0.11	24,24,24,24	0
56	MG	2A	3661	1/1	0.88	0.16	44,44,44,44	0
56	MG	2a	1643	1/1	0.88	0.16	70,70,70,70	0
56	MG	2A	3665	1/1	0.88	0.28	71,71,71,71	0
56	MG	2A	3189	1/1	0.88	0.20	52,52,52,52	0
56	MG	1A	3455	1/1	0.88	0.16	53,53,53,53	0
56	MG	1A	3182	1/1	0.88	0.15	55,55,55,55	0
56	MG	2A	3352	1/1	0.88	0.24	75,75,75,75	0
56	MG	1A	4004	1/1	0.88	0.12	73,73,73,73	0
56	MG	2A	3355	1/1	0.88	0.23	64,64,64,64	0
56	MG	2a	1686	1/1	0.88	0.29	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3676	1/1	0.88	0.12	52,52,52,52	0
56	MG	2a	1692	1/1	0.88	0.27	68,68,68,68	0
56	MG	1A	3289	1/1	0.88	0.19	66,66,66,66	0
56	MG	18	106	1/1	0.88	0.10	74,74,74,74	0
56	MG	1A	3545	1/1	0.88	0.26	61,61,61,61	0
56	MG	2A	3022	1/1	0.88	0.31	62,62,62,62	0
56	MG	2A	3025	1/1	0.88	0.17	57,57,57,57	0
56	MG	2A	3713	1/1	0.88	0.17	69,69,69,69	0
56	MG	2A	3374	1/1	0.88	0.26	65,65,65,65	0
56	MG	2A	3388	1/1	0.88	0.20	55,55,55,55	0
56	MG	1B	225	1/1	0.88	0.11	58,58,58,58	0
56	MG	2a	1733	1/1	0.88	0.35	68,68,68,68	0
56	MG	2A	3042	1/1	0.88	0.33	60,60,60,60	0
56	MG	2A	3738	1/1	0.88	0.15	61,61,61,61	0
56	MG	2A	3400	1/1	0.88	0.13	68,68,68,68	0
56	MG	2A	3403	1/1	0.88	0.11	68,68,68,68	0
56	MG	1A	3788	1/1	0.88	0.09	17,17,17,17	0
56	MG	2a	1769	1/1	0.88	0.14	57,57,57,57	0
56	MG	1A	3054	1/1	0.88	0.15	55,55,55,55	0
56	MG	2A	3764	1/1	0.88	0.18	69,69,69,69	0
56	MG	2A	3767	1/1	0.88	0.17	69,69,69,69	0
56	MG	2A	3425	1/1	0.88	0.15	58,58,58,58	0
56	MG	2A	3433	1/1	0.88	0.26	61,61,61,61	0
56	MG	2A	3050	1/1	0.88	0.25	57,57,57,57	0
56	MG	2A	3053	1/1	0.88	0.18	61,61,61,61	0
56	MG	2a	1786	1/1	0.88	0.15	71,71,71,71	0
56	MG	2a	1789	1/1	0.88	0.20	78,78,78,78	0
56	MG	1A	3579	1/1	0.88	0.14	42,42,42,42	0
56	MG	1a	1641	1/1	0.88	0.24	63,63,63,63	0
56	MG	2A	3450	1/1	0.88	0.18	58,58,58,58	0
56	MG	1A	3948	1/1	0.88	0.07	41,41,41,41	0
56	MG	2A	3254	1/1	0.88	0.18	71,71,71,71	0
56	MG	2A	3807	1/1	0.88	0.14	45,45,45,45	0
56	MG	1A	3618	1/1	0.88	0.15	66,66,66,66	0
56	MG	1A	3163	1/1	0.88	0.20	56,56,56,56	0
56	MG	1a	1661	1/1	0.88	0.17	63,63,63,63	0
56	MG	2a	1816	1/1	0.88	0.17	69,69,69,69	0
56	MG	2A	3822	1/1	0.88	0.12	52,52,52,52	0
56	MG	1A	3827	1/1	0.88	0.10	51,51,51,51	0
56	MG	1A	3631	1/1	0.88	0.14	54,54,54,54	0
56	MG	2f	202	1/1	0.88	0.20	71,71,71,71	0
56	MG	2A	3098	1/1	0.88	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1670	1/1	0.88	0.11	59,59,59,59	0
56	MG	2A	3489	1/1	0.88	0.15	56,56,56,56	0
56	MG	1A	3835	1/1	0.88	0.12	54,54,54,54	0
56	MG	1A	3725	1/1	0.88	0.13	60,60,60,60	0
56	MG	2A	3282	1/1	0.88	0.21	63,63,63,63	0
56	MG	1A	3848	1/1	0.88	0.13	51,51,51,51	0
56	MG	1I	201	1/1	0.88	0.10	67,67,67,67	0
56	MG	1w	101	1/1	0.88	0.18	55,55,55,55	0
56	MG	2x	104	1/1	0.88	0.31	66,66,66,66	0
56	MG	1O	201	1/1	0.88	0.09	56,56,56,56	0
56	MG	2A	3296	1/1	0.88	0.10	58,58,58,58	0
56	MG	2A	3297	1/1	0.88	0.16	62,62,62,62	0
56	MG	1Q	206	1/1	0.88	0.13	47,47,47,47	0
56	MG	2y	105	1/1	0.88	0.23	85,85,85,85	0
56	MG	1A	4076	1/1	0.88	0.24	76,76,76,76	0
56	MG	1a	1768	1/1	0.89	0.19	66,66,66,66	0
56	MG	1A	3770	1/1	0.89	0.10	35,35,35,35	0
56	MG	1A	3259	1/1	0.89	0.17	51,51,51,51	0
56	MG	1a	1772	1/1	0.89	0.21	71,71,71,71	0
56	MG	2A	3187	1/1	0.89	0.08	55,55,55,55	0
56	MG	2A	3407	1/1	0.89	0.22	56,56,56,56	0
56	MG	2A	3819	1/1	0.89	0.11	78,78,78,78	0
56	MG	2A	3410	1/1	0.89	0.21	54,54,54,54	0
56	MG	2A	3411	1/1	0.89	0.24	56,56,56,56	0
56	MG	1a	1780	1/1	0.89	0.14	51,51,51,51	0
56	MG	2A	3200	1/1	0.89	0.15	70,70,70,70	0
56	MG	2A	3204	1/1	0.89	0.17	59,59,59,59	0
56	MG	2A	3842	1/1	0.89	0.20	63,63,63,63	0
56	MG	2A	3426	1/1	0.89	0.12	62,62,62,62	0
56	MG	2B	202	1/1	0.89	0.13	69,69,69,69	0
56	MG	2A	3430	1/1	0.89	0.34	61,61,61,61	0
56	MG	15	102	1/1	0.89	0.18	33,33,33,33	0
56	MG	1A	3682	1/1	0.89	0.11	24,24,24,24	0
56	MG	1A	3942	1/1	0.89	0.10	46,46,46,46	0
56	MG	2B	219	1/1	0.89	0.21	71,71,71,71	0
56	MG	19	101	1/1	0.89	0.14	45,45,45,45	0
56	MG	1A	3943	1/1	0.89	0.14	70,70,70,70	0
56	MG	1A	3683	1/1	0.89	0.08	19,19,19,19	0
56	MG	2A	3457	1/1	0.89	0.14	53,53,53,53	0
56	MG	1A	4090	1/1	0.89	0.11	59,59,59,59	0
56	MG	2A	3467	1/1	0.89	0.30	68,68,68,68	0
56	MG	2A	3469	1/1	0.89	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1612	1/1	0.89	0.09	63,63,63,63	0
56	MG	1l	201	1/1	0.89	0.15	59,59,59,59	0
56	MG	1a	1622	1/1	0.89	0.25	65,65,65,65	0
56	MG	1n	102	1/1	0.89	0.17	60,60,60,60	0
56	MG	1t	201	1/1	0.89	0.26	58,58,58,58	0
56	MG	1A	3262	1/1	0.89	0.18	60,60,60,60	0
56	MG	1a	1637	1/1	0.89	0.20	65,65,65,65	0
56	MG	1A	4096	1/1	0.89	0.26	59,59,59,59	0
56	MG	2a	1613	1/1	0.89	0.27	72,72,72,72	0
56	MG	2A	3238	1/1	0.89	0.16	53,53,53,53	0
56	MG	1B	202	1/1	0.89	0.16	45,45,45,45	0
56	MG	2A	3242	1/1	0.89	0.21	64,64,64,64	0
56	MG	2A	3502	1/1	0.89	0.13	29,29,29,29	0
56	MG	2a	1622	1/1	0.89	0.16	73,73,73,73	0
56	MG	1a	1642	1/1	0.89	0.15	65,65,65,65	0
56	MG	2A	3250	1/1	0.89	0.11	65,65,65,65	0
56	MG	2a	1633	1/1	0.89	0.26	67,67,67,67	0
56	MG	2a	1634	1/1	0.89	0.32	67,67,67,67	0
56	MG	2A	3517	1/1	0.89	0.08	40,40,40,40	0
56	MG	2A	3252	1/1	0.89	0.34	64,64,64,64	0
56	MG	1a	1649	1/1	0.89	0.21	61,61,61,61	0
56	MG	2A	3529	1/1	0.89	0.14	42,42,42,42	0
56	MG	2A	3534	1/1	0.89	0.14	54,54,54,54	0
56	MG	1A	3807	1/1	0.89	0.18	64,64,64,64	0
56	MG	1A	3811	1/1	0.89	0.10	26,26,26,26	0
56	MG	1A	3959	1/1	0.89	0.16	66,66,66,66	0
56	MG	2A	3264	1/1	0.89	0.28	71,71,71,71	0
56	MG	2a	1655	1/1	0.89	0.25	67,67,67,67	0
56	MG	2a	1657	1/1	0.89	0.17	64,64,64,64	0
56	MG	2a	1659	1/1	0.89	0.17	69,69,69,69	0
56	MG	1A	3539	1/1	0.89	0.18	63,63,63,63	0
56	MG	1A	3817	1/1	0.89	0.13	55,55,55,55	0
56	MG	2A	3582	1/1	0.89	0.16	65,65,65,65	0
56	MG	2a	1681	1/1	0.89	0.21	50,50,50,50	0
56	MG	1a	1665	1/1	0.89	0.17	64,64,64,64	0
56	MG	2A	3586	1/1	0.89	0.19	66,66,66,66	0
56	MG	1a	1667	1/1	0.89	0.27	58,58,58,58	0
56	MG	2a	1693	1/1	0.89	0.20	59,59,59,59	0
56	MG	1B	223	1/1	0.89	0.18	63,63,63,63	0
56	MG	1A	3702	1/1	0.89	0.19	55,55,55,55	0
56	MG	2A	3605	1/1	0.89	0.12	42,42,42,42	0
56	MG	2A	3019	1/1	0.89	0.37	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3608	1/1	0.89	0.13	74,74,74,74	0
56	MG	2a	1710	1/1	0.89	0.20	76,76,76,76	0
56	MG	1a	1671	1/1	0.89	0.11	56,56,56,56	0
56	MG	2A	3283	1/1	0.89	0.18	57,57,57,57	0
56	MG	1A	3542	1/1	0.89	0.14	63,63,63,63	0
56	MG	2a	1721	1/1	0.89	0.23	55,55,55,55	0
56	MG	1A	3825	1/1	0.89	0.14	47,47,47,47	0
56	MG	1B	231	1/1	0.89	0.13	63,63,63,63	0
56	MG	1A	3498	1/1	0.89	0.14	49,49,49,49	0
56	MG	1A	3707	1/1	0.89	0.14	55,55,55,55	0
56	MG	1A	4001	1/1	0.89	0.11	45,45,45,45	0
56	MG	1a	1693	1/1	0.89	0.25	52,52,52,52	0
56	MG	2a	1754	1/1	0.89	0.17	70,70,70,70	0
56	MG	2a	1761	1/1	0.89	0.13	54,54,54,54	0
56	MG	2A	3663	1/1	0.89	0.15	68,68,68,68	0
56	MG	1a	1697	1/1	0.89	0.27	64,64,64,64	0
56	MG	1A	3171	1/1	0.89	0.10	44,44,44,44	0
56	MG	1a	1700	1/1	0.89	0.16	57,57,57,57	0
56	MG	1A	3716	1/1	0.89	0.12	53,53,53,53	0
56	MG	2A	3681	1/1	0.89	0.16	57,57,57,57	0
56	MG	1A	3041	1/1	0.89	0.23	56,56,56,56	0
56	MG	2A	3318	1/1	0.89	0.29	66,66,66,66	0
56	MG	1A	3573	1/1	0.89	0.18	67,67,67,67	0
56	MG	1A	3634	1/1	0.89	0.13	62,62,62,62	0
56	MG	2A	3695	1/1	0.89	0.17	40,40,40,40	0
56	MG	2A	3322	1/1	0.89	0.11	49,49,49,49	0
56	MG	2A	3323	1/1	0.89	0.23	60,60,60,60	0
56	MG	2A	3092	1/1	0.89	0.12	64,64,64,64	0
56	MG	2a	1798	1/1	0.89	0.16	68,68,68,68	0
56	MG	2a	1801	1/1	0.89	0.11	68,68,68,68	0
56	MG	2A	3700	1/1	0.89	0.24	60,60,60,60	0
56	MG	2A	3095	1/1	0.89	0.20	60,60,60,60	0
56	MG	1G	202	1/1	0.89	0.18	59,59,59,59	0
56	MG	1G	203	1/1	0.89	0.09	69,69,69,69	0
56	MG	1A	3062	1/1	0.89	0.17	67,67,67,67	0
56	MG	2A	3101	1/1	0.89	0.27	70,70,70,70	0
56	MG	1A	3053	1/1	0.89	0.15	48,48,48,48	0
56	MG	2a	1817	1/1	0.89	0.18	50,50,50,50	0
56	MG	1A	4039	1/1	0.89	0.15	61,61,61,61	0
56	MG	2A	3729	1/1	0.89	0.20	54,54,54,54	0
56	MG	2A	3343	1/1	0.89	0.15	67,67,67,67	0
56	MG	2A	3344	1/1	0.89	0.09	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	3758	1/1	0.89	0.11	45,45,45,45	0
56	MG	2A	3749	1/1	0.89	0.14	54,54,54,54	0
56	MG	1A	3331	1/1	0.89	0.16	54,54,54,54	0
56	MG	1A	3906	1/1	0.89	0.12	33,33,33,33	0
56	MG	2A	3758	1/1	0.89	0.12	55,55,55,55	0
56	MG	1A	4068	1/1	0.89	0.09	49,49,49,49	0
56	MG	1A	3913	1/1	0.89	0.10	64,64,64,64	0
56	MG	2A	3147	1/1	0.89	0.25	49,49,49,49	0
56	MG	2A	3769	1/1	0.89	0.12	70,70,70,70	0
56	MG	1a	1759	1/1	0.89	0.22	66,66,66,66	0
56	MG	2A	3779	1/1	0.89	0.13	51,51,51,51	0
56	MG	2A	3370	1/1	0.89	0.16	67,67,67,67	0
56	MG	1a	1761	1/1	0.89	0.12	50,50,50,50	0
56	MG	2A	3787	1/1	0.89	0.09	61,61,61,61	0
56	MG	1A	3915	1/1	0.89	0.13	42,42,42,42	0
56	MG	2A	3172	1/1	0.89	0.22	51,51,51,51	0
56	MG	1A	3938	1/1	0.90	0.12	63,63,63,63	0
56	MG	1A	3341	1/1	0.90	0.10	58,58,58,58	0
56	MG	2A	3838	1/1	0.90	0.20	55,55,55,55	0
56	MG	1A	3429	1/1	0.90	0.11	55,55,55,55	0
56	MG	1A	3635	1/1	0.90	0.13	54,54,54,54	0
56	MG	1A	3799	1/1	0.90	0.15	58,58,58,58	0
56	MG	1x	107	1/1	0.90	0.14	55,55,55,55	0
56	MG	1A	3644	1/1	0.90	0.16	46,46,46,46	0
56	MG	2A	3248	1/1	0.90	0.13	57,57,57,57	0
56	MG	2B	213	1/1	0.90	0.16	66,66,66,66	0
56	MG	1A	3536	1/1	0.90	0.10	61,61,61,61	0
56	MG	1A	3656	1/1	0.90	0.09	40,40,40,40	0
56	MG	1A	3431	1/1	0.90	0.09	44,44,44,44	0
56	MG	1A	3342	1/1	0.90	0.14	33,33,33,33	0
56	MG	2E	307	1/1	0.90	0.17	53,53,53,53	0
56	MG	1B	224	1/1	0.90	0.14	62,62,62,62	0
56	MG	1A	3437	1/1	0.90	0.14	51,51,51,51	0
56	MG	2Q	203	1/1	0.90	0.09	64,64,64,64	0
56	MG	2R	201	1/1	0.90	0.14	62,62,62,62	0
56	MG	2A	3009	1/1	0.90	0.20	46,46,46,46	0
56	MG	1A	3976	1/1	0.90	0.10	26,26,26,26	0
56	MG	1A	3442	1/1	0.90	0.18	36,36,36,36	0
56	MG	2A	3015	1/1	0.90	0.37	69,69,69,69	0
56	MG	25	102	1/1	0.90	0.15	50,50,50,50	0
56	MG	25	104	1/1	0.90	0.23	53,53,53,53	0
56	MG	1A	3354	1/1	0.90	0.16	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1602	1/1	0.90	0.18	73,73,73,73	0
56	MG	1A	3987	1/1	0.90	0.26	40,40,40,40	0
56	MG	1a	1678	1/1	0.90	0.16	60,60,60,60	0
56	MG	2A	3528	1/1	0.90	0.16	59,59,59,59	0
56	MG	1A	3299	1/1	0.90	0.18	55,55,55,55	0
56	MG	2A	3032	1/1	0.90	0.12	62,62,62,62	0
56	MG	2A	3037	1/1	0.90	0.26	62,62,62,62	0
56	MG	1A	3699	1/1	0.90	0.14	44,44,44,44	0
56	MG	1a	1684	1/1	0.90	0.39	63,63,63,63	0
56	MG	1A	3831	1/1	0.90	0.27	62,62,62,62	0
56	MG	1A	3246	1/1	0.90	0.22	67,67,67,67	0
56	MG	2A	3566	1/1	0.90	0.16	61,61,61,61	0
56	MG	2A	3294	1/1	0.90	0.24	59,59,59,59	0
56	MG	1A	4005	1/1	0.90	0.11	73,73,73,73	0
56	MG	2A	3584	1/1	0.90	0.15	50,50,50,50	0
56	MG	2a	1630	1/1	0.90	0.25	54,54,54,54	0
56	MG	1A	3583	1/1	0.90	0.27	62,62,62,62	0
56	MG	1A	4007	1/1	0.90	0.10	53,53,53,53	0
56	MG	2A	3070	1/1	0.90	0.22	68,68,68,68	0
56	MG	1A	3584	1/1	0.90	0.17	52,52,52,52	0
56	MG	2A	3309	1/1	0.90	0.10	59,59,59,59	0
56	MG	1a	1706	1/1	0.90	0.10	60,60,60,60	0
56	MG	2A	3313	1/1	0.90	0.14	61,61,61,61	0
56	MG	2A	3314	1/1	0.90	0.13	63,63,63,63	0
56	MG	2a	1647	1/1	0.90	0.27	64,64,64,64	0
56	MG	1A	3850	1/1	0.90	0.19	66,66,66,66	0
56	MG	1A	3858	1/1	0.90	0.09	35,35,35,35	0
56	MG	1A	3866	1/1	0.90	0.13	44,44,44,44	0
56	MG	2A	3632	1/1	0.90	0.11	73,73,73,73	0
56	MG	2A	3635	1/1	0.90	0.23	70,70,70,70	0
56	MG	2a	1658	1/1	0.90	0.22	44,44,44,44	0
56	MG	1N	205	1/1	0.90	0.24	62,62,62,62	0
56	MG	2a	1663	1/1	0.90	0.21	54,54,54,54	0
56	MG	2a	1669	1/1	0.90	0.18	61,61,61,61	0
56	MG	1a	1715	1/1	0.90	0.20	62,62,62,62	0
56	MG	2A	3645	1/1	0.90	0.16	57,57,57,57	0
56	MG	2A	3647	1/1	0.90	0.18	64,64,64,64	0
56	MG	1A	3872	1/1	0.90	0.10	35,35,35,35	0
56	MG	1O	205	1/1	0.90	0.20	66,66,66,66	0
56	MG	1A	4035	1/1	0.90	0.10	65,65,65,65	0
56	MG	2a	1691	1/1	0.90	0.49	65,65,65,65	0
56	MG	1S	201	1/1	0.90	0.34	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3362	1/1	0.90	0.15	53,53,53,53	0
56	MG	2A	3328	1/1	0.90	0.09	53,53,53,53	0
56	MG	1A	3364	1/1	0.90	0.09	45,45,45,45	0
56	MG	1W	203	1/1	0.90	0.09	48,48,48,48	0
56	MG	2A	3673	1/1	0.90	0.18	58,58,58,58	0
56	MG	2a	1705	1/1	0.90	0.14	72,72,72,72	0
56	MG	2A	3115	1/1	0.90	0.14	73,73,73,73	0
56	MG	2a	1708	1/1	0.90	0.17	60,60,60,60	0
56	MG	1A	3179	1/1	0.90	0.11	44,44,44,44	0
56	MG	2A	3682	1/1	0.90	0.16	66,66,66,66	0
56	MG	2a	1715	1/1	0.90	0.27	59,59,59,59	0
56	MG	1X	106	1/1	0.90	0.07	32,32,32,32	0
56	MG	2A	3342	1/1	0.90	0.09	54,54,54,54	0
56	MG	1A	4046	1/1	0.90	0.12	55,55,55,55	0
56	MG	2a	1726	1/1	0.90	0.22	77,77,77,77	0
56	MG	2a	1727	1/1	0.90	0.20	55,55,55,55	0
56	MG	2A	3137	1/1	0.90	0.22	65,65,65,65	0
56	MG	2A	3351	1/1	0.90	0.20	73,73,73,73	0
56	MG	2a	1734	1/1	0.90	0.35	65,65,65,65	0
56	MG	1a	1755	1/1	0.90	0.12	64,64,64,64	0
56	MG	1Z	301	1/1	0.90	0.16	59,59,59,59	0
56	MG	2a	1743	1/1	0.90	0.09	66,66,66,66	0
56	MG	1A	3588	1/1	0.90	0.15	50,50,50,50	0
56	MG	2A	3357	1/1	0.90	0.23	64,64,64,64	0
56	MG	2a	1751	1/1	0.90	0.10	41,41,41,41	0
56	MG	1A	4060	1/1	0.90	0.14	43,43,43,43	0
56	MG	2A	3709	1/1	0.90	0.09	56,56,56,56	0
56	MG	2a	1762	1/1	0.90	0.11	70,70,70,70	0
56	MG	2A	3711	1/1	0.90	0.19	58,58,58,58	0
56	MG	2a	1764	1/1	0.90	0.14	64,64,64,64	0
56	MG	1A	4064	1/1	0.90	0.17	60,60,60,60	0
56	MG	2A	3364	1/1	0.90	0.28	71,71,71,71	0
56	MG	2A	3717	1/1	0.90	0.12	59,59,59,59	0
56	MG	2A	3170	1/1	0.90	0.13	58,58,58,58	0
56	MG	1A	3379	1/1	0.90	0.18	76,76,76,76	0
56	MG	15	105	1/1	0.90	0.23	55,55,55,55	0
56	MG	15	110	1/1	0.90	0.08	55,55,55,55	0
56	MG	1a	1775	1/1	0.90	0.24	50,50,50,50	0
56	MG	1A	3325	1/1	0.90	0.16	51,51,51,51	0
56	MG	2a	1788	1/1	0.90	0.20	63,63,63,63	0
56	MG	1A	3594	1/1	0.90	0.22	51,51,51,51	0
56	MG	2a	1791	1/1	0.90	0.12	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	1a	1782	1/1	0.90	0.12	57,57,57,57	0
56	MG	2A	3746	1/1	0.90	0.20	59,59,59,59	0
56	MG	1A	3069	1/1	0.90	0.10	49,49,49,49	0
56	MG	2A	3393	1/1	0.90	0.15	73,73,73,73	0
56	MG	2A	3397	1/1	0.90	0.13	63,63,63,63	0
56	MG	2A	3202	1/1	0.90	0.22	68,68,68,68	0
56	MG	1A	3600	1/1	0.90	0.09	29,29,29,29	0
56	MG	2A	3404	1/1	0.90	0.14	60,60,60,60	0
56	MG	1a	1793	1/1	0.90	0.12	77,77,77,77	0
56	MG	1A	3917	1/1	0.90	0.15	52,52,52,52	0
56	MG	2A	3770	1/1	0.90	0.10	64,64,64,64	0
56	MG	2A	3777	1/1	0.90	0.12	68,68,68,68	0
56	MG	1A	3242	1/1	0.90	0.10	48,48,48,48	0
56	MG	1A	4078	1/1	0.90	0.17	51,51,51,51	0
56	MG	2a	1822	1/1	0.90	0.29	68,68,68,68	0
56	MG	2A	3416	1/1	0.90	0.36	54,54,54,54	0
56	MG	2A	3211	1/1	0.90	0.24	67,67,67,67	0
56	MG	2A	3212	1/1	0.90	0.20	64,64,64,64	0
56	MG	2g	201	1/1	0.90	0.23	72,72,72,72	0
56	MG	2A	3788	1/1	0.90	0.10	69,69,69,69	0
56	MG	1A	3417	1/1	0.90	0.20	56,56,56,56	0
56	MG	2q	203	1/1	0.90	0.20	66,66,66,66	0
56	MG	1A	4084	1/1	0.90	0.16	46,46,46,46	0
56	MG	1f	202	1/1	0.90	0.17	63,63,63,63	0
56	MG	1a	1627	1/1	0.90	0.20	46,46,46,46	0
56	MG	2w	102	1/1	0.90	0.16	82,82,82,82	0
56	MG	2A	3437	1/1	0.90	0.20	69,69,69,69	0
56	MG	2A	3440	1/1	0.90	0.27	56,56,56,56	0
56	MG	2w	105	1/1	0.90	0.11	76,76,76,76	0
56	MG	2A	3808	1/1	0.90	0.08	48,48,48,48	0
56	MG	1a	1632	1/1	0.90	0.18	60,60,60,60	0
56	MG	1a	1635	1/1	0.90	0.24	75,75,75,75	0
56	MG	2A	3446	1/1	0.90	0.27	61,61,61,61	0
56	MG	1A	3207	1/1	0.90	0.09	56,56,56,56	0
56	MG	1a	1638	1/1	0.90	0.34	66,66,66,66	0
56	MG	2A	3824	1/1	0.90	0.08	50,50,50,50	0
56	MG	2A	3454	1/1	0.90	0.20	42,42,42,42	0
56	MG	2y	106	1/1	0.90	0.26	64,64,64,64	0
56	MG	2A	3834	1/1	0.90	0.09	55,55,55,55	0
59	ZN	14	102	1/1	0.90	0.17	134,134,134,134	0
56	MG	1A	4036	1/1	0.91	0.10	75,75,75,75	0
56	MG	1A	4037	1/1	0.91	0.09	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3841	1/1	0.91	0.19	61,61,61,61	0
56	MG	2A	3219	1/1	0.91	0.13	58,58,58,58	0
56	MG	2A	3220	1/1	0.91	0.25	64,64,64,64	0
56	MG	10	102	1/1	0.91	0.11	58,58,58,58	0
56	MG	2B	204	1/1	0.91	0.16	66,66,66,66	0
56	MG	10	107	1/1	0.91	0.16	59,59,59,59	0
56	MG	1a	1796	1/1	0.91	0.10	66,66,66,66	0
56	MG	2A	3228	1/1	0.91	0.23	60,60,60,60	0
56	MG	1A	3015	1/1	0.91	0.11	38,38,38,38	0
56	MG	2B	214	1/1	0.91	0.08	74,74,74,74	0
56	MG	2A	3472	1/1	0.91	0.12	46,46,46,46	0
56	MG	2B	217	1/1	0.91	0.16	62,62,62,62	0
56	MG	1A	4041	1/1	0.91	0.12	60,60,60,60	0
56	MG	1A	4042	1/1	0.91	0.14	38,38,38,38	0
56	MG	1A	3462	1/1	0.91	0.12	56,56,56,56	0
56	MG	2E	306	1/1	0.91	0.10	66,66,66,66	0
56	MG	1A	3466	1/1	0.91	0.11	39,39,39,39	0
56	MG	1A	3212	1/1	0.91	0.07	37,37,37,37	0
56	MG	2F	301	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	4057	1/1	0.91	0.10	50,50,50,50	0
56	MG	2N	201	1/1	0.91	0.15	75,75,75,75	0
56	MG	2O	201	1/1	0.91	0.18	65,65,65,65	0
56	MG	1A	3877	1/1	0.91	0.09	42,42,42,42	0
56	MG	1A	3883	1/1	0.91	0.08	25,25,25,25	0
56	MG	2U	201	1/1	0.91	0.08	60,60,60,60	0
56	MG	1A	4061	1/1	0.91	0.13	50,50,50,50	0
56	MG	1A	3885	1/1	0.91	0.19	70,70,70,70	0
56	MG	2Z	301	1/1	0.91	0.10	77,77,77,77	0
56	MG	1w	102	1/1	0.91	0.24	68,68,68,68	0
56	MG	20	103	1/1	0.91	0.19	56,56,56,56	0
56	MG	1A	4066	1/1	0.91	0.14	51,51,51,51	0
56	MG	1A	3102	1/1	0.91	0.12	65,65,65,65	0
56	MG	2A	3513	1/1	0.91	0.12	49,49,49,49	0
56	MG	27	102	1/1	0.91	0.18	58,58,58,58	0
56	MG	28	102	1/1	0.91	0.23	54,54,54,54	0
56	MG	2A	3515	1/1	0.91	0.10	37,37,37,37	0
56	MG	1w	106	1/1	0.91	0.15	62,62,62,62	0
56	MG	2A	3519	1/1	0.91	0.15	64,64,64,64	0
56	MG	1A	3374	1/1	0.91	0.19	47,47,47,47	0
56	MG	1A	3104	1/1	0.91	0.21	42,42,42,42	0
56	MG	2a	1606	1/1	0.91	0.18	56,56,56,56	0
56	MG	2A	3526	1/1	0.91	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1x	101	1/1	0.91	0.28	57,57,57,57	0
56	MG	1A	3324	1/1	0.91	0.09	45,45,45,45	0
56	MG	1A	3730	1/1	0.91	0.14	62,62,62,62	0
56	MG	1A	4073	1/1	0.91	0.09	52,52,52,52	0
56	MG	2A	3543	1/1	0.91	0.14	38,38,38,38	0
56	MG	1a	1639	1/1	0.91	0.13	54,54,54,54	0
56	MG	2A	3277	1/1	0.91	0.10	65,65,65,65	0
56	MG	2A	3279	1/1	0.91	0.16	56,56,56,56	0
56	MG	2a	1624	1/1	0.91	0.12	63,63,63,63	0
56	MG	2A	3554	1/1	0.91	0.10	39,39,39,39	0
56	MG	1A	3595	1/1	0.91	0.07	28,28,28,28	0
56	MG	1A	3115	1/1	0.91	0.22	40,40,40,40	0
56	MG	2a	1632	1/1	0.91	0.33	60,60,60,60	0
56	MG	2A	3001	1/1	0.91	0.11	54,54,54,54	0
56	MG	1A	3508	1/1	0.91	0.21	37,37,37,37	0
56	MG	1a	1643	1/1	0.91	0.22	56,56,56,56	0
56	MG	1a	1646	1/1	0.91	0.15	54,54,54,54	0
56	MG	1a	1648	1/1	0.91	0.37	61,61,61,61	0
56	MG	2a	1640	1/1	0.91	0.15	60,60,60,60	0
56	MG	2A	3590	1/1	0.91	0.17	67,67,67,67	0
56	MG	2A	3592	1/1	0.91	0.17	63,63,63,63	0
56	MG	1A	3749	1/1	0.91	0.08	20,20,20,20	0
56	MG	1A	4082	1/1	0.91	0.10	36,36,36,36	0
56	MG	1A	3750	1/1	0.91	0.13	44,44,44,44	0
56	MG	2a	1649	1/1	0.91	0.24	71,71,71,71	0
56	MG	2A	3298	1/1	0.91	0.16	58,58,58,58	0
56	MG	2a	1652	1/1	0.91	0.27	57,57,57,57	0
56	MG	1A	3752	1/1	0.91	0.10	22,22,22,22	0
56	MG	2A	3607	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3601	1/1	0.91	0.14	49,49,49,49	0
56	MG	2A	3307	1/1	0.91	0.23	70,70,70,70	0
56	MG	1A	3939	1/1	0.91	0.13	58,58,58,58	0
56	MG	2A	3621	1/1	0.91	0.14	38,38,38,38	0
56	MG	2a	1668	1/1	0.91	0.24	54,54,54,54	0
56	MG	2A	3629	1/1	0.91	0.11	50,50,50,50	0
56	MG	1A	3131	1/1	0.91	0.17	43,43,43,43	0
56	MG	1a	1666	1/1	0.91	0.18	64,64,64,64	0
56	MG	2a	1674	1/1	0.91	0.10	62,62,62,62	0
56	MG	1A	3327	1/1	0.91	0.19	62,62,62,62	0
56	MG	2A	3637	1/1	0.91	0.12	56,56,56,56	0
56	MG	1A	3945	1/1	0.91	0.10	41,41,41,41	0
56	MG	2a	1689	1/1	0.91	0.21	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	3142	1/1	0.91	0.11	50,50,50,50	0
56	MG	2A	3641	1/1	0.91	0.23	65,65,65,65	0
56	MG	2A	3642	1/1	0.91	0.14	67,67,67,67	0
56	MG	2A	3643	1/1	0.91	0.16	63,63,63,63	0
56	MG	1A	3630	1/1	0.91	0.09	48,48,48,48	0
56	MG	2a	1697	1/1	0.91	0.34	67,67,67,67	0
56	MG	2a	1699	1/1	0.91	0.08	70,70,70,70	0
56	MG	1A	3953	1/1	0.91	0.06	44,44,44,44	0
56	MG	1A	3332	1/1	0.91	0.15	52,52,52,52	0
56	MG	1a	1675	1/1	0.91	0.19	59,59,59,59	0
56	MG	2A	3061	1/1	0.91	0.17	61,61,61,61	0
56	MG	2A	3660	1/1	0.91	0.17	68,68,68,68	0
56	MG	2A	3063	1/1	0.91	0.23	66,66,66,66	0
56	MG	2A	3067	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3664	1/1	0.91	0.19	66,66,66,66	0
56	MG	1A	3632	1/1	0.91	0.10	22,22,22,22	0
56	MG	1A	3531	1/1	0.91	0.14	51,51,51,51	0
56	MG	2A	3074	1/1	0.91	0.11	61,61,61,61	0
56	MG	2A	3670	1/1	0.91	0.18	49,49,49,49	0
56	MG	1A	3960	1/1	0.91	0.13	66,66,66,66	0
56	MG	2A	3674	1/1	0.91	0.14	59,59,59,59	0
56	MG	1A	3962	1/1	0.91	0.10	73,73,73,73	0
56	MG	2a	1731	1/1	0.91	0.33	67,67,67,67	0
56	MG	2A	3337	1/1	0.91	0.22	61,61,61,61	0
56	MG	1A	3254	1/1	0.91	0.12	58,58,58,58	0
56	MG	2A	3339	1/1	0.91	0.20	71,71,71,71	0
56	MG	2a	1739	1/1	0.91	0.22	71,71,71,71	0
56	MG	1a	1690	1/1	0.91	0.25	46,46,46,46	0
56	MG	2a	1742	1/1	0.91	0.07	74,74,74,74	0
56	MG	1A	3641	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	3968	1/1	0.91	0.12	71,71,71,71	0
56	MG	2A	3691	1/1	0.91	0.23	65,65,65,65	0
56	MG	1A	3340	1/1	0.91	0.26	62,62,62,62	0
56	MG	1A	3648	1/1	0.91	0.11	48,48,48,48	0
56	MG	1A	3537	1/1	0.91	0.23	60,60,60,60	0
56	MG	1a	1705	1/1	0.91	0.10	59,59,59,59	0
56	MG	1A	3981	1/1	0.91	0.10	54,54,54,54	0
56	MG	1a	1708	1/1	0.91	0.14	70,70,70,70	0
56	MG	2a	1767	1/1	0.91	0.12	59,59,59,59	0
56	MG	1A	3198	1/1	0.91	0.08	43,43,43,43	0
56	MG	2a	1773	1/1	0.91	0.14	59,59,59,59	0
56	MG	1A	3824	1/1	0.91	0.10	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	3658	1/1	0.91	0.09	25,25,25,25	0
56	MG	1F	313	1/1	0.91	0.15	35,35,35,35	0
56	MG	1A	3151	1/1	0.91	0.13	41,41,41,41	0
56	MG	2a	1779	1/1	0.91	0.11	82,82,82,82	0
56	MG	2A	3366	1/1	0.91	0.10	70,70,70,70	0
56	MG	2A	3367	1/1	0.91	0.12	56,56,56,56	0
56	MG	1a	1719	1/1	0.91	0.17	58,58,58,58	0
56	MG	2A	3369	1/1	0.91	0.13	69,69,69,69	0
56	MG	2A	3132	1/1	0.91	0.14	46,46,46,46	0
56	MG	1A	3993	1/1	0.91	0.10	54,54,54,54	0
56	MG	1a	1721	1/1	0.91	0.12	62,62,62,62	0
56	MG	2A	3740	1/1	0.91	0.10	58,58,58,58	0
56	MG	2A	3741	1/1	0.91	0.17	59,59,59,59	0
56	MG	1G	204	1/1	0.91	0.10	50,50,50,50	0
56	MG	2A	3376	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3386	1/1	0.91	0.22	62,62,62,62	0
56	MG	1A	3264	1/1	0.91	0.11	48,48,48,48	0
56	MG	1A	3829	1/1	0.91	0.15	59,59,59,59	0
56	MG	1A	3443	1/1	0.91	0.11	50,50,50,50	0
56	MG	2a	1808	1/1	0.91	0.24	56,56,56,56	0
56	MG	2a	1810	1/1	0.91	0.12	64,64,64,64	0
56	MG	2A	3392	1/1	0.91	0.18	57,57,57,57	0
56	MG	1A	3270	1/1	0.91	0.10	44,44,44,44	0
56	MG	2A	3395	1/1	0.91	0.10	62,62,62,62	0
56	MG	2A	3396	1/1	0.91	0.18	74,74,74,74	0
56	MG	1A	3836	1/1	0.91	0.11	64,64,64,64	0
56	MG	2A	3774	1/1	0.91	0.09	62,62,62,62	0
56	MG	2A	3398	1/1	0.91	0.12	61,61,61,61	0
56	MG	1Q	205	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3178	1/1	0.91	0.13	50,50,50,50	0
56	MG	2A	3780	1/1	0.91	0.11	70,70,70,70	0
56	MG	1A	3450	1/1	0.91	0.14	53,53,53,53	0
56	MG	2A	3783	1/1	0.91	0.10	55,55,55,55	0
56	MG	1R	201	1/1	0.91	0.10	45,45,45,45	0
56	MG	2l	205	1/1	0.91	0.15	67,67,67,67	0
56	MG	2A	3408	1/1	0.91	0.27	47,47,47,47	0
56	MG	2A	3409	1/1	0.91	0.24	47,47,47,47	0
56	MG	1a	1752	1/1	0.91	0.11	56,56,56,56	0
56	MG	2A	3794	1/1	0.91	0.20	60,60,60,60	0
56	MG	1A	3839	1/1	0.91	0.15	58,58,58,58	0
56	MG	2A	3412	1/1	0.91	0.25	45,45,45,45	0
56	MG	1A	4012	1/1	0.91	0.12	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	3288	1/1	0.91	0.17	48,48,48,48	0
56	MG	1T	201	1/1	0.91	0.10	73,73,73,73	0
56	MG	1V	201	1/1	0.91	0.17	37,37,37,37	0
56	MG	1V	206	1/1	0.91	0.09	56,56,56,56	0
56	MG	1A	3580	1/1	0.91	0.09	37,37,37,37	0
56	MG	2A	3432	1/1	0.91	0.28	62,62,62,62	0
56	MG	1A	3855	1/1	0.91	0.15	68,68,68,68	0
56	MG	1A	4024	1/1	0.91	0.08	31,31,31,31	0
56	MG	2y	104	1/1	0.91	0.13	81,81,81,81	0
56	MG	1a	1778	1/1	0.91	0.11	46,46,46,46	0
56	MG	1a	1779	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	4030	1/1	0.91	0.14	34,34,34,34	0
56	MG	1A	3456	1/1	0.91	0.14	61,61,61,61	0
56	MG	2A	3497	1/1	0.92	0.11	41,41,41,41	0
56	MG	1A	3432	1/1	0.92	0.17	51,51,51,51	0
56	MG	2D	308	1/1	0.92	0.09	60,60,60,60	0
56	MG	1x	112	1/1	0.92	0.20	59,59,59,59	0
56	MG	2A	3265	1/1	0.92	0.25	59,59,59,59	0
56	MG	1A	4011	1/1	0.92	0.17	61,61,61,61	0
56	MG	2E	308	1/1	0.92	0.11	42,42,42,42	0
56	MG	1E	306	1/1	0.92	0.11	55,55,55,55	0
56	MG	1A	3741	1/1	0.92	0.10	59,59,59,59	0
56	MG	2F	303	1/1	0.92	0.17	74,74,74,74	0
56	MG	1A	3880	1/1	0.92	0.11	22,22,22,22	0
56	MG	1F	303	1/1	0.92	0.15	55,55,55,55	0
56	MG	1F	304	1/1	0.92	0.29	71,71,71,71	0
56	MG	2Q	201	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	4016	1/1	0.92	0.11	45,45,45,45	0
56	MG	1A	4019	1/1	0.92	0.14	54,54,54,54	0
56	MG	2R	202	1/1	0.92	0.19	49,49,49,49	0
56	MG	1a	1680	1/1	0.92	0.18	67,67,67,67	0
56	MG	1F	314	1/1	0.92	0.10	65,65,65,65	0
56	MG	2W	201	1/1	0.92	0.18	60,60,60,60	0
56	MG	2A	3014	1/1	0.92	0.20	66,66,66,66	0
56	MG	1a	1682	1/1	0.92	0.19	63,63,63,63	0
56	MG	1A	3335	1/1	0.92	0.15	55,55,55,55	0
56	MG	1A	3368	1/1	0.92	0.14	47,47,47,47	0
56	MG	21	101	1/1	0.92	0.17	55,55,55,55	0
56	MG	1A	3107	1/1	0.92	0.25	50,50,50,50	0
56	MG	1A	4026	1/1	0.92	0.08	55,55,55,55	0
56	MG	2A	3558	1/1	0.92	0.15	62,62,62,62	0
56	MG	25	106	1/1	0.92	0.27	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	1A	3890	1/1	0.92	0.09	48,48,48,48	0
56	MG	1A	3372	1/1	0.92	0.10	46,46,46,46	0
56	MG	1a	1694	1/1	0.92	0.27	53,53,53,53	0
56	MG	2A	3578	1/1	0.92	0.11	75,75,75,75	0
56	MG	2A	3579	1/1	0.92	0.18	61,61,61,61	0
56	MG	1a	1695	1/1	0.92	0.26	54,54,54,54	0
56	MG	2A	3301	1/1	0.92	0.12	48,48,48,48	0
56	MG	1N	206	1/1	0.92	0.07	53,53,53,53	0
56	MG	2A	3046	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3757	1/1	0.92	0.11	24,24,24,24	0
56	MG	2A	3591	1/1	0.92	0.21	61,61,61,61	0
56	MG	1A	3028	1/1	0.92	0.12	63,63,63,63	0
56	MG	1a	1702	1/1	0.92	0.21	51,51,51,51	0
56	MG	2A	3598	1/1	0.92	0.14	63,63,63,63	0
56	MG	1a	1703	1/1	0.92	0.06	43,43,43,43	0
56	MG	1P	205	1/1	0.92	0.16	42,42,42,42	0
56	MG	2A	3064	1/1	0.92	0.11	51,51,51,51	0
56	MG	2A	3065	1/1	0.92	0.17	67,67,67,67	0
56	MG	2a	1626	1/1	0.92	0.09	68,68,68,68	0
56	MG	2A	3317	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3376	1/1	0.92	0.24	39,39,39,39	0
56	MG	1A	3766	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3640	1/1	0.92	0.06	25,25,25,25	0
56	MG	1A	3453	1/1	0.92	0.13	51,51,51,51	0
56	MG	2A	3627	1/1	0.92	0.15	60,60,60,60	0
56	MG	2A	3628	1/1	0.92	0.10	38,38,38,38	0
56	MG	1A	3543	1/1	0.92	0.07	63,63,63,63	0
56	MG	2a	1637	1/1	0.92	0.22	55,55,55,55	0
56	MG	1a	1713	1/1	0.92	0.24	49,49,49,49	0
56	MG	1A	3290	1/1	0.92	0.18	71,71,71,71	0
56	MG	1A	3791	1/1	0.92	0.09	56,56,56,56	0
56	MG	1a	1718	1/1	0.92	0.11	58,58,58,58	0
56	MG	2a	1645	1/1	0.92	0.24	62,62,62,62	0
56	MG	1A	3793	1/1	0.92	0.14	47,47,47,47	0
56	MG	1A	3297	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3655	1/1	0.92	0.09	56,56,56,56	0
56	MG	1A	3395	1/1	0.92	0.32	40,40,40,40	0
56	MG	1a	1727	1/1	0.92	0.19	58,58,58,58	0
56	MG	1A	3944	1/1	0.92	0.13	69,69,69,69	0
56	MG	2A	3107	1/1	0.92	0.19	70,70,70,70	0
56	MG	1a	1731	1/1	0.92	0.12	59,59,59,59	0
56	MG	1A	3558	1/1	0.92	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3654	1/1	0.92	0.10	59,59,59,59	0
56	MG	1A	3946	1/1	0.92	0.11	45,45,45,45	0
56	MG	2a	1660	1/1	0.92	0.07	59,59,59,59	0
56	MG	2A	3346	1/1	0.92	0.13	54,54,54,54	0
56	MG	2A	3350	1/1	0.92	0.15	63,63,63,63	0
56	MG	1A	3947	1/1	0.92	0.08	48,48,48,48	0
56	MG	2A	3118	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	3662	1/1	0.92	0.08	39,39,39,39	0
56	MG	1A	3816	1/1	0.92	0.11	32,32,32,32	0
56	MG	2A	3123	1/1	0.92	0.26	57,57,57,57	0
56	MG	2a	1679	1/1	0.92	0.11	64,64,64,64	0
56	MG	2A	3360	1/1	0.92	0.10	57,57,57,57	0
56	MG	2A	3671	1/1	0.92	0.17	50,50,50,50	0
56	MG	10	103	1/1	0.92	0.11	40,40,40,40	0
56	MG	2A	3125	1/1	0.92	0.36	67,67,67,67	0
56	MG	2A	3675	1/1	0.92	0.13	50,50,50,50	0
56	MG	2A	3130	1/1	0.92	0.11	45,45,45,45	0
56	MG	2A	3131	1/1	0.92	0.27	82,82,82,82	0
56	MG	1a	1748	1/1	0.92	0.10	51,51,51,51	0
56	MG	2A	3683	1/1	0.92	0.10	56,56,56,56	0
56	MG	2a	1698	1/1	0.92	0.16	60,60,60,60	0
56	MG	10	104	1/1	0.92	0.16	58,58,58,58	0
56	MG	10	106	1/1	0.92	0.11	50,50,50,50	0
56	MG	2A	3145	1/1	0.92	0.17	54,54,54,54	0
56	MG	2A	3146	1/1	0.92	0.19	61,61,61,61	0
56	MG	1A	3461	1/1	0.92	0.16	50,50,50,50	0
56	MG	1A	3399	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3155	1/1	0.92	0.10	61,61,61,61	0
56	MG	2A	3156	1/1	0.92	0.21	59,59,59,59	0
56	MG	2A	3379	1/1	0.92	0.15	71,71,71,71	0
56	MG	2A	3384	1/1	0.92	0.18	66,66,66,66	0
56	MG	2A	3161	1/1	0.92	0.19	57,57,57,57	0
56	MG	2A	3706	1/1	0.92	0.11	58,58,58,58	0
56	MG	1A	3821	1/1	0.92	0.25	60,60,60,60	0
56	MG	2a	1722	1/1	0.92	0.21	55,55,55,55	0
56	MG	1a	1762	1/1	0.92	0.12	60,60,60,60	0
56	MG	1A	4077	1/1	0.92	0.07	53,53,53,53	0
56	MG	2a	1728	1/1	0.92	0.29	50,50,50,50	0
56	MG	1a	1766	1/1	0.92	0.14	58,58,58,58	0
56	MG	2A	3175	1/1	0.92	0.12	48,48,48,48	0
56	MG	2a	1732	1/1	0.92	0.18	62,62,62,62	0
56	MG	1A	3406	1/1	0.92	0.23	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	3177	1/1	0.92	0.40	56,56,56,56	0
56	MG	1a	1769	1/1	0.92	0.10	68,68,68,68	0
56	MG	16	101	1/1	0.92	0.11	51,51,51,51	0
56	MG	1A	3472	1/1	0.92	0.12	50,50,50,50	0
56	MG	2A	3733	1/1	0.92	0.10	53,53,53,53	0
56	MG	1A	3348	1/1	0.92	0.14	41,41,41,41	0
56	MG	2A	3185	1/1	0.92	0.23	62,62,62,62	0
56	MG	2A	3405	1/1	0.92	0.24	63,63,63,63	0
56	MG	2a	1750	1/1	0.92	0.13	58,58,58,58	0
56	MG	1a	1773	1/1	0.92	0.12	58,58,58,58	0
56	MG	2A	3743	1/1	0.92	0.16	43,43,43,43	0
56	MG	2a	1758	1/1	0.92	0.18	69,69,69,69	0
56	MG	1A	3684	1/1	0.92	0.09	26,26,26,26	0
56	MG	2A	3190	1/1	0.92	0.14	65,65,65,65	0
56	MG	2A	3747	1/1	0.92	0.08	71,71,71,71	0
56	MG	1a	1776	1/1	0.92	0.17	57,57,57,57	0
56	MG	1A	4086	1/1	0.92	0.08	44,44,44,44	0
56	MG	1A	3485	1/1	0.92	0.09	49,49,49,49	0
56	MG	2a	1771	1/1	0.92	0.19	69,69,69,69	0
56	MG	2a	1772	1/1	0.92	0.11	68,68,68,68	0
56	MG	2A	3413	1/1	0.92	0.17	36,36,36,36	0
56	MG	2A	3763	1/1	0.92	0.16	64,64,64,64	0
56	MG	2A	3205	1/1	0.92	0.25	67,67,67,67	0
56	MG	1A	4088	1/1	0.92	0.15	59,59,59,59	0
56	MG	2A	3419	1/1	0.92	0.25	62,62,62,62	0
56	MG	1a	1610	1/1	0.92	0.19	65,65,65,65	0
56	MG	2A	3423	1/1	0.92	0.28	63,63,63,63	0
56	MG	2A	3772	1/1	0.92	0.10	52,52,52,52	0
56	MG	2A	3773	1/1	0.92	0.08	55,55,55,55	0
56	MG	1A	4089	1/1	0.92	0.13	53,53,53,53	0
56	MG	1a	1614	1/1	0.92	0.09	68,68,68,68	0
56	MG	2A	3427	1/1	0.92	0.29	60,60,60,60	0
56	MG	2A	3429	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	3412	1/1	0.92	0.17	69,69,69,69	0
56	MG	2A	3431	1/1	0.92	0.18	63,63,63,63	0
56	MG	2A	3782	1/1	0.92	0.16	65,65,65,65	0
56	MG	2a	1797	1/1	0.92	0.25	58,58,58,58	0
56	MG	1A	3349	1/1	0.92	0.15	46,46,46,46	0
56	MG	2a	1799	1/1	0.92	0.16	73,73,73,73	0
56	MG	1A	3972	1/1	0.92	0.15	54,54,54,54	0
56	MG	1a	1629	1/1	0.92	0.27	63,63,63,63	0
56	MG	2a	1803	1/1	0.92	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3252	1/1	0.92	0.17	57,57,57,57	0
56	MG	2a	1806	1/1	0.92	0.18	80,80,80,80	0
56	MG	1A	3328	1/1	0.92	0.16	49,49,49,49	0
56	MG	1a	1802	1/1	0.92	0.07	60,60,60,60	0
56	MG	2A	3443	1/1	0.92	0.30	54,54,54,54	0
56	MG	1a	1636	1/1	0.92	0.11	51,51,51,51	0
56	MG	1B	210	1/1	0.92	0.17	41,41,41,41	0
56	MG	1e	202	1/1	0.92	0.09	64,64,64,64	0
56	MG	1A	3501	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	3426	1/1	0.92	0.11	44,44,44,44	0
56	MG	2A	3456	1/1	0.92	0.27	67,67,67,67	0
56	MG	2A	3229	1/1	0.92	0.30	55,55,55,55	0
56	MG	1A	3844	1/1	0.92	0.08	53,53,53,53	0
56	MG	2A	3461	1/1	0.92	0.20	72,72,72,72	0
56	MG	2A	3463	1/1	0.92	0.14	54,54,54,54	0
56	MG	2A	3823	1/1	0.92	0.07	47,47,47,47	0
56	MG	2A	3466	1/1	0.92	0.13	62,62,62,62	0
56	MG	1A	3205	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3309	1/1	0.92	0.32	57,57,57,57	0
56	MG	2q	201	1/1	0.92	0.27	69,69,69,69	0
56	MG	1A	3598	1/1	0.92	0.10	30,30,30,30	0
56	MG	2t	201	1/1	0.92	0.21	60,60,60,60	0
56	MG	1A	3997	1/1	0.92	0.10	36,36,36,36	0
56	MG	1A	3517	1/1	0.92	0.10	67,67,67,67	0
56	MG	2A	3840	1/1	0.92	0.12	70,70,70,70	0
56	MG	2A	3241	1/1	0.92	0.17	62,62,62,62	0
56	MG	1A	3363	1/1	0.92	0.14	51,51,51,51	0
56	MG	2A	3845	1/1	0.92	0.12	66,66,66,66	0
56	MG	1A	3867	1/1	0.92	0.16	36,36,36,36	0
56	MG	1A	3869	1/1	0.92	0.15	61,61,61,61	0
56	MG	2x	101	1/1	0.92	0.18	60,60,60,60	0
56	MG	2B	203	1/1	0.92	0.25	63,63,63,63	0
56	MG	1A	3520	1/1	0.92	0.10	53,53,53,53	0
56	MG	1B	234	1/1	0.92	0.09	70,70,70,70	0
56	MG	2B	208	1/1	0.92	0.20	56,56,56,56	0
56	MG	2A	3487	1/1	0.92	0.13	61,61,61,61	0
56	MG	1D	310	1/1	0.92	0.18	47,47,47,47	0
56	MG	2B	212	1/1	0.92	0.18	76,76,76,76	0
56	MG	1A	3734	1/1	0.92	0.06	41,41,41,41	0
56	MG	2A	3492	1/1	0.92	0.13	56,56,56,56	0
56	MG	1x	109	1/1	0.92	0.20	65,65,65,65	0
58	WC9	1A	4098	34/34	0.92	0.12	27,38,47,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3496	1/1	0.92	0.08	52,52,52,52	0
59	ZN	24	501	1/1	0.92	0.19	142,142,142,142	0
56	MG	2A	3500	1/1	0.93	0.11	35,35,35,35	0
56	MG	1A	3926	1/1	0.93	0.13	63,63,63,63	0
56	MG	1A	3036	1/1	0.93	0.06	49,49,49,49	0
56	MG	1A	3387	1/1	0.93	0.16	26,26,26,26	0
56	MG	1a	1647	1/1	0.93	0.12	52,52,52,52	0
56	MG	2A	3259	1/1	0.93	0.15	55,55,55,55	0
56	MG	2F	305	1/1	0.93	0.08	42,42,42,42	0
56	MG	2G	201	1/1	0.93	0.17	67,67,67,67	0
56	MG	1x	103	1/1	0.93	0.22	63,63,63,63	0
56	MG	2A	3262	1/1	0.93	0.14	56,56,56,56	0
56	MG	2P	202	1/1	0.93	0.09	61,61,61,61	0
56	MG	1A	3934	1/1	0.93	0.08	65,65,65,65	0
56	MG	2Q	202	1/1	0.93	0.15	50,50,50,50	0
56	MG	1A	3747	1/1	0.93	0.17	49,49,49,49	0
56	MG	1a	1651	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3112	1/1	0.93	0.14	35,35,35,35	0
56	MG	2T	202	1/1	0.93	0.12	64,64,64,64	0
56	MG	1A	3481	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3270	1/1	0.93	0.15	59,59,59,59	0
56	MG	1a	1659	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3016	1/1	0.93	0.30	57,57,57,57	0
56	MG	1B	214	1/1	0.93	0.23	56,56,56,56	0
56	MG	1A	3597	1/1	0.93	0.08	50,50,50,50	0
56	MG	1A	3488	1/1	0.93	0.08	62,62,62,62	0
56	MG	1A	3400	1/1	0.93	0.13	55,55,55,55	0
56	MG	23	102	1/1	0.93	0.15	54,54,54,54	0
56	MG	1A	3763	1/1	0.93	0.08	22,22,22,22	0
56	MG	1A	3402	1/1	0.93	0.13	44,44,44,44	0
56	MG	2A	3562	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3284	1/1	0.93	0.10	52,52,52,52	0
56	MG	2A	3285	1/1	0.93	0.22	64,64,64,64	0
56	MG	28	101	1/1	0.93	0.25	58,58,58,58	0
56	MG	2A	3573	1/1	0.93	0.12	61,61,61,61	0
56	MG	1a	1669	1/1	0.93	0.15	65,65,65,65	0
56	MG	2A	3287	1/1	0.93	0.08	69,69,69,69	0
56	MG	2A	3288	1/1	0.93	0.11	66,66,66,66	0
56	MG	1A	3949	1/1	0.93	0.13	46,46,46,46	0
56	MG	1A	3607	1/1	0.93	0.07	24,24,24,24	0
56	MG	1A	3776	1/1	0.93	0.06	30,30,30,30	0
56	MG	2A	3589	1/1	0.93	0.13	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	3293	1/1	0.93	0.24	55,55,55,55	0
56	MG	1B	227	1/1	0.93	0.09	41,41,41,41	0
56	MG	2a	1612	1/1	0.93	0.34	69,69,69,69	0
56	MG	1a	1674	1/1	0.93	0.21	62,62,62,62	0
56	MG	1A	3955	1/1	0.93	0.12	43,43,43,43	0
56	MG	2a	1616	1/1	0.93	0.14	67,67,67,67	0
56	MG	1A	3088	1/1	0.93	0.17	50,50,50,50	0
56	MG	2A	3599	1/1	0.93	0.07	35,35,35,35	0
56	MG	1A	3408	1/1	0.93	0.13	54,54,54,54	0
56	MG	2A	3034	1/1	0.93	0.14	60,60,60,60	0
56	MG	2a	1623	1/1	0.93	0.18	64,64,64,64	0
56	MG	2A	3603	1/1	0.93	0.16	46,46,46,46	0
56	MG	2a	1625	1/1	0.93	0.19	58,58,58,58	0
56	MG	1A	3783	1/1	0.93	0.12	60,60,60,60	0
56	MG	2A	3306	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3409	1/1	0.93	0.11	40,40,40,40	0
56	MG	1A	3503	1/1	0.93	0.11	55,55,55,55	0
56	MG	2a	1631	1/1	0.93	0.27	54,54,54,54	0
56	MG	1A	3963	1/1	0.93	0.10	64,64,64,64	0
56	MG	2A	3614	1/1	0.93	0.11	49,49,49,49	0
56	MG	1a	1685	1/1	0.93	0.21	62,62,62,62	0
56	MG	1a	1686	1/1	0.93	0.29	66,66,66,66	0
56	MG	1A	3964	1/1	0.93	0.08	29,29,29,29	0
56	MG	1A	3505	1/1	0.93	0.11	63,63,63,63	0
56	MG	1E	302	1/1	0.93	0.17	50,50,50,50	0
56	MG	1A	3794	1/1	0.93	0.06	22,22,22,22	0
56	MG	1A	3141	1/1	0.93	0.09	43,43,43,43	0
56	MG	1A	3344	1/1	0.93	0.14	48,48,48,48	0
56	MG	2A	3066	1/1	0.93	0.09	49,49,49,49	0
56	MG	1E	314	1/1	0.93	0.09	55,55,55,55	0
56	MG	1A	3804	1/1	0.93	0.17	57,57,57,57	0
56	MG	1a	1699	1/1	0.93	0.41	60,60,60,60	0
56	MG	2A	3072	1/1	0.93	0.18	49,49,49,49	0
56	MG	2A	3326	1/1	0.93	0.36	51,51,51,51	0
56	MG	2A	3644	1/1	0.93	0.12	59,59,59,59	0
56	MG	1A	3974	1/1	0.93	0.09	34,34,34,34	0
56	MG	1A	3805	1/1	0.93	0.17	60,60,60,60	0
56	MG	2A	3329	1/1	0.93	0.23	72,72,72,72	0
56	MG	1A	3511	1/1	0.93	0.37	46,46,46,46	0
56	MG	2A	3333	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3079	1/1	0.93	0.07	41,41,41,41	0
56	MG	2A	3081	1/1	0.93	0.14	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	1704	1/1	0.93	0.10	59,59,59,59	0
56	MG	1A	3980	1/1	0.93	0.11	52,52,52,52	0
56	MG	1A	3809	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3025	1/1	0.93	0.22	53,53,53,53	0
56	MG	1A	3415	1/1	0.93	0.25	56,56,56,56	0
56	MG	2a	1675	1/1	0.93	0.20	56,56,56,56	0
56	MG	1A	3814	1/1	0.93	0.07	38,38,38,38	0
56	MG	1A	3001	1/1	0.93	0.11	37,37,37,37	0
56	MG	2A	3345	1/1	0.93	0.13	60,60,60,60	0
56	MG	2a	1683	1/1	0.93	0.13	58,58,58,58	0
56	MG	2A	3099	1/1	0.93	0.15	57,57,57,57	0
56	MG	2a	1687	1/1	0.93	0.17	43,43,43,43	0
56	MG	1A	3647	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3351	1/1	0.93	0.14	58,58,58,58	0
56	MG	2A	3106	1/1	0.93	0.19	68,68,68,68	0
56	MG	1A	3820	1/1	0.93	0.18	43,43,43,43	0
56	MG	1A	4003	1/1	0.93	0.13	46,46,46,46	0
56	MG	1A	3424	1/1	0.93	0.11	41,41,41,41	0
56	MG	1Q	203	1/1	0.93	0.09	55,55,55,55	0
56	MG	1A	3652	1/1	0.93	0.07	29,29,29,29	0
56	MG	2A	3687	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3527	1/1	0.93	0.25	47,47,47,47	0
56	MG	2A	3119	1/1	0.93	0.24	62,62,62,62	0
56	MG	1a	1725	1/1	0.93	0.18	53,53,53,53	0
56	MG	2a	1704	1/1	0.93	0.09	59,59,59,59	0
56	MG	1a	1726	1/1	0.93	0.15	45,45,45,45	0
56	MG	1A	3217	1/1	0.93	0.13	53,53,53,53	0
56	MG	1A	3826	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3157	1/1	0.93	0.19	58,58,58,58	0
56	MG	2a	1711	1/1	0.93	0.31	59,59,59,59	0
56	MG	1A	3101	1/1	0.93	0.14	68,68,68,68	0
56	MG	2a	1714	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3243	1/1	0.93	0.07	47,47,47,47	0
56	MG	1A	3055	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3135	1/1	0.93	0.07	45,45,45,45	0
56	MG	1A	3035	1/1	0.93	0.35	31,31,31,31	0
56	MG	1A	3541	1/1	0.93	0.09	45,45,45,45	0
56	MG	2A	3380	1/1	0.93	0.10	56,56,56,56	0
56	MG	2A	3715	1/1	0.93	0.25	52,52,52,52	0
56	MG	2A	3144	1/1	0.93	0.28	49,49,49,49	0
56	MG	1A	3365	1/1	0.93	0.16	46,46,46,46	0
56	MG	1A	3249	1/1	0.93	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3843	1/1	0.93	0.14	62,62,62,62	0
56	MG	2A	3390	1/1	0.93	0.11	69,69,69,69	0
56	MG	1a	1750	1/1	0.93	0.22	51,51,51,51	0
56	MG	2a	1735	1/1	0.93	0.27	59,59,59,59	0
56	MG	2A	3731	1/1	0.93	0.13	50,50,50,50	0
56	MG	2A	3151	1/1	0.93	0.22	58,58,58,58	0
56	MG	1A	3180	1/1	0.93	0.19	50,50,50,50	0
56	MG	2A	3394	1/1	0.93	0.06	62,62,62,62	0
56	MG	1a	1753	1/1	0.93	0.08	73,73,73,73	0
56	MG	2a	1745	1/1	0.93	0.12	64,64,64,64	0
56	MG	2a	1747	1/1	0.93	0.13	70,70,70,70	0
56	MG	1A	3691	1/1	0.93	0.06	50,50,50,50	0
56	MG	2A	3162	1/1	0.93	0.24	55,55,55,55	0
56	MG	1A	3693	1/1	0.93	0.06	26,26,26,26	0
56	MG	2A	3399	1/1	0.93	0.08	65,65,65,65	0
56	MG	2a	1753	1/1	0.93	0.10	65,65,65,65	0
56	MG	1A	3853	1/1	0.93	0.12	45,45,45,45	0
56	MG	2a	1757	1/1	0.93	0.19	68,68,68,68	0
56	MG	2A	3166	1/1	0.93	0.13	44,44,44,44	0
56	MG	2A	3751	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3168	1/1	0.93	0.11	54,54,54,54	0
56	MG	1A	3854	1/1	0.93	0.17	56,56,56,56	0
56	MG	1A	3697	1/1	0.93	0.10	28,28,28,28	0
56	MG	1A	3444	1/1	0.93	0.11	50,50,50,50	0
56	MG	1A	3860	1/1	0.93	0.15	33,33,33,33	0
56	MG	2a	1770	1/1	0.93	0.24	63,63,63,63	0
56	MG	2A	3766	1/1	0.93	0.08	51,51,51,51	0
56	MG	1A	3552	1/1	0.93	0.33	42,42,42,42	0
56	MG	1A	3251	1/1	0.93	0.16	47,47,47,47	0
56	MG	1A	3703	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	4052	1/1	0.93	0.08	23,23,23,23	0
56	MG	2A	3183	1/1	0.93	0.17	65,65,65,65	0
56	MG	1A	3448	1/1	0.93	0.09	47,47,47,47	0
56	MG	2A	3418	1/1	0.93	0.17	39,39,39,39	0
56	MG	17	106	1/1	0.93	0.08	49,49,49,49	0
56	MG	2A	3421	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3186	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3571	1/1	0.93	0.19	31,31,31,31	0
56	MG	1a	1777	1/1	0.93	0.09	68,68,68,68	0
56	MG	1A	3105	1/1	0.93	0.10	32,32,32,32	0
56	MG	2A	3193	1/1	0.93	0.29	65,65,65,65	0
56	MG	2A	3196	1/1	0.93	0.20	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	3786	1/1	0.93	0.12	66,66,66,66	0
56	MG	2A	3198	1/1	0.93	0.17	54,54,54,54	0
56	MG	1A	3709	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3183	1/1	0.93	0.19	72,72,72,72	0
56	MG	1A	3881	1/1	0.93	0.09	30,30,30,30	0
56	MG	2A	3434	1/1	0.93	0.23	53,53,53,53	0
56	MG	1A	3377	1/1	0.93	0.08	44,44,44,44	0
56	MG	1a	1607	1/1	0.93	0.17	60,60,60,60	0
56	MG	2A	3438	1/1	0.93	0.22	56,56,56,56	0
56	MG	2a	1805	1/1	0.93	0.12	68,68,68,68	0
56	MG	2A	3439	1/1	0.93	0.19	40,40,40,40	0
56	MG	1A	3884	1/1	0.93	0.08	23,23,23,23	0
56	MG	1A	3717	1/1	0.93	0.11	49,49,49,49	0
56	MG	2a	1809	1/1	0.93	0.14	64,64,64,64	0
56	MG	2A	3814	1/1	0.93	0.14	58,58,58,58	0
56	MG	2a	1812	1/1	0.93	0.12	60,60,60,60	0
56	MG	1a	1795	1/1	0.93	0.17	54,54,54,54	0
56	MG	1a	1613	1/1	0.93	0.18	58,58,58,58	0
56	MG	1A	3720	1/1	0.93	0.07	37,37,37,37	0
56	MG	1a	1616	1/1	0.93	0.14	50,50,50,50	0
56	MG	1A	3257	1/1	0.93	0.10	44,44,44,44	0
56	MG	2a	1820	1/1	0.93	0.08	66,66,66,66	0
56	MG	1A	3457	1/1	0.93	0.17	65,65,65,65	0
56	MG	2A	3829	1/1	0.93	0.15	63,63,63,63	0
56	MG	1a	1804	1/1	0.93	0.16	59,59,59,59	0
56	MG	1a	1805	1/1	0.93	0.20	51,51,51,51	0
56	MG	2e	201	1/1	0.93	0.07	70,70,70,70	0
56	MG	1a	1806	1/1	0.93	0.19	65,65,65,65	0
56	MG	1a	1624	1/1	0.93	0.22	49,49,49,49	0
56	MG	2A	3837	1/1	0.93	0.14	65,65,65,65	0
56	MG	2l	201	1/1	0.93	0.14	62,62,62,62	0
56	MG	2A	3224	1/1	0.93	0.15	55,55,55,55	0
56	MG	2l	203	1/1	0.93	0.11	64,64,64,64	0
56	MG	1a	1626	1/1	0.93	0.16	52,52,52,52	0
56	MG	2m	201	1/1	0.93	0.24	68,68,68,68	0
56	MG	2A	3226	1/1	0.93	0.10	65,65,65,65	0
56	MG	1b	301	1/1	0.93	0.14	66,66,66,66	0
56	MG	2A	3843	1/1	0.93	0.07	62,62,62,62	0
56	MG	1d	301	1/1	0.93	0.43	68,68,68,68	0
56	MG	2A	3471	1/1	0.93	0.14	62,62,62,62	0
56	MG	1A	3728	1/1	0.93	0.08	60,60,60,60	0
56	MG	1A	3729	1/1	0.93	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3382	1/1	0.93	0.11	43,43,43,43	0
56	MG	2B	205	1/1	0.93	0.20	59,59,59,59	0
56	MG	2A	3475	1/1	0.93	0.08	51,51,51,51	0
56	MG	1A	3908	1/1	0.93	0.21	61,61,61,61	0
56	MG	1A	3383	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3236	1/1	0.93	0.08	46,46,46,46	0
56	MG	2x	103	1/1	0.93	0.08	69,69,69,69	0
56	MG	2A	3482	1/1	0.93	0.25	50,50,50,50	0
56	MG	1p	101	1/1	0.93	0.23	49,49,49,49	0
56	MG	1A	3384	1/1	0.93	0.12	53,53,53,53	0
56	MG	2A	3240	1/1	0.93	0.16	56,56,56,56	0
56	MG	2B	216	1/1	0.93	0.20	61,61,61,61	0
56	MG	1A	3916	1/1	0.93	0.08	45,45,45,45	0
56	MG	1A	4085	1/1	0.93	0.13	42,42,42,42	0
56	MG	2D	301	1/1	0.93	0.14	49,49,49,49	0
56	MG	1w	103	1/1	0.93	0.11	64,64,64,64	0
56	MG	2A	3247	1/1	0.93	0.09	62,62,62,62	0
58	WC9	2A	3846	34/34	0.93	0.12	43,52,58,60	0
56	MG	1A	3736	1/1	0.93	0.20	52,52,52,52	0
56	MG	1A	3463	1/1	0.93	0.23	57,57,57,57	0
56	MG	1A	3565	1/1	0.94	0.21	50,50,50,50	0
56	MG	1x	102	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3488	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3361	1/1	0.94	0.18	55,55,55,55	0
56	MG	1A	3902	1/1	0.94	0.14	34,34,34,34	0
56	MG	1x	105	1/1	0.94	0.20	66,66,66,66	0
56	MG	2D	306	1/1	0.94	0.22	42,42,42,42	0
56	MG	1A	3084	1/1	0.94	0.19	39,39,39,39	0
56	MG	1A	3577	1/1	0.94	0.13	42,42,42,42	0
56	MG	1A	3446	1/1	0.94	0.28	63,63,63,63	0
56	MG	2A	3498	1/1	0.94	0.19	48,48,48,48	0
56	MG	1A	3909	1/1	0.94	0.06	34,34,34,34	0
56	MG	1A	3735	1/1	0.94	0.05	16,16,16,16	0
56	MG	1A	3293	1/1	0.94	0.08	38,38,38,38	0
56	MG	2A	3504	1/1	0.94	0.24	46,46,46,46	0
56	MG	2F	302	1/1	0.94	0.15	43,43,43,43	0
56	MG	1A	3581	1/1	0.94	0.09	45,45,45,45	0
56	MG	1a	1655	1/1	0.94	0.18	52,52,52,52	0
56	MG	1A	3740	1/1	0.94	0.06	32,32,32,32	0
56	MG	2A	3516	1/1	0.94	0.07	37,37,37,37	0
56	MG	1a	1657	1/1	0.94	0.13	64,64,64,64	0
56	MG	2A	3274	1/1	0.94	0.12	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	3919	1/1	0.94	0.08	46,46,46,46	0
56	MG	1B	201	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3525	1/1	0.94	0.19	53,53,53,53	0
56	MG	1A	3296	1/1	0.94	0.12	62,62,62,62	0
56	MG	1B	206	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3281	1/1	0.94	0.26	67,67,67,67	0
56	MG	1A	3449	1/1	0.94	0.13	48,48,48,48	0
56	MG	1a	1664	1/1	0.94	0.12	60,60,60,60	0
56	MG	2U	202	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3221	1/1	0.94	0.06	49,49,49,49	0
56	MG	1B	211	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3546	1/1	0.94	0.10	40,40,40,40	0
56	MG	1A	3748	1/1	0.94	0.11	50,50,50,50	0
56	MG	2A	3027	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3028	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3555	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3366	1/1	0.94	0.12	63,63,63,63	0
56	MG	2A	3290	1/1	0.94	0.13	68,68,68,68	0
56	MG	1A	3367	1/1	0.94	0.14	45,45,45,45	0
56	MG	2A	3564	1/1	0.94	0.08	36,36,36,36	0
56	MG	25	105	1/1	0.94	0.15	52,52,52,52	0
56	MG	2A	3033	1/1	0.94	0.09	35,35,35,35	0
56	MG	1A	3060	1/1	0.94	0.18	57,57,57,57	0
56	MG	27	103	1/1	0.94	0.32	52,52,52,52	0
56	MG	2A	3570	1/1	0.94	0.18	51,51,51,51	0
56	MG	2A	3571	1/1	0.94	0.14	47,47,47,47	0
56	MG	1A	3941	1/1	0.94	0.09	56,56,56,56	0
56	MG	2A	3038	1/1	0.94	0.18	62,62,62,62	0
56	MG	1A	3753	1/1	0.94	0.12	36,36,36,36	0
56	MG	1A	3756	1/1	0.94	0.09	20,20,20,20	0
56	MG	2A	3583	1/1	0.94	0.16	61,61,61,61	0
56	MG	1A	3589	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3233	1/1	0.94	0.09	55,55,55,55	0
56	MG	2A	3303	1/1	0.94	0.08	48,48,48,48	0
56	MG	2a	1610	1/1	0.94	0.27	64,64,64,64	0
56	MG	2A	3587	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	3304	1/1	0.94	0.17	51,51,51,51	0
56	MG	2A	3305	1/1	0.94	0.13	58,58,58,58	0
56	MG	2a	1614	1/1	0.94	0.21	54,54,54,54	0
56	MG	1A	3305	1/1	0.94	0.32	60,60,60,60	0
56	MG	2A	3055	1/1	0.94	0.19	65,65,65,65	0
56	MG	1B	230	1/1	0.94	0.08	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	3764	1/1	0.94	0.12	26,26,26,26	0
56	MG	2A	3310	1/1	0.94	0.15	46,46,46,46	0
56	MG	2A	3311	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3601	1/1	0.94	0.09	37,37,37,37	0
56	MG	1A	3375	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3950	1/1	0.94	0.06	24,24,24,24	0
56	MG	2A	3604	1/1	0.94	0.16	40,40,40,40	0
56	MG	1A	3768	1/1	0.94	0.07	35,35,35,35	0
56	MG	1B	235	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3952	1/1	0.94	0.07	49,49,49,49	0
56	MG	2A	3068	1/1	0.94	0.14	63,63,63,63	0
56	MG	2A	3609	1/1	0.94	0.09	43,43,43,43	0
56	MG	1A	3167	1/1	0.94	0.09	38,38,38,38	0
56	MG	2A	3612	1/1	0.94	0.11	50,50,50,50	0
56	MG	1A	3774	1/1	0.94	0.06	69,69,69,69	0
56	MG	1A	3775	1/1	0.94	0.09	39,39,39,39	0
56	MG	2A	3617	1/1	0.94	0.10	42,42,42,42	0
56	MG	2A	3619	1/1	0.94	0.10	61,61,61,61	0
56	MG	2a	1639	1/1	0.94	0.10	58,58,58,58	0
56	MG	2A	3073	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3626	1/1	0.94	0.12	58,58,58,58	0
56	MG	2a	1642	1/1	0.94	0.20	54,54,54,54	0
56	MG	1A	3464	1/1	0.94	0.15	65,65,65,65	0
56	MG	1E	303	1/1	0.94	0.23	45,45,45,45	0
56	MG	1a	1696	1/1	0.94	0.13	49,49,49,49	0
56	MG	1A	3170	1/1	0.94	0.18	41,41,41,41	0
56	MG	2A	3631	1/1	0.94	0.12	37,37,37,37	0
56	MG	1A	3468	1/1	0.94	0.08	64,64,64,64	0
56	MG	2A	3634	1/1	0.94	0.09	51,51,51,51	0
56	MG	2a	1651	1/1	0.94	0.13	63,63,63,63	0
56	MG	2A	3082	1/1	0.94	0.10	50,50,50,50	0
56	MG	1E	310	1/1	0.94	0.07	17,17,17,17	0
56	MG	1A	3961	1/1	0.94	0.09	60,60,60,60	0
56	MG	2a	1656	1/1	0.94	0.15	76,76,76,76	0
56	MG	2A	3639	1/1	0.94	0.18	49,49,49,49	0
56	MG	2A	3332	1/1	0.94	0.19	63,63,63,63	0
56	MG	1a	1701	1/1	0.94	0.22	61,61,61,61	0
56	MG	2A	3334	1/1	0.94	0.09	51,51,51,51	0
56	MG	2a	1662	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3335	1/1	0.94	0.11	57,57,57,57	0
56	MG	1A	3314	1/1	0.94	0.11	46,46,46,46	0
56	MG	1A	3784	1/1	0.94	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3315	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3609	1/1	0.94	0.10	10,10,10,10	0
56	MG	1F	312	1/1	0.94	0.13	57,57,57,57	0
56	MG	1a	1707	1/1	0.94	0.18	60,60,60,60	0
56	MG	2A	3657	1/1	0.94	0.11	63,63,63,63	0
56	MG	2A	3658	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3479	1/1	0.94	0.18	45,45,45,45	0
56	MG	2A	3104	1/1	0.94	0.12	48,48,48,48	0
56	MG	2a	1685	1/1	0.94	0.30	54,54,54,54	0
56	MG	1A	3480	1/1	0.94	0.09	41,41,41,41	0
56	MG	1F	315	1/1	0.94	0.09	41,41,41,41	0
56	MG	2a	1688	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3109	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3348	1/1	0.94	0.09	60,60,60,60	0
56	MG	1A	3970	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3622	1/1	0.94	0.07	35,35,35,35	0
56	MG	1A	3318	1/1	0.94	0.19	51,51,51,51	0
56	MG	2A	3353	1/1	0.94	0.22	56,56,56,56	0
56	MG	2a	1696	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3672	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3803	1/1	0.94	0.09	62,62,62,62	0
56	MG	1A	3628	1/1	0.94	0.08	23,23,23,23	0
56	MG	1A	3629	1/1	0.94	0.10	43,43,43,43	0
56	MG	2A	3676	1/1	0.94	0.08	74,74,74,74	0
56	MG	2A	3358	1/1	0.94	0.10	54,54,54,54	0
56	MG	2A	3359	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3806	1/1	0.94	0.10	30,30,30,30	0
56	MG	2a	1706	1/1	0.94	0.24	57,57,57,57	0
56	MG	1A	3482	1/1	0.94	0.11	56,56,56,56	0
56	MG	1O	202	1/1	0.94	0.10	53,53,53,53	0
56	MG	1a	1724	1/1	0.94	0.23	57,57,57,57	0
56	MG	1O	204	1/1	0.94	0.07	61,61,61,61	0
56	MG	1A	3244	1/1	0.94	0.19	48,48,48,48	0
56	MG	1A	3486	1/1	0.94	0.07	49,49,49,49	0
56	MG	1A	3017	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3133	1/1	0.94	0.22	61,61,61,61	0
56	MG	2a	1719	1/1	0.94	0.19	48,48,48,48	0
56	MG	2A	3134	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	3490	1/1	0.94	0.13	33,33,33,33	0
56	MG	2A	3136	1/1	0.94	0.07	62,62,62,62	0
56	MG	2a	1724	1/1	0.94	0.23	53,53,53,53	0
56	MG	1a	1736	1/1	0.94	0.14	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	2A	3375	1/1	0.94	0.18	52,52,52,52	0
56	MG	2A	3703	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3704	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3138	1/1	0.94	0.11	55,55,55,55	0
56	MG	2A	3378	1/1	0.94	0.29	55,55,55,55	0
56	MG	1A	3638	1/1	0.94	0.08	38,38,38,38	0
56	MG	1A	3068	1/1	0.94	0.06	33,33,33,33	0
56	MG	1A	3388	1/1	0.94	0.16	27,27,27,27	0
56	MG	2a	1737	1/1	0.94	0.22	59,59,59,59	0
56	MG	2A	3385	1/1	0.94	0.13	55,55,55,55	0
56	MG	1A	3389	1/1	0.94	0.12	45,45,45,45	0
56	MG	1A	3499	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3393	1/1	0.94	0.29	61,61,61,61	0
56	MG	1U	209	1/1	0.94	0.14	54,54,54,54	0
56	MG	2a	1744	1/1	0.94	0.11	71,71,71,71	0
56	MG	2A	3725	1/1	0.94	0.16	59,59,59,59	0
56	MG	2A	3726	1/1	0.94	0.11	74,74,74,74	0
56	MG	2A	3152	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3116	1/1	0.94	0.17	33,33,33,33	0
56	MG	1A	3122	1/1	0.94	0.07	42,42,42,42	0
56	MG	2A	3732	1/1	0.94	0.13	38,38,38,38	0
56	MG	2A	3158	1/1	0.94	0.20	39,39,39,39	0
56	MG	2A	3734	1/1	0.94	0.17	45,45,45,45	0
56	MG	2A	3736	1/1	0.94	0.15	53,53,53,53	0
56	MG	1a	1751	1/1	0.94	0.17	53,53,53,53	0
56	MG	2a	1760	1/1	0.94	0.24	59,59,59,59	0
56	MG	1A	3329	1/1	0.94	0.09	38,38,38,38	0
56	MG	1W	206	1/1	0.94	0.13	27,27,27,27	0
56	MG	1a	1754	1/1	0.94	0.13	59,59,59,59	0
56	MG	2A	3742	1/1	0.94	0.08	36,36,36,36	0
56	MG	1A	3129	1/1	0.94	0.10	66,66,66,66	0
56	MG	1a	1758	1/1	0.94	0.12	59,59,59,59	0
56	MG	2A	3401	1/1	0.94	0.06	59,59,59,59	0
56	MG	1X	104	1/1	0.94	0.25	43,43,43,43	0
56	MG	1a	1760	1/1	0.94	0.11	62,62,62,62	0
56	MG	1A	3405	1/1	0.94	0.08	51,51,51,51	0
56	MG	2A	3752	1/1	0.94	0.16	68,68,68,68	0
56	MG	1Y	202	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3754	1/1	0.94	0.11	81,81,81,81	0
56	MG	2A	3755	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	3661	1/1	0.94	0.09	29,29,29,29	0
56	MG	1Y	205	1/1	0.94	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1782	1/1	0.94	0.17	61,61,61,61	0
56	MG	2a	1783	1/1	0.94	0.07	62,62,62,62	0
56	MG	2A	3759	1/1	0.94	0.11	69,69,69,69	0
56	MG	2A	3180	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3007	1/1	0.94	0.08	39,39,39,39	0
56	MG	2A	3765	1/1	0.94	0.07	48,48,48,48	0
56	MG	1A	3673	1/1	0.94	0.06	27,27,27,27	0
56	MG	2a	1790	1/1	0.94	0.22	60,60,60,60	0
56	MG	1A	3333	1/1	0.94	0.21	52,52,52,52	0
56	MG	1A	3334	1/1	0.94	0.23	56,56,56,56	0
56	MG	2A	3415	1/1	0.94	0.26	49,49,49,49	0
56	MG	1A	3194	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3338	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	4025	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3420	1/1	0.94	0.14	50,50,50,50	0
56	MG	2A	3775	1/1	0.94	0.13	64,64,64,64	0
56	MG	1A	3051	1/1	0.94	0.09	24,24,24,24	0
56	MG	11	103	1/1	0.94	0.17	62,62,62,62	0
56	MG	11	105	1/1	0.94	0.10	62,62,62,62	0
56	MG	12	101	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	4029	1/1	0.94	0.11	32,32,32,32	0
56	MG	1A	3845	1/1	0.94	0.12	24,24,24,24	0
56	MG	1A	3846	1/1	0.94	0.09	30,30,30,30	0
56	MG	1a	1784	1/1	0.94	0.11	49,49,49,49	0
56	MG	15	109	1/1	0.94	0.10	39,39,39,39	0
56	MG	2a	1811	1/1	0.94	0.19	60,60,60,60	0
56	MG	1A	3103	1/1	0.94	0.06	25,25,25,25	0
56	MG	1A	3849	1/1	0.94	0.21	36,36,36,36	0
56	MG	2A	3789	1/1	0.94	0.08	44,44,44,44	0
56	MG	17	105	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3261	1/1	0.94	0.12	60,60,60,60	0
56	MG	2A	3795	1/1	0.94	0.12	59,59,59,59	0
56	MG	2a	1819	1/1	0.94	0.22	66,66,66,66	0
56	MG	1A	3851	1/1	0.94	0.06	47,47,47,47	0
56	MG	1A	3419	1/1	0.94	0.13	50,50,50,50	0
56	MG	1a	1799	1/1	0.94	0.21	59,59,59,59	0
56	MG	1A	3146	1/1	0.94	0.09	34,34,34,34	0
56	MG	2A	3441	1/1	0.94	0.27	53,53,53,53	0
56	MG	2d	301	1/1	0.94	0.30	59,59,59,59	0
56	MG	2A	3216	1/1	0.94	0.16	52,52,52,52	0
56	MG	2A	3809	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3694	1/1	0.94	0.06	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3263	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3445	1/1	0.94	0.25	49,49,49,49	0
56	MG	2A	3817	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	4051	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3345	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3449	1/1	0.94	0.34	53,53,53,53	0
56	MG	1A	3538	1/1	0.94	0.13	47,47,47,47	0
56	MG	2A	3451	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3452	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3701	1/1	0.94	0.07	47,47,47,47	0
56	MG	2A	3455	1/1	0.94	0.10	69,69,69,69	0
56	MG	1a	1809	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3147	1/1	0.94	0.24	44,44,44,44	0
56	MG	1A	3540	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	3268	1/1	0.94	0.21	56,56,56,56	0
56	MG	1f	201	1/1	0.94	0.11	59,59,59,59	0
56	MG	1a	1618	1/1	0.94	0.06	55,55,55,55	0
56	MG	1A	3081	1/1	0.94	0.08	51,51,51,51	0
56	MG	1A	4067	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3844	1/1	0.94	0.11	63,63,63,63	0
56	MG	1A	3353	1/1	0.94	0.06	50,50,50,50	0
56	MG	1a	1625	1/1	0.94	0.22	58,58,58,58	0
56	MG	1A	3287	1/1	0.94	0.05	45,45,45,45	0
56	MG	1A	3156	1/1	0.94	0.16	38,38,38,38	0
56	MG	1A	3438	1/1	0.94	0.22	45,45,45,45	0
56	MG	1a	1631	1/1	0.94	0.27	57,57,57,57	0
56	MG	1A	3554	1/1	0.94	0.20	49,49,49,49	0
56	MG	2B	207	1/1	0.94	0.12	68,68,68,68	0
56	MG	1A	3439	1/1	0.94	0.31	44,44,44,44	0
56	MG	1A	3213	1/1	0.94	0.15	46,46,46,46	0
56	MG	1A	3562	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3894	1/1	0.94	0.14	41,41,41,41	0
56	MG	2A	3484	1/1	0.94	0.10	68,68,68,68	0
56	MG	1A	3355	1/1	0.95	0.19	47,47,47,47	0
56	MG	1A	3706	1/1	0.95	0.06	26,26,26,26	0
56	MG	1A	3879	1/1	0.95	0.05	43,43,43,43	0
56	MG	2A	3007	1/1	0.95	0.32	58,58,58,58	0
56	MG	1a	1644	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3357	1/1	0.95	0.09	60,60,60,60	0
56	MG	2F	306	1/1	0.95	0.11	53,53,53,53	0
56	MG	2A	3560	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3708	1/1	0.95	0.12	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3548	1/1	0.95	0.11	57,57,57,57	0
56	MG	2P	201	1/1	0.95	0.10	63,63,63,63	0
56	MG	1A	4083	1/1	0.95	0.12	56,56,56,56	0
56	MG	2A	3565	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3017	1/1	0.95	0.23	50,50,50,50	0
56	MG	2A	3018	1/1	0.95	0.24	49,49,49,49	0
56	MG	2A	3569	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3127	1/1	0.95	0.15	56,56,56,56	0
56	MG	1a	1654	1/1	0.95	0.06	48,48,48,48	0
56	MG	2T	203	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3553	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3886	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	3271	1/1	0.95	0.08	38,38,38,38	0
56	MG	2V	202	1/1	0.95	0.05	56,56,56,56	0
56	MG	1A	3718	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3300	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3719	1/1	0.95	0.09	39,39,39,39	0
56	MG	2A	3302	1/1	0.95	0.28	45,45,45,45	0
56	MG	1A	3895	1/1	0.95	0.21	24,24,24,24	0
56	MG	20	104	1/1	0.95	0.11	61,61,61,61	0
56	MG	1A	3896	1/1	0.95	0.12	53,53,53,53	0
56	MG	2A	3588	1/1	0.95	0.27	67,67,67,67	0
56	MG	2A	3036	1/1	0.95	0.12	44,44,44,44	0
56	MG	1a	1662	1/1	0.95	0.13	65,65,65,65	0
56	MG	25	103	1/1	0.95	0.18	50,50,50,50	0
56	MG	1A	3555	1/1	0.95	0.28	47,47,47,47	0
56	MG	1A	3898	1/1	0.95	0.18	49,49,49,49	0
56	MG	1A	3723	1/1	0.95	0.09	64,64,64,64	0
56	MG	26	101	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3595	1/1	0.95	0.10	47,47,47,47	0
56	MG	2A	3596	1/1	0.95	0.09	50,50,50,50	0
56	MG	1B	204	1/1	0.95	0.20	56,56,56,56	0
56	MG	1A	3901	1/1	0.95	0.10	30,30,30,30	0
56	MG	2A	3047	1/1	0.95	0.14	39,39,39,39	0
56	MG	2a	1601	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3281	1/1	0.95	0.13	29,29,29,29	0
56	MG	2A	3052	1/1	0.95	0.12	30,30,30,30	0
56	MG	1A	3203	1/1	0.95	0.10	22,22,22,22	0
56	MG	1A	3727	1/1	0.95	0.06	36,36,36,36	0
56	MG	1B	212	1/1	0.95	0.17	56,56,56,56	0
56	MG	1B	213	1/1	0.95	0.13	56,56,56,56	0
56	MG	2a	1608	1/1	0.95	0.26	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	3907	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3559	1/1	0.95	0.12	34,34,34,34	0
56	MG	1A	3560	1/1	0.95	0.08	36,36,36,36	0
56	MG	2A	3610	1/1	0.95	0.06	35,35,35,35	0
56	MG	1A	3047	1/1	0.95	0.04	27,27,27,27	0
56	MG	1A	3206	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3613	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3569	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3451	1/1	0.95	0.08	56,56,56,56	0
56	MG	1A	3918	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3013	1/1	0.95	0.14	29,29,29,29	0
56	MG	1A	3454	1/1	0.95	0.18	43,43,43,43	0
56	MG	2A	3623	1/1	0.95	0.07	39,39,39,39	0
56	MG	2A	3330	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3136	1/1	0.95	0.27	39,39,39,39	0
56	MG	1a	1687	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3077	1/1	0.95	0.15	59,59,59,59	0
56	MG	1a	1688	1/1	0.95	0.23	52,52,52,52	0
56	MG	1A	3929	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3080	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3294	1/1	0.95	0.18	43,43,43,43	0
56	MG	1A	3743	1/1	0.95	0.07	35,35,35,35	0
56	MG	2A	3636	1/1	0.95	0.17	39,39,39,39	0
56	MG	1a	1692	1/1	0.95	0.23	47,47,47,47	0
56	MG	1A	3295	1/1	0.95	0.18	54,54,54,54	0
56	MG	2A	3085	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3086	1/1	0.95	0.30	45,45,45,45	0
56	MG	1A	3935	1/1	0.95	0.06	66,66,66,66	0
56	MG	1A	3936	1/1	0.95	0.08	48,48,48,48	0
56	MG	2A	3093	1/1	0.95	0.14	53,53,53,53	0
56	MG	1D	306	1/1	0.95	0.07	38,38,38,38	0
56	MG	2A	3347	1/1	0.95	0.31	77,77,77,77	0
56	MG	2A	3646	1/1	0.95	0.18	59,59,59,59	0
56	MG	2A	3096	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	3027	1/1	0.95	0.09	47,47,47,47	0
56	MG	2A	3649	1/1	0.95	0.15	62,62,62,62	0
56	MG	1A	3089	1/1	0.95	0.07	44,44,44,44	0
56	MG	2A	3652	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3653	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3940	1/1	0.95	0.08	54,54,54,54	0
56	MG	2A	3656	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	3373	1/1	0.95	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3214	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3216	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3105	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3302	1/1	0.95	0.09	29,29,29,29	0
56	MG	2A	3662	1/1	0.95	0.07	47,47,47,47	0
56	MG	1E	308	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3754	1/1	0.95	0.08	28,28,28,28	0
56	MG	2a	1666	1/1	0.95	0.24	61,61,61,61	0
56	MG	1A	3467	1/1	0.95	0.12	52,52,52,52	0
56	MG	1A	3143	1/1	0.95	0.09	38,38,38,38	0
56	MG	2A	3668	1/1	0.95	0.19	49,49,49,49	0
56	MG	2a	1671	1/1	0.95	0.22	55,55,55,55	0
56	MG	1A	3591	1/1	0.95	0.15	44,44,44,44	0
56	MG	2A	3114	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3471	1/1	0.95	0.10	52,52,52,52	0
56	MG	2a	1676	1/1	0.95	0.23	56,56,56,56	0
56	MG	1A	3219	1/1	0.95	0.14	47,47,47,47	0
56	MG	2a	1678	1/1	0.95	0.10	55,55,55,55	0
56	MG	1F	307	1/1	0.95	0.11	45,45,45,45	0
56	MG	1F	308	1/1	0.95	0.18	31,31,31,31	0
56	MG	1A	3308	1/1	0.95	0.05	43,43,43,43	0
56	MG	1A	3477	1/1	0.95	0.17	59,59,59,59	0
56	MG	2A	3678	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3090	1/1	0.95	0.15	38,38,38,38	0
56	MG	1A	3954	1/1	0.95	0.07	34,34,34,34	0
56	MG	2A	3127	1/1	0.95	0.12	46,46,46,46	0
56	MG	1A	3312	1/1	0.95	0.16	44,44,44,44	0
56	MG	1A	3771	1/1	0.95	0.06	49,49,49,49	0
56	MG	1A	3223	1/1	0.95	0.09	44,44,44,44	0
56	MG	1a	1723	1/1	0.95	0.24	47,47,47,47	0
56	MG	2a	1694	1/1	0.95	0.07	51,51,51,51	0
56	MG	2A	3383	1/1	0.95	0.07	64,64,64,64	0
56	MG	1A	3224	1/1	0.95	0.16	40,40,40,40	0
56	MG	1A	3602	1/1	0.95	0.07	28,28,28,28	0
56	MG	1A	3604	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3605	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3782	1/1	0.95	0.11	64,64,64,64	0
56	MG	1A	3225	1/1	0.95	0.12	56,56,56,56	0
56	MG	1a	1734	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3004	1/1	0.95	0.05	27,27,27,27	0
56	MG	1O	203	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3487	1/1	0.95	0.08	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	3967	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3789	1/1	0.95	0.07	37,37,37,37	0
56	MG	2a	1709	1/1	0.95	0.12	69,69,69,69	0
56	MG	1a	1743	1/1	0.95	0.08	42,42,42,42	0
56	MG	1A	3320	1/1	0.95	0.18	36,36,36,36	0
56	MG	1A	3619	1/1	0.95	0.07	27,27,27,27	0
56	MG	2A	3157	1/1	0.95	0.20	64,64,64,64	0
56	MG	1A	3621	1/1	0.95	0.04	33,33,33,33	0
56	MG	2A	3402	1/1	0.95	0.06	56,56,56,56	0
56	MG	1A	3795	1/1	0.95	0.04	19,19,19,19	0
56	MG	2A	3720	1/1	0.95	0.05	71,71,71,71	0
56	MG	1A	3798	1/1	0.95	0.28	27,27,27,27	0
56	MG	1A	3232	1/1	0.95	0.25	42,42,42,42	0
56	MG	1A	3397	1/1	0.95	0.21	41,41,41,41	0
56	MG	2a	1725	1/1	0.95	0.17	62,62,62,62	0
56	MG	2A	3727	1/1	0.95	0.08	69,69,69,69	0
56	MG	1A	3493	1/1	0.95	0.23	40,40,40,40	0
56	MG	2A	3167	1/1	0.95	0.09	41,41,41,41	0
56	MG	1T	202	1/1	0.95	0.15	50,50,50,50	0
56	MG	2A	3169	1/1	0.95	0.11	59,59,59,59	0
56	MG	1U	202	1/1	0.95	0.16	35,35,35,35	0
56	MG	1U	204	1/1	0.95	0.18	37,37,37,37	0
56	MG	2A	3173	1/1	0.95	0.20	65,65,65,65	0
56	MG	2A	3174	1/1	0.95	0.10	61,61,61,61	0
56	MG	1A	3984	1/1	0.95	0.08	44,44,44,44	0
56	MG	1A	3031	1/1	0.95	0.20	26,26,26,26	0
56	MG	1V	205	1/1	0.95	0.11	31,31,31,31	0
56	MG	1A	3496	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3497	1/1	0.95	0.10	47,47,47,47	0
56	MG	1A	3236	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	3401	1/1	0.95	0.10	49,49,49,49	0
56	MG	1X	102	1/1	0.95	0.15	39,39,39,39	0
56	MG	1A	3096	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3998	1/1	0.95	0.07	25,25,25,25	0
56	MG	1A	3100	1/1	0.95	0.07	62,62,62,62	0
56	MG	1A	3160	1/1	0.95	0.17	36,36,36,36	0
56	MG	1A	3407	1/1	0.95	0.08	48,48,48,48	0
56	MG	1A	3642	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3059	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3194	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3164	1/1	0.95	0.21	36,36,36,36	0
56	MG	2A	3761	1/1	0.95	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3509	1/1	0.95	0.34	44,44,44,44	0
56	MG	1A	3002	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3512	1/1	0.95	0.12	37,37,37,37	0
56	MG	1A	3654	1/1	0.95	0.07	21,21,21,21	0
56	MG	2a	1765	1/1	0.95	0.07	52,52,52,52	0
56	MG	1a	1783	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3513	1/1	0.95	0.14	54,54,54,54	0
56	MG	2A	3207	1/1	0.95	0.16	52,52,52,52	0
56	MG	1a	1786	1/1	0.95	0.17	67,67,67,67	0
56	MG	1A	3514	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3061	1/1	0.95	0.10	27,27,27,27	0
56	MG	2A	3447	1/1	0.95	0.21	55,55,55,55	0
56	MG	1a	1790	1/1	0.95	0.05	54,54,54,54	0
56	MG	1a	1791	1/1	0.95	0.12	66,66,66,66	0
56	MG	1A	3413	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3214	1/1	0.95	0.11	53,53,53,53	0
56	MG	2a	1780	1/1	0.95	0.18	66,66,66,66	0
56	MG	13	103	1/1	0.95	0.09	52,52,52,52	0
56	MG	2A	3453	1/1	0.95	0.08	63,63,63,63	0
56	MG	1A	3011	1/1	0.95	0.20	46,46,46,46	0
56	MG	1A	3666	1/1	0.95	0.04	22,22,22,22	0
56	MG	15	103	1/1	0.95	0.17	38,38,38,38	0
56	MG	2A	3785	1/1	0.95	0.06	51,51,51,51	0
56	MG	1A	3671	1/1	0.95	0.12	38,38,38,38	0
56	MG	15	106	1/1	0.95	0.13	43,43,43,43	0
56	MG	2A	3221	1/1	0.95	0.09	69,69,69,69	0
56	MG	2A	3462	1/1	0.95	0.11	54,54,54,54	0
56	MG	2A	3790	1/1	0.95	0.09	44,44,44,44	0
56	MG	2a	1793	1/1	0.95	0.07	59,59,59,59	0
56	MG	15	108	1/1	0.95	0.07	47,47,47,47	0
56	MG	2a	1795	1/1	0.95	0.20	76,76,76,76	0
56	MG	2A	3793	1/1	0.95	0.08	34,34,34,34	0
56	MG	2A	3465	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3067	1/1	0.95	0.08	30,30,30,30	0
56	MG	1A	4027	1/1	0.95	0.09	38,38,38,38	0
56	MG	1A	3838	1/1	0.95	0.13	43,43,43,43	0
56	MG	1A	3524	1/1	0.95	0.24	32,32,32,32	0
56	MG	1A	4031	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	4033	1/1	0.95	0.08	41,41,41,41	0
56	MG	1a	1810	1/1	0.95	0.23	56,56,56,56	0
56	MG	1A	3840	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3810	1/1	0.95	0.07	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	3841	1/1	0.95	0.08	20,20,20,20	0
56	MG	2A	3813	1/1	0.95	0.13	80,80,80,80	0
56	MG	2A	3476	1/1	0.95	0.08	39,39,39,39	0
56	MG	1e	201	1/1	0.95	0.30	59,59,59,59	0
56	MG	2A	3478	1/1	0.95	0.22	63,63,63,63	0
56	MG	2A	3818	1/1	0.95	0.05	31,31,31,31	0
56	MG	2A	3235	1/1	0.95	0.09	50,50,50,50	0
56	MG	1a	1601	1/1	0.95	0.20	52,52,52,52	0
56	MG	1a	1602	1/1	0.95	0.13	64,64,64,64	0
56	MG	1A	3525	1/1	0.95	0.09	36,36,36,36	0
56	MG	2a	1818	1/1	0.95	0.16	62,62,62,62	0
56	MG	1A	3037	1/1	0.95	0.12	37,37,37,37	0
56	MG	2A	3826	1/1	0.95	0.16	59,59,59,59	0
56	MG	1m	3001	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3832	1/1	0.95	0.13	58,58,58,58	0
56	MG	2a	1823	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	4040	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3681	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3255	1/1	0.95	0.14	65,65,65,65	0
56	MG	1A	3847	1/1	0.95	0.07	32,32,32,32	0
56	MG	1A	3528	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3251	1/1	0.95	0.15	59,59,59,59	0
56	MG	1A	3181	1/1	0.95	0.20	53,53,53,53	0
56	MG	1A	4048	1/1	0.95	0.10	45,45,45,45	0
56	MG	1a	1617	1/1	0.95	0.05	54,54,54,54	0
56	MG	2A	3499	1/1	0.95	0.22	71,71,71,71	0
56	MG	2l	204	1/1	0.95	0.07	68,68,68,68	0
56	MG	1A	3686	1/1	0.95	0.11	27,27,27,27	0
56	MG	2A	3257	1/1	0.95	0.13	54,54,54,54	0
56	MG	1a	1621	1/1	0.95	0.26	61,61,61,61	0
56	MG	1A	3111	1/1	0.95	0.13	37,37,37,37	0
56	MG	2A	3506	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3018	1/1	0.95	0.08	36,36,36,36	0
56	MG	1A	3533	1/1	0.95	0.21	47,47,47,47	0
56	MG	2A	3514	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3072	1/1	0.95	0.12	28,28,28,28	0
56	MG	1A	3857	1/1	0.95	0.10	40,40,40,40	0
56	MG	2B	209	1/1	0.95	0.14	48,48,48,48	0
56	MG	1A	4063	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3347	1/1	0.95	0.19	38,38,38,38	0
56	MG	2A	3522	1/1	0.95	0.12	63,63,63,63	0
56	MG	2A	3269	1/1	0.95	0.16	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	3859	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3042	1/1	0.95	0.06	32,32,32,32	0
56	MG	1x	110	1/1	0.95	0.31	67,67,67,67	0
56	MG	1A	3862	1/1	0.95	0.12	39,39,39,39	0
56	MG	1A	3078	1/1	0.95	0.25	54,54,54,54	0
56	MG	2A	3530	1/1	0.95	0.14	42,42,42,42	0
56	MG	2D	303	1/1	0.95	0.28	55,55,55,55	0
56	MG	2A	3531	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3533	1/1	0.95	0.11	48,48,48,48	0
56	MG	1A	3350	1/1	0.95	0.16	30,30,30,30	0
57	K	2A	3459	1/1	0.95	0.10	73,73,73,73	0
56	MG	1A	3265	1/1	0.95	0.07	52,52,52,52	0
56	MG	1A	3267	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3197	1/1	0.95	0.21	41,41,41,41	0
56	MG	2A	3545	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3491	1/1	0.96	0.13	37,37,37,37	0
56	MG	2A	3020	1/1	0.96	0.20	44,44,44,44	0
56	MG	2F	307	1/1	0.96	0.14	39,39,39,39	0
56	MG	1A	3910	1/1	0.96	0.06	65,65,65,65	0
56	MG	2A	3572	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3024	1/1	0.96	0.06	47,47,47,47	0
56	MG	2A	3575	1/1	0.96	0.14	60,60,60,60	0
56	MG	2A	3577	1/1	0.96	0.08	70,70,70,70	0
56	MG	1B	203	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3026	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3404	1/1	0.96	0.12	51,51,51,51	0
56	MG	2Q	204	1/1	0.96	0.10	57,57,57,57	0
56	MG	1a	1650	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3914	1/1	0.96	0.06	54,54,54,54	0
56	MG	2R	203	1/1	0.96	0.16	56,56,56,56	0
56	MG	1a	1652	1/1	0.96	0.08	50,50,50,50	0
56	MG	1a	1653	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3603	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3063	1/1	0.96	0.29	63,63,63,63	0
56	MG	1A	3337	1/1	0.96	0.22	44,44,44,44	0
56	MG	1A	3755	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3040	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3066	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3052	1/1	0.96	0.15	29,29,29,29	0
56	MG	2A	3594	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	3269	1/1	0.96	0.23	49,49,49,49	0
56	MG	1A	3759	1/1	0.96	0.07	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	219	1/1	0.96	0.24	53,53,53,53	0
56	MG	23	101	1/1	0.96	0.06	50,50,50,50	0
56	MG	2A	3048	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3049	1/1	0.96	0.11	32,32,32,32	0
56	MG	1B	220	1/1	0.96	0.09	41,41,41,41	0
56	MG	1A	3760	1/1	0.96	0.05	26,26,26,26	0
56	MG	1A	3614	1/1	0.96	0.08	38,38,38,38	0
56	MG	2A	3054	1/1	0.96	0.08	44,44,44,44	0
56	MG	1A	3762	1/1	0.96	0.09	47,47,47,47	0
56	MG	2A	3056	1/1	0.96	0.27	56,56,56,56	0
56	MG	1A	3616	1/1	0.96	0.14	43,43,43,43	0
56	MG	2A	3059	1/1	0.96	0.10	56,56,56,56	0
56	MG	2A	3060	1/1	0.96	0.21	52,52,52,52	0
56	MG	1A	3617	1/1	0.96	0.09	54,54,54,54	0
56	MG	1A	3158	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	3411	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3159	1/1	0.96	0.13	32,32,32,32	0
56	MG	1A	3343	1/1	0.96	0.13	39,39,39,39	0
56	MG	1A	3272	1/1	0.96	0.19	57,57,57,57	0
56	MG	2A	3616	1/1	0.96	0.13	52,52,52,52	0
56	MG	1A	3627	1/1	0.96	0.07	28,28,28,28	0
56	MG	2A	3618	1/1	0.96	0.09	55,55,55,55	0
56	MG	1A	3275	1/1	0.96	0.16	48,48,48,48	0
56	MG	1A	3276	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3622	1/1	0.96	0.14	51,51,51,51	0
56	MG	1a	1679	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3780	1/1	0.96	0.08	21,21,21,21	0
56	MG	1B	236	1/1	0.96	0.06	39,39,39,39	0
56	MG	1D	302	1/1	0.96	0.09	26,26,26,26	0
56	MG	1D	304	1/1	0.96	0.16	36,36,36,36	0
56	MG	1A	3418	1/1	0.96	0.06	40,40,40,40	0
56	MG	1D	309	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3093	1/1	0.96	0.10	27,27,27,27	0
56	MG	2a	1619	1/1	0.96	0.07	74,74,74,74	0
56	MG	2A	3633	1/1	0.96	0.08	52,52,52,52	0
56	MG	2a	1621	1/1	0.96	0.17	82,82,82,82	0
56	MG	1A	3285	1/1	0.96	0.17	54,54,54,54	0
56	MG	1A	3422	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3423	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	3636	1/1	0.96	0.10	24,24,24,24	0
56	MG	1A	3790	1/1	0.96	0.06	41,41,41,41	0
56	MG	1A	3118	1/1	0.96	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1628	1/1	0.96	0.31	61,61,61,61	0
56	MG	1A	3639	1/1	0.96	0.05	28,28,28,28	0
56	MG	2A	3349	1/1	0.96	0.06	67,67,67,67	0
56	MG	2A	3090	1/1	0.96	0.32	58,58,58,58	0
56	MG	1A	3425	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3121	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3797	1/1	0.96	0.05	23,23,23,23	0
56	MG	1E	313	1/1	0.96	0.11	40,40,40,40	0
56	MG	1A	3427	1/1	0.96	0.16	50,50,50,50	0
56	MG	2A	3356	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3522	1/1	0.96	0.07	40,40,40,40	0
56	MG	1A	3645	1/1	0.96	0.08	43,43,43,43	0
56	MG	2A	3651	1/1	0.96	0.08	34,34,34,34	0
56	MG	1F	305	1/1	0.96	0.17	35,35,35,35	0
56	MG	1A	3801	1/1	0.96	0.04	38,38,38,38	0
56	MG	1A	3523	1/1	0.96	0.14	43,43,43,43	0
56	MG	2a	1644	1/1	0.96	0.08	76,76,76,76	0
56	MG	2A	3655	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3165	1/1	0.96	0.17	35,35,35,35	0
56	MG	1F	311	1/1	0.96	0.16	48,48,48,48	0
56	MG	1A	3094	1/1	0.96	0.17	52,52,52,52	0
56	MG	1A	3650	1/1	0.96	0.10	34,34,34,34	0
56	MG	1A	3291	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3969	1/1	0.96	0.10	63,63,63,63	0
56	MG	1G	201	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3653	1/1	0.96	0.07	22,22,22,22	0
56	MG	2a	1654	1/1	0.96	0.08	60,60,60,60	0
56	MG	1A	3810	1/1	0.96	0.06	37,37,37,37	0
56	MG	2A	3117	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3356	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3433	1/1	0.96	0.24	51,51,51,51	0
56	MG	1A	3975	1/1	0.96	0.09	38,38,38,38	0
56	MG	2A	3377	1/1	0.96	0.20	41,41,41,41	0
56	MG	2a	1661	1/1	0.96	0.16	61,61,61,61	0
56	MG	1N	204	1/1	0.96	0.20	43,43,43,43	0
56	MG	1A	3228	1/1	0.96	0.14	37,37,37,37	0
56	MG	2a	1665	1/1	0.96	0.16	44,44,44,44	0
56	MG	1A	3530	1/1	0.96	0.15	39,39,39,39	0
56	MG	2A	3381	1/1	0.96	0.17	58,58,58,58	0
56	MG	1A	3979	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3436	1/1	0.96	0.23	46,46,46,46	0
56	MG	2A	3128	1/1	0.96	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3679	1/1	0.96	0.06	65,65,65,65	0
56	MG	2a	1673	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3818	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3387	1/1	0.96	0.12	64,64,64,64	0
56	MG	1A	3982	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3124	1/1	0.96	0.23	41,41,41,41	0
56	MG	1A	3664	1/1	0.96	0.06	23,23,23,23	0
56	MG	1Q	201	1/1	0.96	0.12	33,33,33,33	0
56	MG	2a	1680	1/1	0.96	0.26	65,65,65,65	0
56	MG	1a	1730	1/1	0.96	0.10	51,51,51,51	0
56	MG	2a	1682	1/1	0.96	0.25	54,54,54,54	0
56	MG	2A	3688	1/1	0.96	0.07	30,30,30,30	0
56	MG	2a	1684	1/1	0.96	0.14	50,50,50,50	0
56	MG	1A	3231	1/1	0.96	0.10	57,57,57,57	0
56	MG	1Q	204	1/1	0.96	0.11	56,56,56,56	0
56	MG	1A	3125	1/1	0.96	0.21	33,33,33,33	0
56	MG	2A	3693	1/1	0.96	0.14	55,55,55,55	0
56	MG	2A	3140	1/1	0.96	0.13	52,52,52,52	0
56	MG	2A	3696	1/1	0.96	0.10	44,44,44,44	0
56	MG	2A	3141	1/1	0.96	0.06	55,55,55,55	0
56	MG	1A	3672	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3143	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3178	1/1	0.96	0.11	36,36,36,36	0
56	MG	1R	205	1/1	0.96	0.16	33,33,33,33	0
56	MG	1A	3298	1/1	0.96	0.13	39,39,39,39	0
56	MG	1a	1742	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3148	1/1	0.96	0.21	35,35,35,35	0
56	MG	1A	3235	1/1	0.96	0.09	31,31,31,31	0
56	MG	2A	3406	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3126	1/1	0.96	0.23	34,34,34,34	0
56	MG	1A	3679	1/1	0.96	0.05	29,29,29,29	0
56	MG	2A	3153	1/1	0.96	0.10	40,40,40,40	0
56	MG	2A	3154	1/1	0.96	0.26	48,48,48,48	0
56	MG	1a	1746	1/1	0.96	0.05	59,59,59,59	0
56	MG	1a	1747	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3830	1/1	0.96	0.05	33,33,33,33	0
56	MG	2A	3722	1/1	0.96	0.08	65,65,65,65	0
56	MG	1A	3237	1/1	0.96	0.17	34,34,34,34	0
56	MG	1U	203	1/1	0.96	0.09	38,38,38,38	0
56	MG	2a	1712	1/1	0.96	0.28	59,59,59,59	0
56	MG	1A	3833	1/1	0.96	0.06	58,58,58,58	0
56	MG	1U	207	1/1	0.96	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3241	1/1	0.96	0.23	47,47,47,47	0
56	MG	1A	3026	1/1	0.96	0.13	41,41,41,41	0
56	MG	2a	1718	1/1	0.96	0.11	45,45,45,45	0
56	MG	2A	3730	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3369	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3685	1/1	0.96	0.06	63,63,63,63	0
56	MG	1W	202	1/1	0.96	0.16	41,41,41,41	0
56	MG	1A	3005	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	4014	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3737	1/1	0.96	0.06	50,50,50,50	0
56	MG	1A	3687	1/1	0.96	0.07	38,38,38,38	0
56	MG	1X	101	1/1	0.96	0.27	44,44,44,44	0
56	MG	1A	3688	1/1	0.96	0.09	41,41,41,41	0
56	MG	1a	1767	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3019	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	4020	1/1	0.96	0.09	51,51,51,51	0
56	MG	1X	107	1/1	0.96	0.06	52,52,52,52	0
56	MG	2A	3745	1/1	0.96	0.14	66,66,66,66	0
56	MG	1Y	201	1/1	0.96	0.12	52,52,52,52	0
56	MG	1A	3310	1/1	0.96	0.24	63,63,63,63	0
56	MG	2A	3748	1/1	0.96	0.10	67,67,67,67	0
56	MG	1A	3692	1/1	0.96	0.09	29,29,29,29	0
56	MG	2a	1741	1/1	0.96	0.06	72,72,72,72	0
56	MG	2A	3750	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3132	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3184	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	3695	1/1	0.96	0.10	54,54,54,54	0
56	MG	2a	1746	1/1	0.96	0.12	58,58,58,58	0
56	MG	1Z	303	1/1	0.96	0.06	49,49,49,49	0
56	MG	1A	3248	1/1	0.96	0.26	50,50,50,50	0
56	MG	10	101	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3698	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3134	1/1	0.96	0.09	42,42,42,42	0
56	MG	2a	1752	1/1	0.96	0.16	48,48,48,48	0
56	MG	2A	3195	1/1	0.96	0.10	34,34,34,34	0
56	MG	2A	3762	1/1	0.96	0.08	54,54,54,54	0
56	MG	2a	1755	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	3852	1/1	0.96	0.07	50,50,50,50	0
56	MG	10	105	1/1	0.96	0.10	62,62,62,62	0
56	MG	1A	4032	1/1	0.96	0.05	44,44,44,44	0
56	MG	2A	3201	1/1	0.96	0.21	70,70,70,70	0
56	MG	1A	3460	1/1	0.96	0.26	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	10	108	1/1	0.96	0.07	44,44,44,44	0
56	MG	11	102	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3378	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3316	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3381	1/1	0.96	0.15	29,29,29,29	0
56	MG	13	102	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3563	1/1	0.96	0.10	52,52,52,52	0
56	MG	2A	3776	1/1	0.96	0.18	62,62,62,62	0
56	MG	1A	3193	1/1	0.96	0.26	30,30,30,30	0
56	MG	2a	1774	1/1	0.96	0.16	50,50,50,50	0
56	MG	1A	3465	1/1	0.96	0.09	60,60,60,60	0
56	MG	1A	3570	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3863	1/1	0.96	0.15	31,31,31,31	0
56	MG	1a	1803	1/1	0.96	0.06	58,58,58,58	0
56	MG	2A	3468	1/1	0.96	0.06	55,55,55,55	0
56	MG	1A	3864	1/1	0.96	0.21	38,38,38,38	0
56	MG	15	107	1/1	0.96	0.19	39,39,39,39	0
56	MG	1A	3135	1/1	0.96	0.21	30,30,30,30	0
56	MG	1A	3321	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3712	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3870	1/1	0.96	0.06	40,40,40,40	0
56	MG	17	102	1/1	0.96	0.16	34,34,34,34	0
56	MG	2a	1787	1/1	0.96	0.10	51,51,51,51	0
56	MG	2A	3223	1/1	0.96	0.35	42,42,42,42	0
56	MG	1A	4053	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	4054	1/1	0.96	0.06	42,42,42,42	0
56	MG	18	101	1/1	0.96	0.18	57,57,57,57	0
56	MG	1A	4056	1/1	0.96	0.05	44,44,44,44	0
56	MG	2A	3797	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3575	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	4058	1/1	0.96	0.07	52,52,52,52	0
56	MG	1k	201	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3576	1/1	0.96	0.17	53,53,53,53	0
56	MG	1l	202	1/1	0.96	0.07	57,57,57,57	0
56	MG	1A	3874	1/1	0.96	0.07	29,29,29,29	0
56	MG	2a	1800	1/1	0.96	0.17	57,57,57,57	0
56	MG	1A	3875	1/1	0.96	0.09	28,28,28,28	0
56	MG	1A	3323	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3578	1/1	0.96	0.08	48,48,48,48	0
56	MG	1a	1606	1/1	0.96	0.08	54,54,54,54	0
56	MG	1A	3469	1/1	0.96	0.14	51,51,51,51	0
56	MG	1a	1608	1/1	0.96	0.06	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	3057	1/1	0.96	0.17	45,45,45,45	0
56	MG	1a	1611	1/1	0.96	0.14	27,27,27,27	0
56	MG	2A	3244	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3029	1/1	0.96	0.32	29,29,29,29	0
56	MG	1A	3882	1/1	0.96	0.11	21,21,21,21	0
56	MG	1A	3473	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3475	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3825	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3507	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3508	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3830	1/1	0.96	0.07	66,66,66,66	0
56	MG	1A	3043	1/1	0.96	0.21	27,27,27,27	0
56	MG	2A	3512	1/1	0.96	0.09	71,71,71,71	0
56	MG	1A	3392	1/1	0.96	0.07	50,50,50,50	0
56	MG	1a	1619	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3478	1/1	0.96	0.10	49,49,49,49	0
56	MG	2A	3256	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3201	1/1	0.96	0.09	32,32,32,32	0
56	MG	1x	106	1/1	0.96	0.08	41,41,41,41	0
56	MG	2A	3520	1/1	0.96	0.08	31,31,31,31	0
56	MG	1A	3892	1/1	0.96	0.18	48,48,48,48	0
56	MG	1x	108	1/1	0.96	0.16	58,58,58,58	0
56	MG	1A	3893	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3394	1/1	0.96	0.12	66,66,66,66	0
56	MG	1A	3258	1/1	0.96	0.04	39,39,39,39	0
56	MG	1A	3024	1/1	0.96	0.08	29,29,29,29	0
56	MG	1a	1628	1/1	0.96	0.08	51,51,51,51	0
56	MG	1x	114	1/1	0.96	0.12	62,62,62,62	0
56	MG	1A	3483	1/1	0.96	0.18	48,48,48,48	0
56	MG	2A	3271	1/1	0.96	0.06	65,65,65,65	0
56	MG	1A	3737	1/1	0.96	0.10	52,52,52,52	0
56	MG	2A	3535	1/1	0.96	0.10	39,39,39,39	0
56	MG	2A	3536	1/1	0.96	0.07	35,35,35,35	0
56	MG	2A	3537	1/1	0.96	0.07	50,50,50,50	0
56	MG	2A	3538	1/1	0.96	0.09	40,40,40,40	0
56	MG	2v	103	1/1	0.96	0.15	50,50,50,50	0
56	MG	1A	3593	1/1	0.96	0.07	39,39,39,39	0
56	MG	2A	3542	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3002	1/1	0.96	0.15	43,43,43,43	0
56	MG	1a	1634	1/1	0.96	0.26	58,58,58,58	0
56	MG	2A	3004	1/1	0.96	0.10	48,48,48,48	0
56	MG	2A	3278	1/1	0.96	0.07	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	2B	218	1/1	0.96	0.19	68,68,68,68	0
56	MG	1A	3087	1/1	0.96	0.31	38,38,38,38	0
56	MG	1A	3006	1/1	0.96	0.21	54,54,54,54	0
56	MG	2A	3552	1/1	0.96	0.07	37,37,37,37	0
56	MG	2x	105	1/1	0.96	0.07	61,61,61,61	0
56	MG	2D	304	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3149	1/1	0.96	0.18	39,39,39,39	0
56	MG	2A	3008	1/1	0.96	0.09	41,41,41,41	0
56	MG	2A	3557	1/1	0.96	0.10	57,57,57,57	0
56	MG	2y	103	1/1	0.96	0.05	66,66,66,66	0
56	MG	1A	3150	1/1	0.96	0.08	35,35,35,35	0
56	MG	2A	3559	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3010	1/1	0.96	0.28	57,57,57,57	0
56	MG	1A	4091	1/1	0.96	0.20	65,65,65,65	0
56	MG	1A	3489	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	4094	1/1	0.96	0.09	47,47,47,47	0
56	MG	1A	4095	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3403	1/1	0.96	0.17	48,48,48,48	0
56	MG	1A	4097	1/1	0.96	0.16	42,42,42,42	0
56	MG	2A	3087	1/1	0.97	0.06	48,48,48,48	0
56	MG	2W	203	1/1	0.97	0.11	58,58,58,58	0
56	MG	2X	101	1/1	0.97	0.06	59,59,59,59	0
56	MG	1P	202	1/1	0.97	0.19	32,32,32,32	0
56	MG	1A	3322	1/1	0.97	0.13	35,35,35,35	0
56	MG	2A	3091	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3396	1/1	0.97	0.04	28,28,28,28	0
56	MG	1a	1710	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	4010	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3020	1/1	0.97	0.11	54,54,54,54	0
56	MG	1A	3398	1/1	0.97	0.10	40,40,40,40	0
56	MG	1A	4013	1/1	0.97	0.07	50,50,50,50	0
56	MG	1A	3044	1/1	0.97	0.17	30,30,30,30	0
56	MG	2A	3625	1/1	0.97	0.05	43,43,43,43	0
56	MG	1a	1716	1/1	0.97	0.13	44,44,44,44	0
56	MG	1R	202	1/1	0.97	0.08	43,43,43,43	0
56	MG	2A	3102	1/1	0.97	0.10	39,39,39,39	0
56	MG	27	101	1/1	0.97	0.04	44,44,44,44	0
56	MG	2A	3103	1/1	0.97	0.11	44,44,44,44	0
56	MG	1R	203	1/1	0.97	0.14	28,28,28,28	0
56	MG	1R	204	1/1	0.97	0.25	37,37,37,37	0
56	MG	1A	3711	1/1	0.97	0.15	48,48,48,48	0
56	MG	1R	206	1/1	0.97	0.17	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3253	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3714	1/1	0.97	0.08	48,48,48,48	0
56	MG	1A	3196	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	4021	1/1	0.97	0.06	43,43,43,43	0
56	MG	2A	3113	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	3148	1/1	0.97	0.11	27,27,27,27	0
56	MG	2A	3362	1/1	0.97	0.05	59,59,59,59	0
56	MG	1a	1728	1/1	0.97	0.15	54,54,54,54	0
56	MG	2A	3116	1/1	0.97	0.17	53,53,53,53	0
56	MG	1U	201	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3856	1/1	0.97	0.09	27,27,27,27	0
56	MG	1A	3256	1/1	0.97	0.13	39,39,39,39	0
56	MG	1a	1732	1/1	0.97	0.08	48,48,48,48	0
56	MG	2A	3121	1/1	0.97	0.15	40,40,40,40	0
56	MG	1a	1733	1/1	0.97	0.09	47,47,47,47	0
56	MG	1A	3030	1/1	0.97	0.08	29,29,29,29	0
56	MG	1U	205	1/1	0.97	0.16	37,37,37,37	0
56	MG	2A	3373	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	3330	1/1	0.97	0.06	36,36,36,36	0
56	MG	2A	3126	1/1	0.97	0.07	46,46,46,46	0
56	MG	1U	208	1/1	0.97	0.22	30,30,30,30	0
56	MG	1A	3199	1/1	0.97	0.20	25,25,25,25	0
56	MG	1A	4028	1/1	0.97	0.11	31,31,31,31	0
56	MG	1A	3861	1/1	0.97	0.04	37,37,37,37	0
56	MG	1A	3722	1/1	0.97	0.08	27,27,27,27	0
56	MG	1W	201	1/1	0.97	0.12	41,41,41,41	0
56	MG	2A	3382	1/1	0.97	0.10	54,54,54,54	0
56	MG	1A	3200	1/1	0.97	0.06	36,36,36,36	0
56	MG	1A	3260	1/1	0.97	0.08	50,50,50,50	0
56	MG	1W	205	1/1	0.97	0.08	39,39,39,39	0
56	MG	1A	3865	1/1	0.97	0.22	31,31,31,31	0
56	MG	1A	4034	1/1	0.97	0.08	23,23,23,23	0
56	MG	2A	3139	1/1	0.97	0.12	49,49,49,49	0
56	MG	2A	3667	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3119	1/1	0.97	0.10	36,36,36,36	0
56	MG	1A	3120	1/1	0.97	0.30	42,42,42,42	0
56	MG	1X	103	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3868	1/1	0.97	0.20	41,41,41,41	0
56	MG	1X	105	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	4038	1/1	0.97	0.17	63,63,63,63	0
56	MG	1a	1757	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3495	1/1	0.97	0.10	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	3599	1/1	0.97	0.08	42,42,42,42	0
56	MG	1A	3336	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3731	1/1	0.97	0.04	54,54,54,54	0
56	MG	1Y	204	1/1	0.97	0.21	52,52,52,52	0
56	MG	1a	1763	1/1	0.97	0.10	55,55,55,55	0
56	MG	1A	3154	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3155	1/1	0.97	0.27	36,36,36,36	0
56	MG	1A	3073	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3049	1/1	0.97	0.10	33,33,33,33	0
56	MG	1A	3416	1/1	0.97	0.06	50,50,50,50	0
56	MG	2A	3159	1/1	0.97	0.06	38,38,38,38	0
56	MG	2A	3160	1/1	0.97	0.11	47,47,47,47	0
56	MG	1A	3606	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3209	1/1	0.97	0.08	45,45,45,45	0
56	MG	2A	3692	1/1	0.97	0.05	53,53,53,53	0
56	MG	1A	3608	1/1	0.97	0.04	33,33,33,33	0
56	MG	1A	3504	1/1	0.97	0.16	45,45,45,45	0
56	MG	2A	3165	1/1	0.97	0.06	58,58,58,58	0
56	MG	1a	1774	1/1	0.97	0.10	60,60,60,60	0
56	MG	1A	3210	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3746	1/1	0.97	0.10	48,48,48,48	0
56	MG	2a	1664	1/1	0.97	0.15	44,44,44,44	0
56	MG	1A	3076	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	3507	1/1	0.97	0.26	32,32,32,32	0
56	MG	2a	1667	1/1	0.97	0.05	43,43,43,43	0
56	MG	2A	3702	1/1	0.97	0.04	49,49,49,49	0
56	MG	2A	3171	1/1	0.97	0.08	59,59,59,59	0
56	MG	11	101	1/1	0.97	0.29	43,43,43,43	0
56	MG	1A	3888	1/1	0.97	0.07	54,54,54,54	0
56	MG	2A	3708	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3889	1/1	0.97	0.09	25,25,25,25	0
56	MG	2A	3424	1/1	0.97	0.23	51,51,51,51	0
56	MG	1A	3050	1/1	0.97	0.06	22,22,22,22	0
56	MG	11	106	1/1	0.97	0.07	54,54,54,54	0
56	MG	2A	3714	1/1	0.97	0.06	56,56,56,56	0
56	MG	1A	3079	1/1	0.97	0.19	45,45,45,45	0
56	MG	2A	3428	1/1	0.97	0.29	62,62,62,62	0
56	MG	12	102	1/1	0.97	0.11	44,44,44,44	0
56	MG	2A	3179	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3346	1/1	0.97	0.16	32,32,32,32	0
56	MG	2A	3721	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3620	1/1	0.97	0.05	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	3723	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3274	1/1	0.97	0.06	39,39,39,39	0
56	MG	15	101	1/1	0.97	0.16	35,35,35,35	0
56	MG	2A	3435	1/1	0.97	0.20	49,49,49,49	0
56	MG	1A	3161	1/1	0.97	0.36	34,34,34,34	0
56	MG	1A	3624	1/1	0.97	0.08	27,27,27,27	0
56	MG	1A	3039	1/1	0.97	0.31	43,43,43,43	0
56	MG	1A	3218	1/1	0.97	0.16	40,40,40,40	0
56	MG	1A	3900	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3283	1/1	0.97	0.39	32,32,32,32	0
56	MG	2A	3191	1/1	0.97	0.13	56,56,56,56	0
56	MG	2A	3192	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3352	1/1	0.97	0.13	49,49,49,49	0
56	MG	1a	1801	1/1	0.97	0.05	58,58,58,58	0
56	MG	1A	3519	1/1	0.97	0.04	49,49,49,49	0
56	MG	2a	1700	1/1	0.97	0.06	48,48,48,48	0
56	MG	1A	3284	1/1	0.97	0.08	48,48,48,48	0
56	MG	17	101	1/1	0.97	0.15	40,40,40,40	0
56	MG	2A	3199	1/1	0.97	0.07	40,40,40,40	0
56	MG	1A	3521	1/1	0.97	0.08	52,52,52,52	0
56	MG	17	103	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3633	1/1	0.97	0.04	15,15,15,15	0
56	MG	1A	3128	1/1	0.97	0.07	31,31,31,31	0
56	MG	1A	3767	1/1	0.97	0.07	47,47,47,47	0
56	MG	18	102	1/1	0.97	0.09	47,47,47,47	0
56	MG	18	103	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	3912	1/1	0.97	0.06	47,47,47,47	0
56	MG	18	105	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3286	1/1	0.97	0.06	31,31,31,31	0
56	MG	1A	3434	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3637	1/1	0.97	0.05	30,30,30,30	0
56	MG	2a	1716	1/1	0.97	0.11	64,64,64,64	0
56	MG	2A	3464	1/1	0.97	0.20	40,40,40,40	0
56	MG	1A	3772	1/1	0.97	0.11	65,65,65,65	0
56	MG	1A	3773	1/1	0.97	0.11	25,25,25,25	0
56	MG	2A	3757	1/1	0.97	0.07	59,59,59,59	0
56	MG	1A	3220	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	4093	1/1	0.97	0.06	43,43,43,43	0
56	MG	2a	1723	1/1	0.97	0.26	52,52,52,52	0
56	MG	2A	3760	1/1	0.97	0.06	66,66,66,66	0
56	MG	1A	3083	1/1	0.97	0.15	28,28,28,28	0
56	MG	1A	3166	1/1	0.97	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3922	1/1	0.97	0.05	65,65,65,65	0
56	MG	1a	1609	1/1	0.97	0.15	48,48,48,48	0
56	MG	2a	1729	1/1	0.97	0.17	66,66,66,66	0
56	MG	1A	3777	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3927	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3778	1/1	0.97	0.04	29,29,29,29	0
56	MG	1A	3359	1/1	0.97	0.19	59,59,59,59	0
56	MG	1A	3130	1/1	0.97	0.10	38,38,38,38	0
56	MG	1a	1615	1/1	0.97	0.08	53,53,53,53	0
56	MG	2a	1736	1/1	0.97	0.23	57,57,57,57	0
56	MG	2A	3479	1/1	0.97	0.08	47,47,47,47	0
56	MG	1B	205	1/1	0.97	0.10	53,53,53,53	0
56	MG	1A	3933	1/1	0.97	0.11	59,59,59,59	0
56	MG	1A	3643	1/1	0.97	0.06	28,28,28,28	0
56	MG	1B	208	1/1	0.97	0.11	54,54,54,54	0
56	MG	1a	1620	1/1	0.97	0.05	47,47,47,47	0
56	MG	2A	3232	1/1	0.97	0.50	47,47,47,47	0
56	MG	2A	3486	1/1	0.97	0.15	43,43,43,43	0
56	MG	1B	209	1/1	0.97	0.08	52,52,52,52	0
56	MG	1A	3441	1/1	0.97	0.15	40,40,40,40	0
56	MG	1A	3168	1/1	0.97	0.14	59,59,59,59	0
56	MG	1A	3937	1/1	0.97	0.04	43,43,43,43	0
56	MG	2A	3237	1/1	0.97	0.16	47,47,47,47	0
56	MG	2A	3493	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3646	1/1	0.97	0.08	33,33,33,33	0
56	MG	1A	3787	1/1	0.97	0.09	24,24,24,24	0
56	MG	1A	3292	1/1	0.97	0.13	25,25,25,25	0
56	MG	1B	216	1/1	0.97	0.06	58,58,58,58	0
56	MG	1B	217	1/1	0.97	0.09	45,45,45,45	0
56	MG	2a	1756	1/1	0.97	0.09	39,39,39,39	0
56	MG	1A	3226	1/1	0.97	0.07	28,28,28,28	0
56	MG	2A	3501	1/1	0.97	0.09	34,34,34,34	0
56	MG	2a	1759	1/1	0.97	0.10	66,66,66,66	0
56	MG	1A	3534	1/1	0.97	0.04	22,22,22,22	0
56	MG	2A	3245	1/1	0.97	0.11	44,44,44,44	0
56	MG	2A	3796	1/1	0.97	0.07	32,32,32,32	0
56	MG	2A	3246	1/1	0.97	0.13	47,47,47,47	0
56	MG	2A	3799	1/1	0.97	0.16	36,36,36,36	0
56	MG	1a	1633	1/1	0.97	0.12	35,35,35,35	0
56	MG	2a	1766	1/1	0.97	0.17	55,55,55,55	0
56	MG	2A	3803	1/1	0.97	0.06	55,55,55,55	0
56	MG	1A	3535	1/1	0.97	0.15	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	2A	3249	1/1	0.97	0.08	55,55,55,55	0
56	MG	1A	3792	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3445	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3227	1/1	0.97	0.08	23,23,23,23	0
56	MG	1A	3169	1/1	0.97	0.04	39,39,39,39	0
56	MG	1A	3229	1/1	0.97	0.11	47,47,47,47	0
56	MG	1A	3040	1/1	0.97	0.21	28,28,28,28	0
56	MG	1A	3085	1/1	0.97	0.09	34,34,34,34	0
56	MG	2A	3518	1/1	0.97	0.09	54,54,54,54	0
56	MG	1B	228	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3659	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	3172	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3011	1/1	0.97	0.17	42,42,42,42	0
56	MG	2A	3820	1/1	0.97	0.06	54,54,54,54	0
56	MG	1a	1645	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3370	1/1	0.97	0.16	47,47,47,47	0
56	MG	1A	3177	1/1	0.97	0.09	18,18,18,18	0
56	MG	1A	3301	1/1	0.97	0.10	35,35,35,35	0
56	MG	2A	3016	1/1	0.97	0.20	50,50,50,50	0
56	MG	1A	3667	1/1	0.97	0.08	22,22,22,22	0
56	MG	1A	3669	1/1	0.97	0.06	28,28,28,28	0
56	MG	2A	3532	1/1	0.97	0.13	45,45,45,45	0
56	MG	2A	3831	1/1	0.97	0.13	57,57,57,57	0
56	MG	1A	3958	1/1	0.97	0.10	55,55,55,55	0
56	MG	1D	301	1/1	0.97	0.08	32,32,32,32	0
56	MG	2A	3021	1/1	0.97	0.13	46,46,46,46	0
56	MG	1A	3808	1/1	0.97	0.15	24,24,24,24	0
56	MG	1D	303	1/1	0.97	0.14	44,44,44,44	0
56	MG	2A	3276	1/1	0.97	0.24	47,47,47,47	0
56	MG	1A	3546	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3547	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3234	1/1	0.97	0.21	34,34,34,34	0
56	MG	1A	3812	1/1	0.97	0.08	34,34,34,34	0
56	MG	1D	311	1/1	0.97	0.21	33,33,33,33	0
56	MG	1A	3549	1/1	0.97	0.19	35,35,35,35	0
56	MG	1A	3550	1/1	0.97	0.05	29,29,29,29	0
56	MG	1A	3815	1/1	0.97	0.06	42,42,42,42	0
56	MG	2A	3550	1/1	0.97	0.07	30,30,30,30	0
56	MG	1E	301	1/1	0.97	0.17	41,41,41,41	0
56	MG	1A	3551	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3133	1/1	0.97	0.07	43,43,43,43	0
56	MG	2A	3556	1/1	0.97	0.06	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3039	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3458	1/1	0.97	0.09	35,35,35,35	0
56	MG	2A	3041	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3064	1/1	0.97	0.13	46,46,46,46	0
56	MG	1A	3306	1/1	0.97	0.12	45,45,45,45	0
56	MG	2A	3044	1/1	0.97	0.21	50,50,50,50	0
56	MG	1A	3108	1/1	0.97	0.28	27,27,27,27	0
56	MG	1A	3822	1/1	0.97	0.05	43,43,43,43	0
56	MG	1A	3240	1/1	0.97	0.18	32,32,32,32	0
56	MG	1A	3109	1/1	0.97	0.05	36,36,36,36	0
56	MG	1E	315	1/1	0.97	0.04	36,36,36,36	0
56	MG	1F	301	1/1	0.97	0.07	44,44,44,44	0
56	MG	1A	3977	1/1	0.97	0.07	30,30,30,30	0
56	MG	1a	1677	1/1	0.97	0.06	38,38,38,38	0
56	MG	2D	302	1/1	0.97	0.21	51,51,51,51	0
56	MG	2d	302	1/1	0.97	0.06	58,58,58,58	0
56	MG	1A	3311	1/1	0.97	0.05	51,51,51,51	0
56	MG	2f	201	1/1	0.97	0.07	43,43,43,43	0
56	MG	2A	3574	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3561	1/1	0.97	0.06	17,17,17,17	0
56	MG	2A	3576	1/1	0.97	0.08	74,74,74,74	0
56	MG	1F	306	1/1	0.97	0.07	37,37,37,37	0
56	MG	2A	3057	1/1	0.97	0.09	55,55,55,55	0
56	MG	2E	303	1/1	0.97	0.15	49,49,49,49	0
56	MG	2E	304	1/1	0.97	0.18	49,49,49,49	0
56	MG	2E	305	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3138	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3690	1/1	0.97	0.09	28,28,28,28	0
56	MG	2q	202	1/1	0.97	0.05	77,77,77,77	0
56	MG	1A	3010	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	3009	1/1	0.97	0.08	24,24,24,24	0
56	MG	2A	3062	1/1	0.97	0.10	27,27,27,27	0
56	MG	1A	3567	1/1	0.97	0.08	25,25,25,25	0
56	MG	1A	3185	1/1	0.97	0.03	32,32,32,32	0
56	MG	1A	3990	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3386	1/1	0.97	0.21	26,26,26,26	0
56	MG	1A	3696	1/1	0.97	0.09	28,28,28,28	0
56	MG	1A	3470	1/1	0.97	0.13	42,42,42,42	0
56	MG	2F	308	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3994	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3995	1/1	0.97	0.07	28,28,28,28	0
56	MG	2A	3071	1/1	0.97	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3321	1/1	0.97	0.07	62,62,62,62	0
56	MG	1A	3996	1/1	0.97	0.04	25,25,25,25	0
56	MG	1A	3114	1/1	0.97	0.09	36,36,36,36	0
56	MG	1N	201	1/1	0.97	0.14	36,36,36,36	0
56	MG	2A	3075	1/1	0.97	0.12	54,54,54,54	0
56	MG	1N	202	1/1	0.97	0.07	38,38,38,38	0
56	MG	1N	203	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3317	1/1	0.97	0.16	46,46,46,46	0
56	MG	1A	4000	1/1	0.97	0.06	38,38,38,38	0
56	MG	2T	201	1/1	0.97	0.07	61,61,61,61	0
56	MG	1A	3188	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3474	1/1	0.97	0.07	42,42,42,42	0
57	K	1A	3557	1/1	0.97	0.10	64,64,64,64	0
56	MG	1A	3842	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3319	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3192	1/1	0.97	0.28	39,39,39,39	0
56	MG	1A	3145	1/1	0.97	0.09	30,30,30,30	0
56	MG	1P	201	1/1	0.97	0.17	31,31,31,31	0
56	MG	2D	305	1/1	0.98	0.08	25,25,25,25	0
56	MG	1A	3502	1/1	0.98	0.12	32,32,32,32	0
56	MG	17	104	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	4062	1/1	0.98	0.06	31,31,31,31	0
56	MG	2E	301	1/1	0.98	0.05	52,52,52,52	0
56	MG	2A	3258	1/1	0.98	0.07	56,56,56,56	0
56	MG	1A	3391	1/1	0.98	0.08	60,60,60,60	0
56	MG	2A	3260	1/1	0.98	0.05	65,65,65,65	0
56	MG	2A	3549	1/1	0.98	0.07	55,55,55,55	0
56	MG	1A	3082	1/1	0.98	0.10	35,35,35,35	0
56	MG	2A	3551	1/1	0.98	0.05	57,57,57,57	0
56	MG	1A	4065	1/1	0.98	0.14	43,43,43,43	0
56	MG	2A	3263	1/1	0.98	0.04	57,57,57,57	0
56	MG	1A	3239	1/1	0.98	0.21	29,29,29,29	0
56	MG	2A	3716	1/1	0.98	0.13	39,39,39,39	0
56	MG	1A	3046	1/1	0.98	0.05	28,28,28,28	0
56	MG	1A	3710	1/1	0.98	0.15	45,45,45,45	0
56	MG	1a	1717	1/1	0.98	0.11	35,35,35,35	0
56	MG	1A	3568	1/1	0.98	0.32	33,33,33,33	0
56	MG	1A	3056	1/1	0.98	0.03	24,24,24,24	0
56	MG	1A	3033	1/1	0.98	0.17	26,26,26,26	0
56	MG	1A	3452	1/1	0.98	0.15	38,38,38,38	0
56	MG	1H	201	1/1	0.98	0.15	60,60,60,60	0
56	MG	1A	3878	1/1	0.98	0.09	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4074	1/1	0.98	0.05	53,53,53,53	0
56	MG	1A	3796	1/1	0.98	0.04	50,50,50,50	0
56	MG	2A	3568	1/1	0.98	0.07	33,33,33,33	0
56	MG	1A	3572	1/1	0.98	0.05	29,29,29,29	0
56	MG	1A	3510	1/1	0.98	0.19	40,40,40,40	0
56	MG	1A	3574	1/1	0.98	0.03	41,41,41,41	0
56	MG	2A	3417	1/1	0.98	0.23	50,50,50,50	0
56	MG	1A	4079	1/1	0.98	0.05	48,48,48,48	0
56	MG	1A	3162	1/1	0.98	0.21	51,51,51,51	0
56	MG	2R	204	1/1	0.98	0.12	48,48,48,48	0
56	MG	2A	3735	1/1	0.98	0.17	64,64,64,64	0
56	MG	1A	4081	1/1	0.98	0.05	60,60,60,60	0
56	MG	1A	3106	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3802	1/1	0.98	0.05	48,48,48,48	0
56	MG	1A	3721	1/1	0.98	0.05	26,26,26,26	0
56	MG	1a	1735	1/1	0.98	0.09	39,39,39,39	0
56	MG	2A	3580	1/1	0.98	0.06	32,32,32,32	0
56	MG	1A	3202	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3086	1/1	0.98	0.18	31,31,31,31	0
56	MG	2A	3150	1/1	0.98	0.14	39,39,39,39	0
56	MG	1P	203	1/1	0.98	0.21	24,24,24,24	0
56	MG	1A	3515	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3247	1/1	0.98	0.15	37,37,37,37	0
56	MG	20	102	1/1	0.98	0.09	52,52,52,52	0
56	MG	1a	1741	1/1	0.98	0.11	53,53,53,53	0
56	MG	1A	3891	1/1	0.98	0.05	45,45,45,45	0
56	MG	1A	3986	1/1	0.98	0.05	11,11,11,11	0
56	MG	2A	3295	1/1	0.98	0.07	52,52,52,52	0
56	MG	1A	3726	1/1	0.98	0.04	44,44,44,44	0
56	MG	1A	3204	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3058	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	3651	1/1	0.98	0.03	26,26,26,26	0
56	MG	1A	3071	1/1	0.98	0.04	11,11,11,11	0
56	MG	1A	3110	1/1	0.98	0.18	29,29,29,29	0
56	MG	2A	3029	1/1	0.98	0.05	46,46,46,46	0
56	MG	1A	3034	1/1	0.98	0.21	29,29,29,29	0
56	MG	1A	3733	1/1	0.98	0.07	31,31,31,31	0
56	MG	1A	3137	1/1	0.98	0.05	40,40,40,40	0
56	MG	1A	3303	1/1	0.98	0.16	24,24,24,24	0
56	MG	2A	3035	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3999	1/1	0.98	0.04	39,39,39,39	0
56	MG	2a	1768	1/1	0.98	0.09	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	3657	1/1	0.98	0.06	38,38,38,38	0
56	MG	1A	3022	1/1	0.98	0.10	37,37,37,37	0
56	MG	1A	4002	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3211	1/1	0.98	0.10	31,31,31,31	0
56	MG	1A	3739	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3660	1/1	0.98	0.05	22,22,22,22	0
56	MG	2A	3771	1/1	0.98	0.09	41,41,41,41	0
56	MG	1A	3139	1/1	0.98	0.12	36,36,36,36	0
56	MG	1U	206	1/1	0.98	0.25	35,35,35,35	0
56	MG	1A	3742	1/1	0.98	0.05	41,41,41,41	0
56	MG	1a	1765	1/1	0.98	0.07	53,53,53,53	0
56	MG	1A	3911	1/1	0.98	0.08	48,48,48,48	0
56	MG	2A	3460	1/1	0.98	0.14	25,25,25,25	0
56	MG	1A	3307	1/1	0.98	0.08	39,39,39,39	0
56	MG	1A	3744	1/1	0.98	0.03	20,20,20,20	0
56	MG	2A	3620	1/1	0.98	0.05	37,37,37,37	0
56	MG	1V	202	1/1	0.98	0.19	31,31,31,31	0
56	MG	2A	3051	1/1	0.98	0.17	49,49,49,49	0
56	MG	1V	203	1/1	0.98	0.08	28,28,28,28	0
56	MG	2A	3624	1/1	0.98	0.04	49,49,49,49	0
56	MG	1V	204	1/1	0.98	0.11	39,39,39,39	0
56	MG	1A	3113	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3173	1/1	0.98	0.31	33,33,33,33	0
56	MG	1A	3215	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3668	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	3174	1/1	0.98	0.14	25,25,25,25	0
56	MG	1W	204	1/1	0.98	0.14	37,37,37,37	0
56	MG	2A	3792	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3832	1/1	0.98	0.08	38,38,38,38	0
56	MG	1A	4017	1/1	0.98	0.03	24,24,24,24	0
56	MG	1A	4018	1/1	0.98	0.05	53,53,53,53	0
56	MG	2A	3197	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3175	1/1	0.98	0.04	30,30,30,30	0
56	MG	1A	3834	1/1	0.98	0.04	59,59,59,59	0
56	MG	2A	3800	1/1	0.98	0.07	40,40,40,40	0
56	MG	1A	3925	1/1	0.98	0.06	35,35,35,35	0
56	MG	2A	3802	1/1	0.98	0.06	53,53,53,53	0
56	MG	1A	3751	1/1	0.98	0.06	40,40,40,40	0
56	MG	1a	1785	1/1	0.98	0.05	52,52,52,52	0
56	MG	2A	3203	1/1	0.98	0.04	52,52,52,52	0
56	MG	1A	3008	1/1	0.98	0.08	25,25,25,25	0
56	MG	1a	1787	1/1	0.98	0.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3928	1/1	0.98	0.04	57,57,57,57	0
56	MG	1A	3092	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3930	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	3021	1/1	0.98	0.06	30,30,30,30	0
56	MG	2A	3812	1/1	0.98	0.05	34,34,34,34	0
56	MG	1a	1792	1/1	0.98	0.05	60,60,60,60	0
56	MG	2A	3490	1/1	0.98	0.08	61,61,61,61	0
56	MG	1A	3421	1/1	0.98	0.13	44,44,44,44	0
56	MG	2A	3816	1/1	0.98	0.08	64,64,64,64	0
56	MG	1a	1794	1/1	0.98	0.07	58,58,58,58	0
56	MG	1A	3117	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3266	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	3077	1/1	0.98	0.03	27,27,27,27	0
56	MG	1A	3038	1/1	0.98	0.10	24,24,24,24	0
56	MG	1A	3045	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3097	1/1	0.98	0.10	32,32,32,32	0
56	MG	1A	3098	1/1	0.98	0.10	19,19,19,19	0
56	MG	1a	1676	1/1	0.98	0.14	52,52,52,52	0
56	MG	1D	305	1/1	0.98	0.07	18,18,18,18	0
56	MG	2A	3827	1/1	0.98	0.12	55,55,55,55	0
56	MG	2A	3828	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3186	1/1	0.98	0.14	38,38,38,38	0
56	MG	1D	307	1/1	0.98	0.14	28,28,28,28	0
56	MG	2A	3088	1/1	0.98	0.13	32,32,32,32	0
56	MG	1A	3611	1/1	0.98	0.09	28,28,28,28	0
56	MG	1A	3612	1/1	0.98	0.06	53,53,53,53	0
56	MG	2A	3509	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	3273	1/1	0.98	0.07	29,29,29,29	0
56	MG	2A	3511	1/1	0.98	0.05	47,47,47,47	0
56	MG	1A	3152	1/1	0.98	0.09	32,32,32,32	0
56	MG	1A	3769	1/1	0.98	0.06	25,25,25,25	0
56	MG	2A	3839	1/1	0.98	0.15	42,42,42,42	0
56	MG	2A	3094	1/1	0.98	0.06	49,49,49,49	0
56	MG	1A	3153	1/1	0.98	0.09	36,36,36,36	0
56	MG	1A	3189	1/1	0.98	0.07	37,37,37,37	0
56	MG	11	104	1/1	0.98	0.04	43,43,43,43	0
56	MG	1A	4044	1/1	0.98	0.03	22,22,22,22	0
56	MG	1A	3277	1/1	0.98	0.06	33,33,33,33	0
56	MG	2A	3677	1/1	0.98	0.04	33,33,33,33	0
56	MG	1E	304	1/1	0.98	0.11	27,27,27,27	0
56	MG	1E	305	1/1	0.98	0.17	33,33,33,33	0
56	MG	13	101	1/1	0.98	0.04	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3278	1/1	0.98	0.14	24,24,24,24	0
56	MG	1A	4047	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3279	1/1	0.98	0.10	34,34,34,34	0
56	MG	2A	3527	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	4049	1/1	0.98	0.05	10,10,10,10	0
56	MG	1E	311	1/1	0.98	0.12	22,22,22,22	0
56	MG	2A	3108	1/1	0.98	0.12	58,58,58,58	0
56	MG	1A	3280	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3190	1/1	0.98	0.21	42,42,42,42	0
56	MG	1A	3623	1/1	0.98	0.05	18,18,18,18	0
56	MG	1A	3440	1/1	0.98	0.14	43,43,43,43	0
56	MG	1A	4055	1/1	0.98	0.05	28,28,28,28	0
56	MG	2A	3694	1/1	0.98	0.06	35,35,35,35	0
56	MG	1A	3282	1/1	0.98	0.17	30,30,30,30	0
56	MG	1A	3123	1/1	0.98	0.14	35,35,35,35	0
56	MG	1A	3099	1/1	0.98	0.06	42,42,42,42	0
56	MG	2A	3540	1/1	0.98	0.11	40,40,40,40	0
56	MG	1A	3080	1/1	0.98	0.04	23,23,23,23	0
59	ZN	2Y	501	1/1	0.98	0.04	95,95,95,95	0
56	MG	1A	3065	1/1	0.98	0.08	37,37,37,37	0
56	MG	2A	3553	1/1	0.99	0.06	41,41,41,41	0
56	MG	1A	3074	1/1	0.99	0.04	16,16,16,16	0
56	MG	1A	3191	1/1	0.99	0.08	42,42,42,42	0
56	MG	1A	3484	1/1	0.99	0.18	38,38,38,38	0
56	MG	1F	309	1/1	0.99	0.12	31,31,31,31	0
56	MG	1A	3923	1/1	0.99	0.07	32,32,32,32	0
56	MG	1A	3924	1/1	0.99	0.04	40,40,40,40	0
56	MG	1A	3670	1/1	0.99	0.04	27,27,27,27	0
56	MG	1A	3014	1/1	0.99	0.04	28,28,28,28	0
56	MG	1A	3140	1/1	0.99	0.04	16,16,16,16	0
56	MG	2A	3686	1/1	0.99	0.03	64,64,64,64	0
56	MG	2A	3563	1/1	0.99	0.08	39,39,39,39	0
56	MG	1A	3012	1/1	0.99	0.04	30,30,30,30	0
56	MG	2A	3505	1/1	0.99	0.04	40,40,40,40	0
56	MG	1A	3003	1/1	0.99	0.06	23,23,23,23	0
56	MG	2A	3023	1/1	0.99	0.04	38,38,38,38	0
56	MG	1A	3675	1/1	0.99	0.08	20,20,20,20	0
56	MG	2A	3129	1/1	0.99	0.06	37,37,37,37	0
56	MG	1A	4050	1/1	0.99	0.08	24,24,24,24	0
56	MG	1A	3626	1/1	0.99	0.04	44,44,44,44	0
56	MG	1A	3765	1/1	0.99	0.03	38,38,38,38	0
56	MG	1A	3677	1/1	0.99	0.03	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	15	104	1/1	0.99	0.28	29,29,29,29	0
56	MG	2A	3188	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3582	1/1	0.99	0.13	33,33,33,33	0
56	MG	2A	3031	1/1	0.99	0.11	34,34,34,34	0
56	MG	1a	1630	1/1	0.99	0.20	45,45,45,45	0
56	MG	1A	3070	1/1	0.99	0.10	17,17,17,17	0
56	MG	1A	3973	1/1	0.99	0.09	19,19,19,19	0
56	MG	2A	3705	1/1	0.99	0.10	33,33,33,33	0
56	MG	2A	3521	1/1	0.99	0.08	41,41,41,41	0
56	MG	2A	3707	1/1	0.99	0.07	39,39,39,39	0
56	MG	1D	308	1/1	0.99	0.08	32,32,32,32	0
56	MG	1A	3680	1/1	0.99	0.06	27,27,27,27	0
56	MG	2A	3710	1/1	0.99	0.05	37,37,37,37	0
56	MG	1A	3144	1/1	0.99	0.13	24,24,24,24	0
56	MG	1A	3564	1/1	0.99	0.18	39,39,39,39	0
56	MG	1A	3390	1/1	0.99	0.13	30,30,30,30	0
56	MG	1A	3566	1/1	0.99	0.11	36,36,36,36	0
56	MG	1A	3903	1/1	0.99	0.04	23,23,23,23	0
56	MG	1A	3904	1/1	0.99	0.04	35,35,35,35	0
56	MG	2X	102	1/1	0.99	0.08	51,51,51,51	0
56	MG	1A	3222	1/1	0.99	0.10	32,32,32,32	0
56	MG	1A	3871	1/1	0.99	0.03	26,26,26,26	0
56	MG	1A	3983	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3023	1/1	0.99	0.03	12,12,12,12	0
56	MG	1P	204	1/1	0.99	0.03	40,40,40,40	0
56	MG	1A	3176	1/1	0.99	0.10	27,27,27,27	0
56	MG	2A	3597	1/1	0.99	0.14	66,66,66,66	0
56	MG	1E	307	1/1	0.99	0.06	25,25,25,25	0
56	MG	1A	3238	1/1	0.99	0.08	32,32,32,32	0
56	MG	1A	3032	1/1	0.99	0.12	27,27,27,27	0
56	MG	2A	3539	1/1	0.99	0.08	31,31,31,31	0
56	MG	1A	3988	1/1	0.99	0.08	23,23,23,23	0
56	MG	1A	3989	1/1	0.99	0.05	38,38,38,38	0
56	MG	1A	3615	1/1	0.99	0.10	29,29,29,29	0
56	MG	1A	3380	1/1	0.99	0.22	29,29,29,29	0
56	MG	1A	3663	1/1	0.99	0.02	34,34,34,34	0
56	MG	2A	3798	1/1	0.99	0.03	45,45,45,45	0
56	MG	1A	3048	1/1	0.99	0.09	37,37,37,37	0
56	MG	1A	3665	1/1	0.99	0.06	22,22,22,22	0
56	MG	1F	302	1/1	0.99	0.15	26,26,26,26	0
56	MG	1a	1756	1/1	0.99	0.06	55,55,55,55	0
56	MG	1A	3430	1/1	0.99	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	ZN	1Y	206	1/1	0.99	0.03	75,75,75,75	0
56	MG	1A	3785	1/1	0.99	0.03	17,17,17,17	0
59	ZN	1n	103	1/1	0.99	0.03	66,66,66,66	0
56	MG	1A	3786	1/1	0.99	0.04	17,17,17,17	0
56	MG	2A	3494	1/1	0.99	0.07	48,48,48,48	0
59	ZN	29	501	1/1	0.99	0.03	72,72,72,72	0
59	ZN	2n	501	1/1	0.99	0.03	84,84,84,84	0
60	SF4	1d	302	8/8	0.99	0.04	60,64,69,72	0
60	SF4	2d	303	8/8	0.99	0.04	52,65,72,78	0
59	ZN	19	102	1/1	1.00	0.03	42,42,42,42	0
56	MG	1A	3920	1/1	1.00	0.02	13,13,13,13	0
56	MG	1A	3610	1/1	1.00	0.05	32,32,32,32	0
56	MG	1A	3713	1/1	1.00	0.05	17,17,17,17	0
59	ZN	25	107	1/1	1.00	0.05	55,55,55,55	0
59	ZN	26	102	1/1	1.00	0.03	61,61,61,61	0
56	MG	1Q	202	1/1	1.00	0.02	31,31,31,31	0
56	MG	2A	3581	1/1	1.00	0.02	39,39,39,39	0
59	ZN	15	111	1/1	1.00	0.07	47,47,47,47	0
59	ZN	16	102	1/1	1.00	0.02	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.