wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 07:08 AM EST

PDB ID	:	6ND5
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with chloramphenicol and bound to mRNA and A-, P-, and E-site tRNAs at 2.60A resolution
Authors	:	Svetlov, M.S.; Plessa, E.; Chen, C.-W.; Bougas, A.; Krokidis, M.G.; Dinos, G.P.; Polikanov, Y.S.
Deposited on	:	2018-12-13
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:

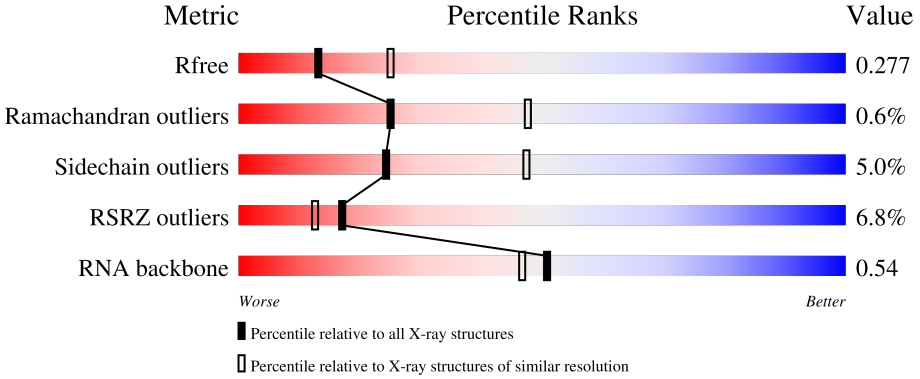
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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	2% 82% 16% •
1	2A	2915	2% 79% 17% •
2	1B	121	89% 9% ••
2	2B	121	70% 29% •
3	1D	276	2% 94% 6%

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Mol	Chain	Length	Quality of chain
3	2D	276	4% 94% 5%
4	1E	206	% 92% 7%
4	2E	206	3% 95%
5	1F	210	90% 7%
5	2F	210	3% 90% 7%
6	1G	182	% 96%
6	2G	182	13% 91% 8%
7	1H	180	92%
7	2H	180	26% 93%
8	1I	148	% 95%
8	2I	148	7% 93% 6%
9	1N	140	% 95% 5%
9	2N	140	21% 97%
10	1O	122	98%
10	2O	122	4% 98%
11	1P	150	3% 96%
11	2P	150	30% 97%
12	1Q	141	% 96%
12	2Q	141	11% 98%
13	1R	118	91% 9%
13	2R	118	91% 9%
14	1S	112	95%
14	2S	112	9% 97%
15	1T	146	87% 10%
15	2T	146	3% 88% 10%

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Mol	Chain	Length	Quality of chain
16	1U	118	%, 95%
16	2U	118	14%, 96%
17	1V	101	89%, 10%
17	2V	101	14%, 91%, 8%
18	1W	113	95%
18	2W	113	2%, 96%
19	1X	96	97%
19	2X	96	3%, 97%
20	1Y	110	92%, 5%
20	2Y	110	15%, 93%, 5%
21	1Z	206	71%, 25%
21	2Z	206	2%, 77%, 22%
22	10	85	8%, 94%
22	20	85	22%, 96%
23	11	98	2%, 94%, 5%
23	21	98	16%, 95%
24	12	72	%, 94%
24	22	72	%, 97%
25	13	60	2%, 93%, 5%
25	23	60	45%, 95%
26	14	71	83%, 13%
26	24	71	10%, 92%, 6%
27	15	60	2%, 93%, 5%
27	25	60	3%, 95%
28	16	54	94%

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Mol	Chain	Length	Quality of chain
28	26	54	19% 94%
29	17	49	6% 88% 10%
29	27	49	14% 88% 10%
30	18	65	3% 92% 6%
30	28	65	26% 95%
31	19	37	97%
31	29	37	30% 95% 5%
32	1a	1521	2% 82% 16%
32	2a	1521	3% 79% 19%
33	1b	256	3% 85% 5% 10%
33	2b	256	25% 85% 5% 10%
34	1c	239	15% 84% 14%
34	2c	239	38% 83% 14%
35	1d	209	6% 93% 6%
35	2d	209	% 94% 6%
36	1e	162	2% 88% 9%
36	2e	162	12% 90% 9%
37	1f	101	94% 5%
37	2f	101	2% 96%
38	1g	156	12% 95%
38	2g	156	21% 96%
39	1h	138	4% 95%
39	2h	138	8% 95%
40	1i	128	8% 97%
40	2i	128	44% 95%

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Mol	Chain	Length	Quality of chain
41	1j	105	14% 86% 7% 8%
41	2j	105	46% 82% 10% 9%
42	1k	129	13% 85% • 12%
42	2k	129	17% 86% • 12%
43	1l	132	2% 88% 5% 8%
43	2l	132	9% 89% • 8%
44	1m	126	4% 96% • •
44	2m	126	34% 92% 5% •
45	1n	61	20% 90% 8% •
45	2n	61	72% 90% 8% •
46	1o	89	2% 98% ••
46	2o	89	4% 98% ••
47	1p	88	6% 90% • 7%
47	2p	88	89% 5% 7%
48	1q	105	2% 90% 5% 6%
48	2q	105	16% 93% • 6%
49	1r	88	7% 74% • 23%
49	2r	88	7% 73% 5% 23%
50	1s	93	88% • 11%
50	2s	93	29% 83% 6% 11%
51	1t	106	6% 84% 7% 9%
51	2t	106	10% 88% • 9%
52	1u	27	11% 81% • 15%
52	2u	27	41% 85% 15%
53	1v	24	21% 46% 8% 46%

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Mol	Chain	Length	Quality of chain
53	2v	24	21% 38% 17% 46%
54	1w	76	25% 58% 37%
54	1y	76	24% 63% 32%
54	2w	76	51% 58% 36% 5%
54	2y	76	43% 59% 34%
55	1x	77	% 79% 17%
55	2x	77	% 75% 23%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	PSU	2y	55	-	-	-	X
56	MG	1A	3411	-	-	-	X
56	MG	1A	3489	-	-	-	X
56	MG	1A	3503	-	-	-	X
56	MG	2A	3040	-	-	-	X
56	MG	2A	3243	-	-	-	X
56	MG	2A	3382	-	-	-	X
56	MG	2A	3812	-	-	-	X
56	MG	2a	3031	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 300833 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	15	59	455	285	89	76	5	0	0	0
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
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
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
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
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 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-site and E-site tRNAs.

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 tRNA.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1A	1101	1101	1101	0	0
56	1B	39	39	39	0	0
56	1D	13	13	13	0	0
56	1E	15	15	15	0	0
56	1F	10	10	10	0	0
56	1G	4	4	4	0	0
56	1I	1	1	1	0	0
56	1N	6	6	6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1O	5	5	5	0	0
56	1P	9	9	9	0	0
56	1Q	8	8	8	0	0
56	1R	3	3	3	0	0
56	1S	3	3	3	0	0
56	1T	4	4	4	0	0
56	1U	12	12	12	0	0
56	1V	7	7	7	0	0
56	1W	5	5	5	0	0
56	1X	5	5	5	0	0
56	1Y	3	3	3	0	0
56	1Z	3	3	3	0	0
56	10	6	6	6	0	0
56	11	5	5	5	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	5	5	5	0	0
56	16	3	3	3	0	0
56	17	8	8	8	0	0
56	18	7	7	7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	19	1	1	1	0	0
56	1a	233	233	233	0	0
56	1b	2	2	2	0	0
56	1d	1	1	1	0	0
56	1e	2	2	2	0	0
56	1f	2	2	2	0	0
56	1h	1	1	1	0	0
56	1l	2	2	2	0	0
56	1m	2	2	2	0	0
56	1n	1	1	1	0	0
56	1s	1	1	1	0	0
56	1t	1	1	1	0	0
56	1v	1	1	1	0	0
56	1w	12	12	12	0	0
56	1x	18	18	18	0	0
56	2A	887	887	887	0	0
56	2B	20	20	20	0	0
56	2D	10	10	10	0	0
56	2E	4	4	4	0	0
56	2F	6	6	6	0	0
56	2G	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	2N	1	1	1	0	0
56	2O	1	1	1	0	0
56	2P	4	4	4	0	0
56	2Q	4	4	4	0	0
56	2R	2	2	2	0	0
56	2T	4	4	4	0	0
56	2U	3	3	3	0	0
56	2V	3	3	3	0	0
56	2W	3	3	3	0	0
56	2X	1	1	1	0	0
56	2Z	1	1	1	0	0
56	20	3	3	3	0	0
56	21	1	1	1	0	0
56	23	3	3	3	0	0
56	25	5	5	5	0	0
56	27	2	2	2	0	0
56	28	3	3	3	0	0
56	2a	241	241	241	0	0
56	2d	1	1	1	0	0
56	2e	1	1	1	0	0
56	2f	2	2	2	0	0

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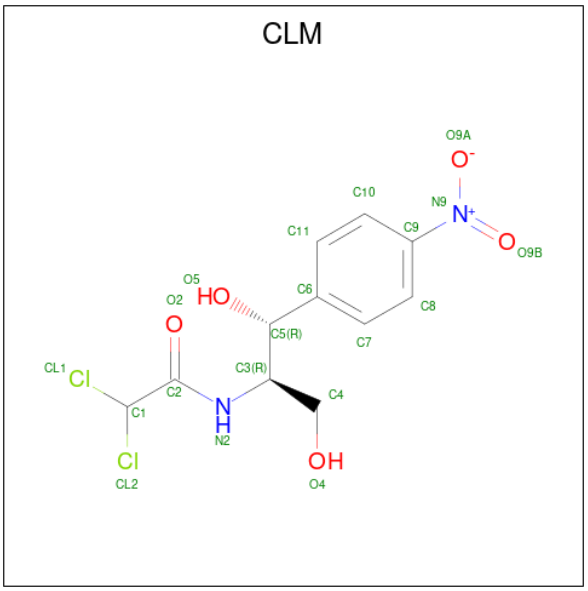
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	2g	1	1	1	0	0
56	2i	1	1	1	0	0
56	2j	1	1	1	0	0
56	2k	1	1	1	0	0
56	2l	4	4	4	0	0
56	2m	1	1	1	0	0
56	2q	2	2	2	0	0
56	2r	1	1	1	0	0
56	2t	1	1	1	0	0
56	2v	1	1	1	0	0
56	2w	4	4	4	0	0
56	2x	5	5	5	0	0
56	2y	6	6	6	0	0

- Molecule 57 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
57	1A	1	20	11	2	2	5	0	0
57	2A	1	20	11	2	2	5	0	0

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
59	1Y	1	1	1	0	0
59	14	1	1	1	0	0
59	15	1	1	1	0	0
59	16	1	1	1	0	0
59	19	1	1	1	0	0

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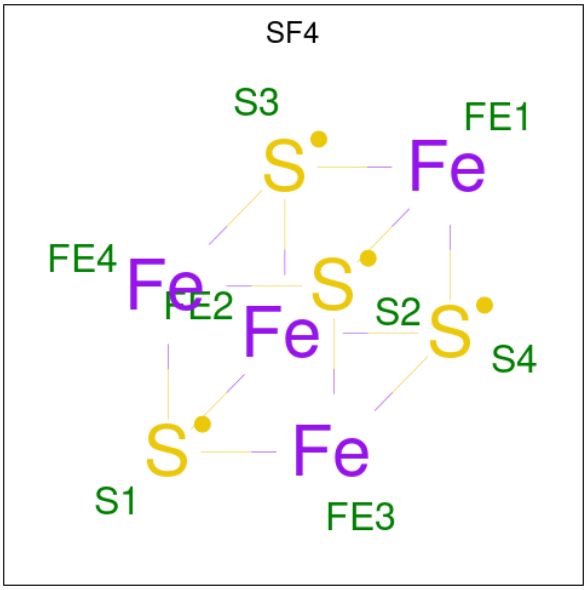
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
59	1n	1	1	1	0	0
59	2Y	1	1	1	0	0
59	24	1	1	1	0	0
59	25	1	1	1	0	0
59	26	1	1	1	0	0
59	29	1	1	1	0	0
59	2n	1	1	1	0	0

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	6	Total O 6 6	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	3	Total O 3 3	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	6	Total O 6 6	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	6	Total O 6 6	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	6	Total O 6 6	0	0
61	1A	500	Total O 500 500	0	0
61	1B	3	Total O 3 3	0	0
61	1B	1	Total O 1 1	0	0
61	1B	5	Total O 5 5	0	0
61	1B	4	Total O 4 4	0	0
61	1B	3	Total O 3 3	0	0
61	1B	1	Total O 1 1	0	0
61	1B	1	Total O 1 1	0	0
61	1B	1	Total O 1 1	0	0
61	1B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1B	1	Total O 1 1	0	0
61	1B	2	Total O 2 2	0	0
61	1B	2	Total O 2 2	0	0
61	1B	1	Total O 1 1	0	0
61	1B	2	Total O 2 2	0	0
61	1B	1	Total O 1 1	0	0
61	1B	6	Total O 6 6	0	0
61	1B	1	Total O 1 1	0	0
61	1B	2	Total O 2 2	0	0
61	1B	1	Total O 1 1	0	0
61	1B	1	Total O 1 1	0	0
61	1B	3	Total O 3 3	0	0
61	1B	2	Total O 2 2	0	0
61	1B	1	Total O 1 1	0	0
61	1B	2	Total O 2 2	0	0
61	1B	1	Total O 1 1	0	0
61	1B	3	Total O 3 3	0	0
61	1B	5	Total O 5 5	0	0
61	1B	16	Total O 16 16	0	0
61	1D	5	Total O 5 5	0	0
61	1D	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1D	1	Total O 1 1	0	0
61	1D	1	Total O 1 1	0	0
61	1D	15	Total O 15 15	0	0
61	1E	2	Total O 2 2	0	0
61	1E	2	Total O 2 2	0	0
61	1E	2	Total O 2 2	0	0
61	1E	2	Total O 2 2	0	0
61	1E	6	Total O 6 6	0	0
61	1E	13	Total O 13 13	0	0
61	1F	1	Total O 1 1	0	0
61	1F	8	Total O 8 8	0	0
61	1G	2	Total O 2 2	0	0
61	1G	3	Total O 3 3	0	0
61	1H	1	Total O 1 1	0	0
61	1I	2	Total O 2 2	0	0
61	1N	4	Total O 4 4	0	0
61	1O	2	Total O 2 2	0	0
61	1O	1	Total O 1 1	0	0
61	1O	4	Total O 4 4	0	0
61	1P	5	Total O 5 5	0	0
61	1P	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1P	2	Total O 2 2	0	0
61	1P	1	Total O 1 1	0	0
61	1P	6	Total O 6 6	0	0
61	1P	5	Total O 5 5	0	0
61	1Q	6	Total O 6 6	0	0
61	1Q	1	Total O 1 1	0	0
61	1Q	4	Total O 4 4	0	0
61	1R	1	Total O 1 1	0	0
61	1R	7	Total O 7 7	0	0
61	1S	2	Total O 2 2	0	0
61	1S	2	Total O 2 2	0	0
61	1T	1	Total O 1 1	0	0
61	1T	1	Total O 1 1	0	0
61	1T	4	Total O 4 4	0	0
61	1U	9	Total O 9 9	0	0
61	1V	1	Total O 1 1	0	0
61	1V	6	Total O 6 6	0	0
61	1W	9	Total O 9 9	0	0
61	1X	4	Total O 4 4	0	0
61	1X	3	Total O 3 3	0	0
61	1Y	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1Z	1	Total O 1 1	0	0
61	10	3	Total O 3 3	0	0
61	10	2	Total O 2 2	0	0
61	10	7	Total O 7 7	0	0
61	11	1	Total O 1 1	0	0
61	11	1	Total O 1 1	0	0
61	11	8	Total O 8 8	0	0
61	12	4	Total O 4 4	0	0
61	13	1	Total O 1 1	0	0
61	13	3	Total O 3 3	0	0
61	14	2	Total O 2 2	0	0
61	15	2	Total O 2 2	0	0
61	15	5	Total O 5 5	0	0
61	16	1	Total O 1 1	0	0
61	17	2	Total O 2 2	0	0
61	17	5	Total O 5 5	0	0
61	18	5	Total O 5 5	0	0
61	18	2	Total O 2 2	0	0
61	18	1	Total O 1 1	0	0
61	18	2	Total O 2 2	0	0
61	18	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	18	3	Total O 3 3	0	0
61	1a	2	Total O 2 2	0	0
61	1a	3	Total O 3 3	0	0
61	1a	4	Total O 4 4	0	0
61	1a	1	Total O 1 1	0	0
61	1a	2	Total O 2 2	0	0
61	1a	2	Total O 2 2	0	0
61	1a	1	Total O 1 1	0	0
61	1a	5	Total O 5 5	0	0
61	1a	4	Total O 4 4	0	0
61	1a	4	Total O 4 4	0	0
61	1a	5	Total O 5 5	0	0
61	1a	4	Total O 4 4	0	0
61	1a	4	Total O 4 4	0	0
61	1a	1	Total O 1 1	0	0
61	1a	2	Total O 2 2	0	0
61	1a	1	Total O 1 1	0	0
61	1a	3	Total O 3 3	0	0
61	1a	2	Total O 2 2	0	0
61	1a	3	Total O 3 3	0	0
61	1a	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1a	6	Total O 6 6	0	0
61	1a	3	Total O 3 3	0	0
61	1a	5	Total O 5 5	0	0
61	1a	5	Total O 5 5	0	0
61	1a	3	Total O 3 3	0	0
61	1a	1	Total O 1 1	0	0
61	1a	5	Total O 5 5	0	0
61	1a	2	Total O 2 2	0	0
61	1a	4	Total O 4 4	0	0
61	1a	1	Total O 1 1	0	0
61	1a	1	Total O 1 1	0	0
61	1a	6	Total O 6 6	0	0
61	1a	5	Total O 5 5	0	0
61	1a	4	Total O 4 4	0	0
61	1a	1	Total O 1 1	0	0
61	1a	4	Total O 4 4	0	0
61	1a	2	Total O 2 2	0	0
61	1a	1	Total O 1 1	0	0
61	1a	1	Total O 1 1	0	0
61	1a	1	Total O 1 1	0	0
61	1a	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1a	3	Total O 3 3	0	0
61	1a	1	Total O 1 1	0	0
61	1a	6	Total O 6 6	0	0
61	1a	3	Total O 3 3	0	0
61	1a	1	Total O 1 1	0	0
61	1a	3	Total O 3 3	0	0
61	1a	1	Total O 1 1	0	0
61	1a	4	Total O 4 4	0	0
61	1a	4	Total O 4 4	0	0
61	1a	6	Total O 6 6	0	0
61	1a	5	Total O 5 5	0	0
61	1a	5	Total O 5 5	0	0
61	1a	5	Total O 5 5	0	0
61	1a	5	Total O 5 5	0	0
61	1a	6	Total O 6 6	0	0
61	1a	4	Total O 4 4	0	0
61	1a	4	Total O 4 4	0	0
61	1a	6	Total O 6 6	0	0
61	1a	4	Total O 4 4	0	0
61	1a	4	Total O 4 4	0	0
61	1a	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1a	4	Total O 4 4	0	0
61	1a	6	Total O 6 6	0	0
61	1a	4	Total O 4 4	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	5	Total O 5 5	0	0
61	1a	4	Total O 4 4	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	2	Total O 2 2	0	0
61	1a	4	Total O 4 4	0	0
61	1a	5	Total O 5 5	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1a	4	Total O 4 4	0	0
61	1a	6	Total O 6 6	0	0
61	1a	5	Total O 5 5	0	0
61	1a	6	Total O 6 6	0	0
61	1a	2	Total O 2 2	0	0
61	1a	1	Total O 1 1	0	0
61	1a	1	Total O 1 1	0	0
61	1a	1	Total O 1 1	0	0
61	1a	2	Total O 2 2	0	0
61	1a	1	Total O 1 1	0	0
61	1a	1	Total O 1 1	0	0
61	1a	2	Total O 2 2	0	0
61	1a	1	Total O 1 1	0	0
61	1a	78	Total O 78 78	0	0
61	1b	1	Total O 1 1	0	0
61	1d	1	Total O 1 1	0	0
61	1f	1	Total O 1 1	0	0
61	1l	6	Total O 6 6	0	0
61	1l	1	Total O 1 1	0	0
61	1q	4	Total O 4 4	0	0
61	1w	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1w	1	Total O 1 1	0	0
61	1w	9	Total O 9 9	0	0
61	1x	3	Total O 3 3	0	0
61	1x	2	Total O 2 2	0	0
61	1x	1	Total O 1 1	0	0
61	1x	2	Total O 2 2	0	0
61	1x	1	Total O 1 1	0	0
61	1x	1	Total O 1 1	0	0
61	1x	5	Total O 5 5	0	0
61	1y	1	Total O 1 1	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	6	Total O 6 6	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	5	Total O 5 5	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	2	Total O 2 2	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	6	Total O 6 6	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0
61	2A	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	6	Total O 6 6	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0
61	2A	5	Total O 5 5	0	0
61	2A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	6	Total O 6 6	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	3	Total O 3 3	0	0
61	2A	6	Total O 6 6	0	0
61	2A	2	Total O 2 2	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	2	Total O 2 2	0	0
61	2A	6	Total O 6 6	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	6	Total O 6 6	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	6	Total O 6 6	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	2	Total O 2 2	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0
61	2A	3	Total O 3 3	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	6	Total O 6 6	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	6	Total O 6 6	0	0
61	2A	222	Total O 222 222	0	0
61	2B	2	Total O 2 2	0	0
61	2B	3	Total O 3 3	0	0
61	2B	3	Total O 3 3	0	0
61	2B	1	Total O 1 1	0	0
61	2B	2	Total O 2 2	0	0
61	2B	1	Total O 1 1	0	0
61	2B	1	Total O 1 1	0	0
61	2B	12	Total O 12 12	0	0
61	2D	5	Total O 5 5	0	0
61	2D	3	Total O 3 3	0	0
61	2D	2	Total O 2 2	0	0
61	2D	7	Total O 7 7	0	0
61	2E	3	Total O 3 3	0	0
61	2F	6	Total O 6 6	0	0
61	2I	3	Total O 3 3	0	0
61	2N	1	Total O 1 1	0	0
61	2O	1	Total O 1 1	0	0
61	2P	5	Total O 5 5	0	0
61	2P	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2P	4	Total O 4 4	0	0
61	2Q	1	Total O 1 1	0	0
61	2Q	1	Total O 1 1	0	0
61	2R	1	Total O 1 1	0	0
61	2R	2	Total O 2 2	0	0
61	2T	2	Total O 2 2	0	0
61	2T	3	Total O 3 3	0	0
61	2U	2	Total O 2 2	0	0
61	2W	3	Total O 3 3	0	0
61	2Z	1	Total O 1 1	0	0
61	20	6	Total O 6 6	0	0
61	20	2	Total O 2 2	0	0
61	20	2	Total O 2 2	0	0
61	21	6	Total O 6 6	0	0
61	22	1	Total O 1 1	0	0
61	25	4	Total O 4 4	0	0
61	27	1	Total O 1 1	0	0
61	27	1	Total O 1 1	0	0
61	28	4	Total O 4 4	0	0
61	28	1	Total O 1 1	0	0
61	28	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	29	1	Total O 1 1	0	0
61	2a	6	Total O 6 6	0	0
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	5	Total O 5 5	0	0
61	2a	4	Total O 4 4	0	0
61	2a	6	Total O 6 6	0	0
61	2a	6	Total O 6 6	0	0
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	5	Total O 5 5	0	0
61	2a	3	Total O 3 3	0	0
61	2a	5	Total O 5 5	0	0
61	2a	4	Total O 4 4	0	0
61	2a	6	Total O 6 6	0	0
61	2a	3	Total O 3 3	0	0
61	2a	5	Total O 5 5	0	0
61	2a	6	Total O 6 6	0	0
61	2a	4	Total O 4 4	0	0
61	2a	4	Total O 4 4	0	0
61	2a	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	3	Total O 3 3	0	0
61	2a	6	Total O 6 6	0	0
61	2a	3	Total O 3 3	0	0
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	4	Total O 4 4	0	0
61	2a	3	Total O 3 3	0	0
61	2a	5	Total O 5 5	0	0
61	2a	6	Total O 6 6	0	0
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	5	Total O 5 5	0	0
61	2a	2	Total O 2 2	0	0
61	2a	4	Total O 4 4	0	0
61	2a	6	Total O 6 6	0	0
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	5	Total O 5 5	0	0
61	2a	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2a	5	Total O 5 5	0	0
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	6	Total O 6 6	0	0
61	2a	3	Total O 3 3	0	0
61	2a	6	Total O 6 6	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0
61	2a	3	Total O 3 3	0	0
61	2a	2	Total O 2 2	0	0
61	2a	5	Total O 5 5	0	0
61	2a	4	Total O 4 4	0	0
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	5	Total O 5 5	0	0
61	2a	1	Total O 1 1	0	0
61	2a	4	Total O 4 4	0	0
61	2a	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	3	Total O 3 3	0	0
61	2a	3	Total O 3 3	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	3	Total O 3 3	0	0
61	2a	2	Total O 2 2	0	0
61	2a	3	Total O 3 3	0	0
61	2a	4	Total O 4 4	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	4	Total O 4 4	0	0
61	2a	4	Total O 4 4	0	0
61	2a	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0

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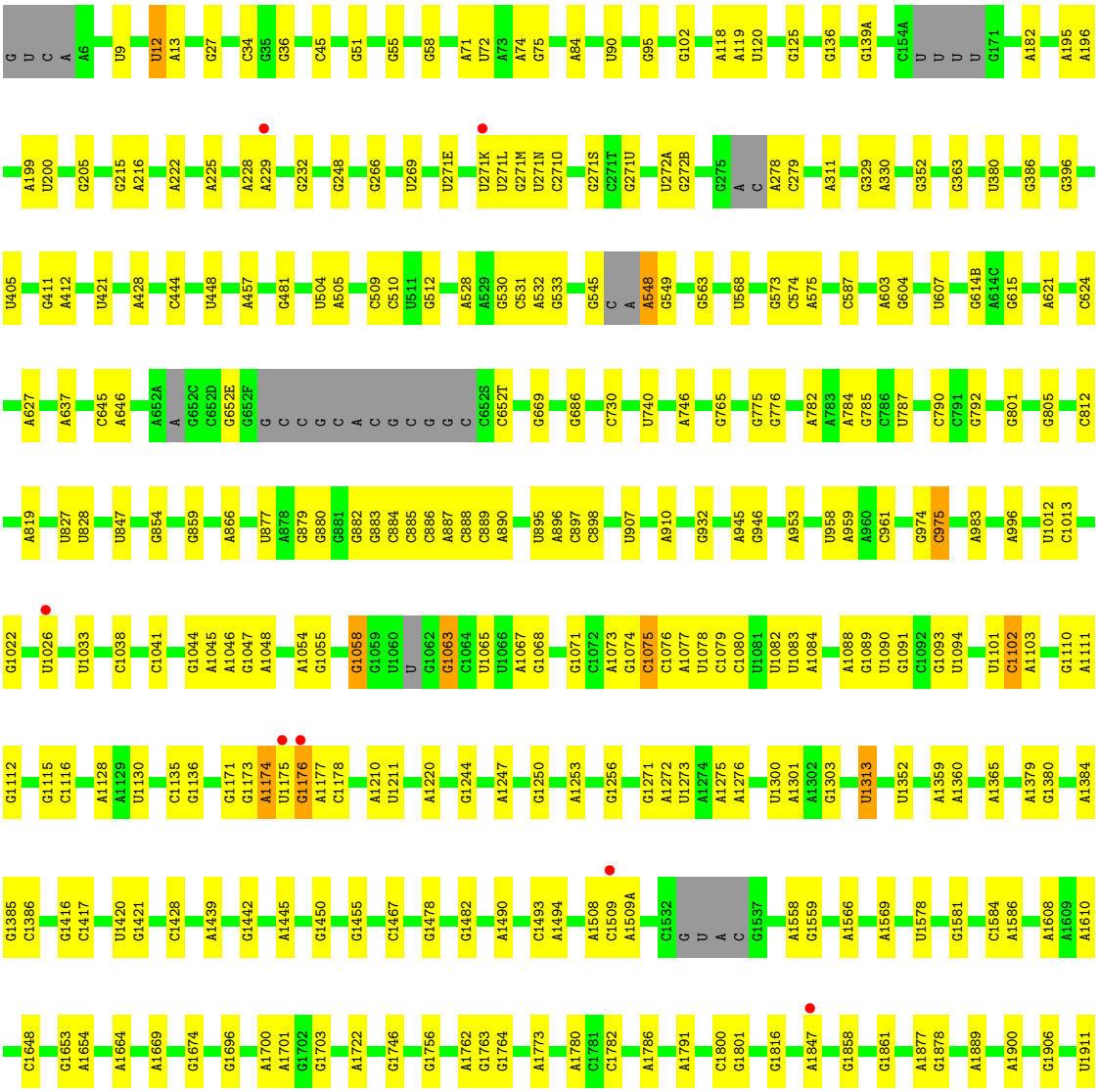
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	40	Total O 40 40	0	0
61	2d	1	Total O 1 1	0	0
61	2g	1	Total O 1 1	0	0
61	2i	1	Total O 1 1	0	0
61	2j	2	Total O 2 2	0	0
61	2j	1	Total O 1 1	0	0
61	2l	1	Total O 1 1	0	0
61	2l	1	Total O 1 1	0	0
61	2p	1	Total O 1 1	0	0
61	2r	1	Total O 1 1	0	0
61	2t	2	Total O 2 2	0	0
61	2x	2	Total O 2 2	0	0
61	2x	2	Total O 2 2	0	0
61	2x	3	Total O 3 3	0	0
61	2y	6	Total O 6 6	0	0
61	2y	1	Total O 1 1	0	0
61	2y	6	Total O 6 6	0	0

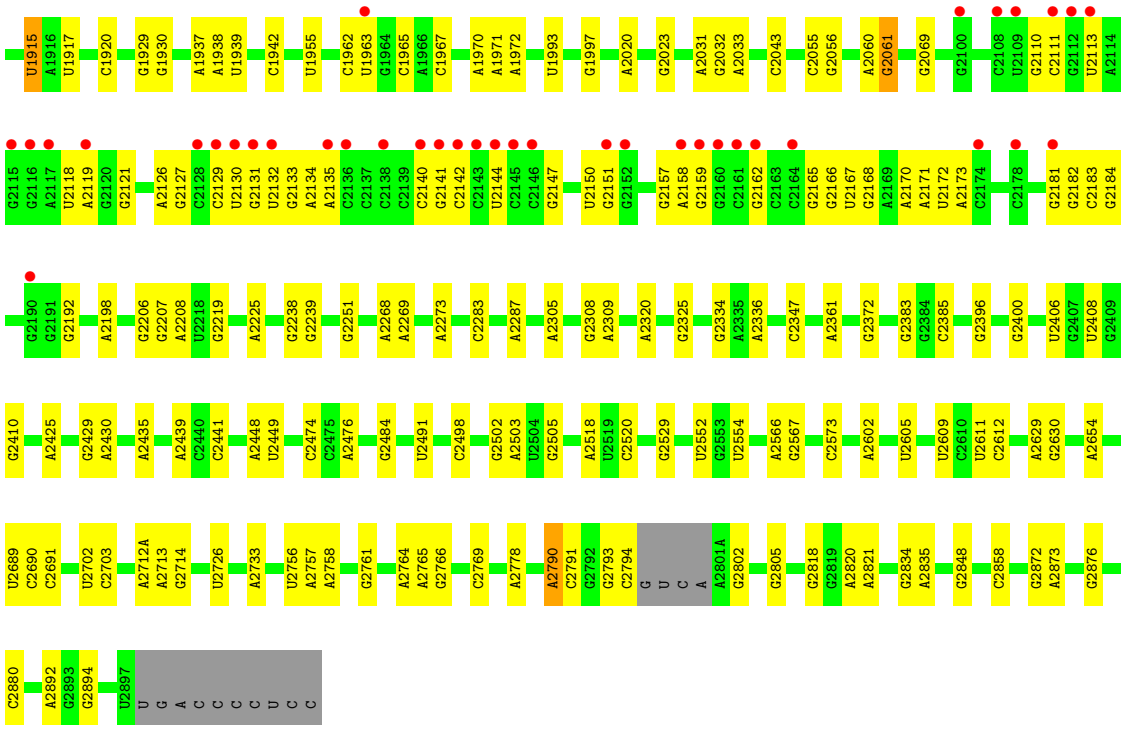
3 Residue-property plots (i)

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

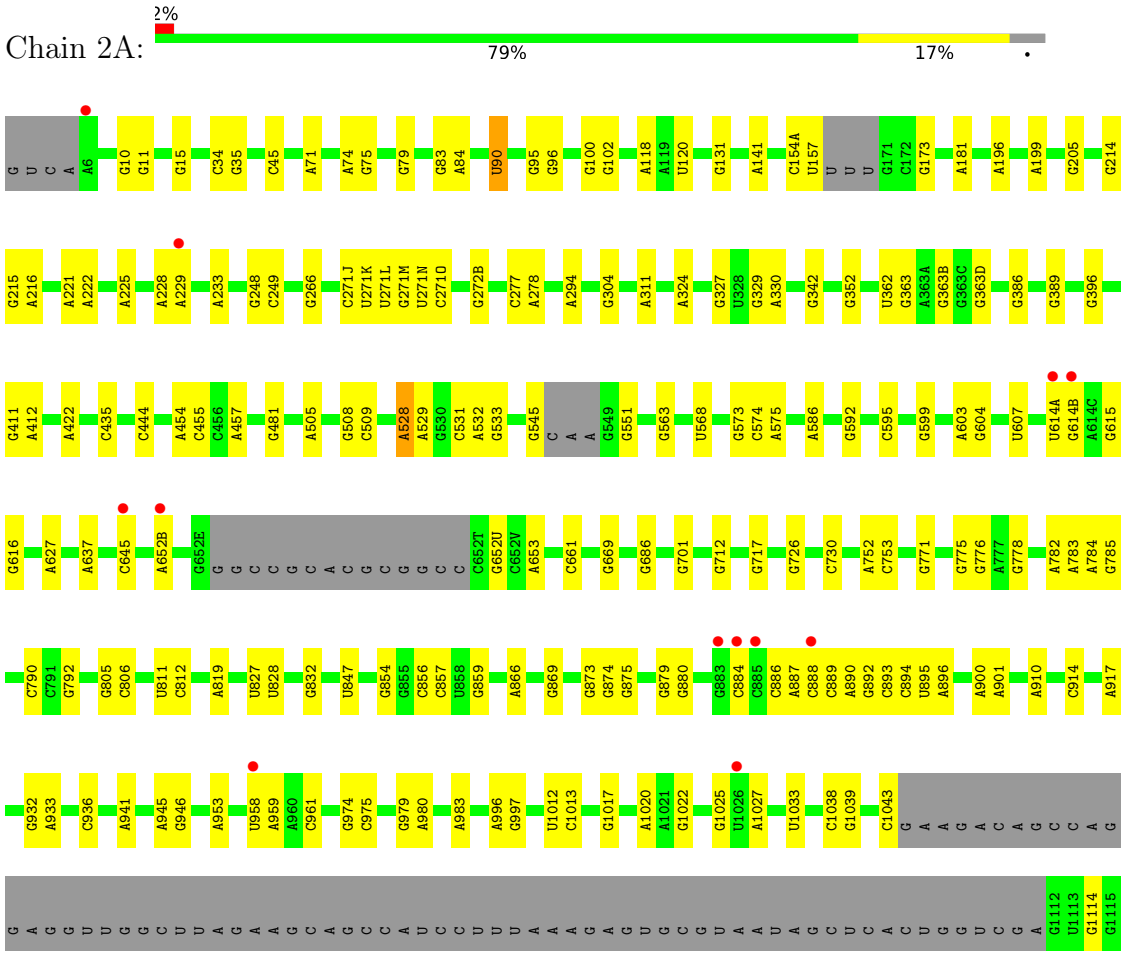
Chain 1A: 2% 82% 16%

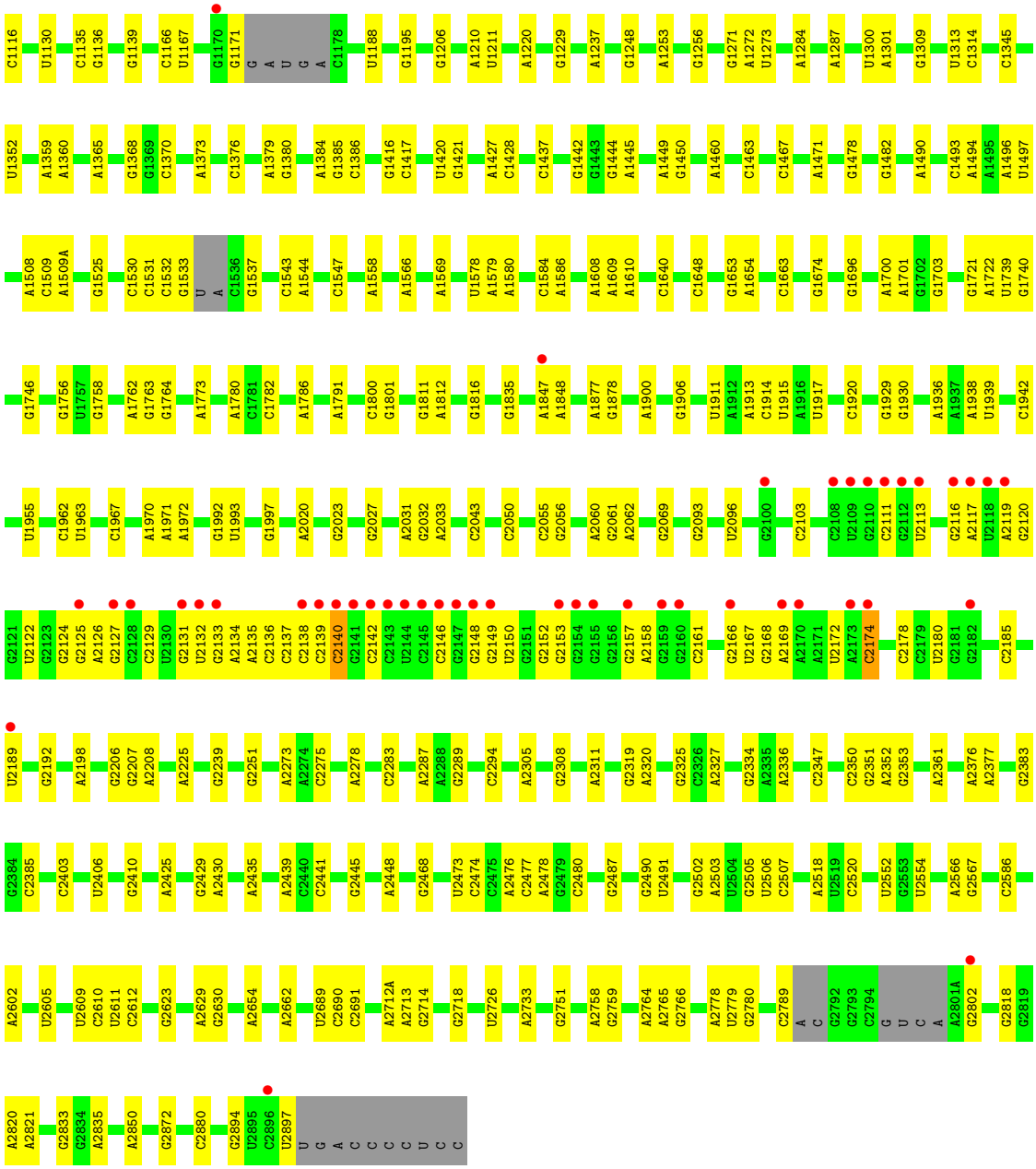




- Molecule 1: 23S Ribosomal RNA

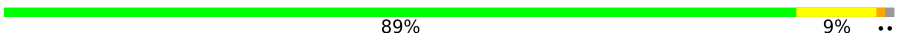
Chain 2A:

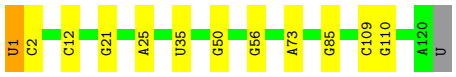




- Molecule 2: 5S Ribosomal RNA

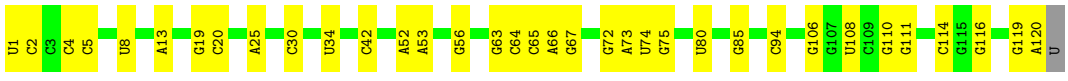
Chain 1B:





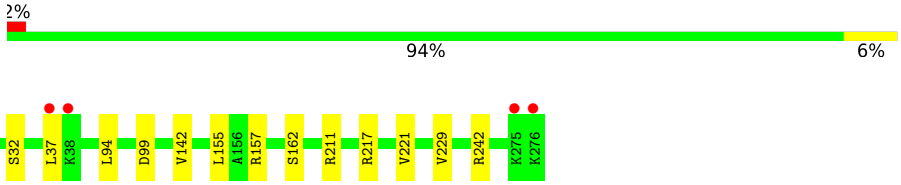
- Molecule 2: 5S Ribosomal RNA

Chain 2B:



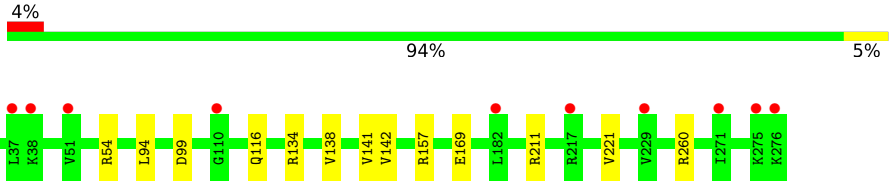
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



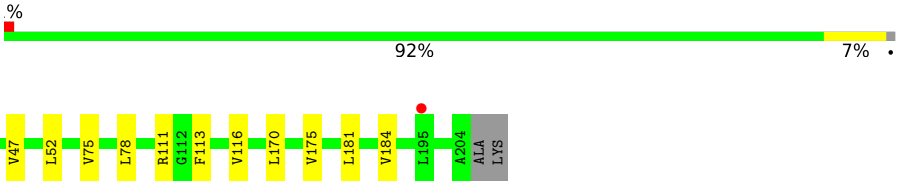
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



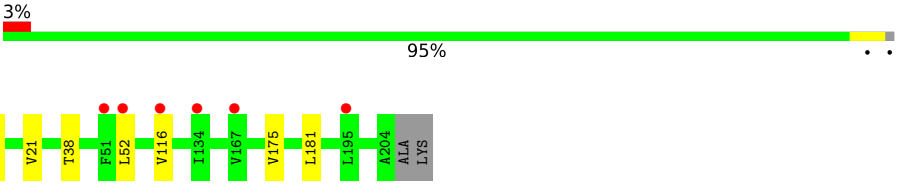
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



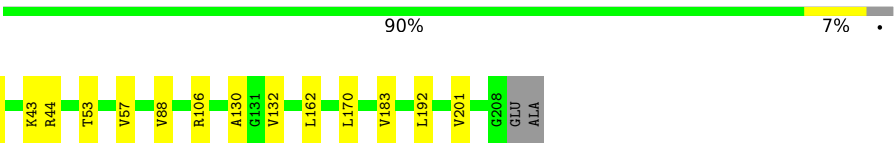
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



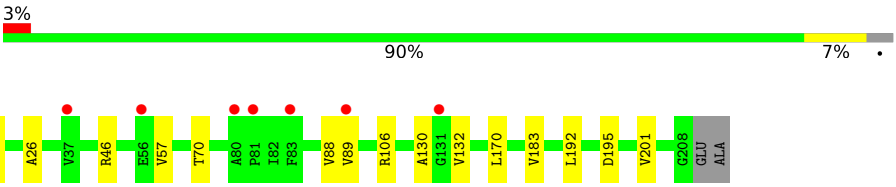
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



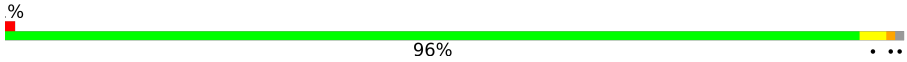
• Molecule 5: 50S ribosomal protein L4

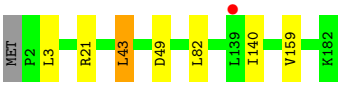
Chain 2F:



• Molecule 6: 50S ribosomal protein L5

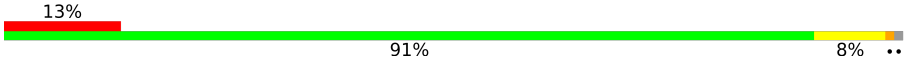
Chain 1G:

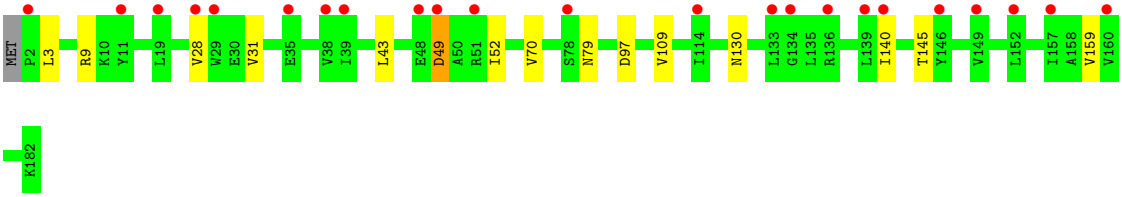




• Molecule 6: 50S ribosomal protein L5

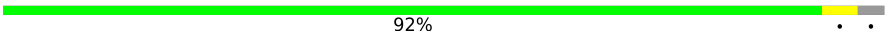
Chain 2G:





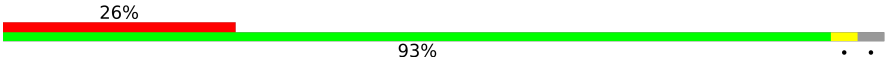
• Molecule 7: 50S ribosomal protein L6

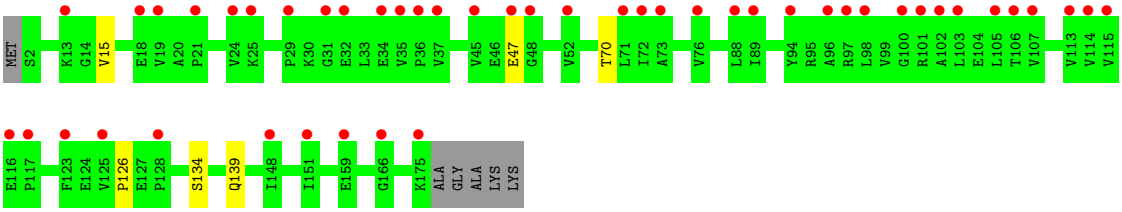
Chain 1H:



• Molecule 7: 50S ribosomal protein L6

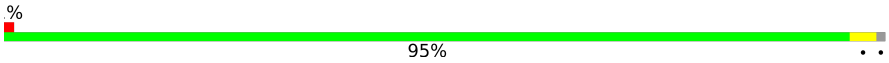
Chain 2H:





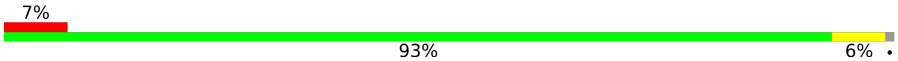
• Molecule 8: 50S ribosomal protein L9

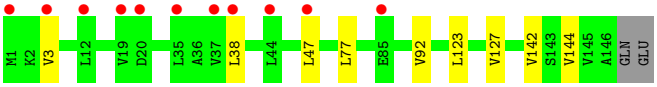
Chain 1I:



• Molecule 8: 50S ribosomal protein L9

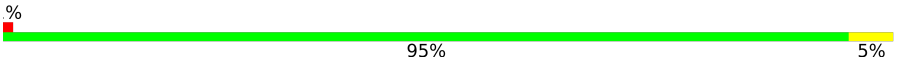
Chain 2I:

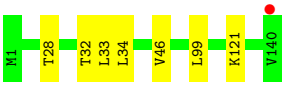




• Molecule 9: 50S ribosomal protein L13

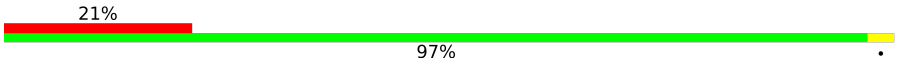
Chain 1N:

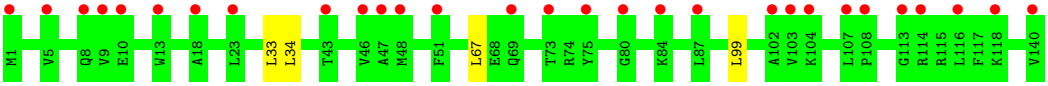




• Molecule 9: 50S ribosomal protein L13

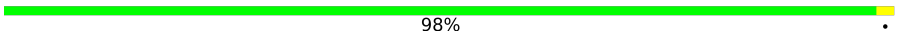
Chain 2N:

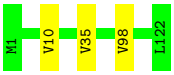




• Molecule 10: 50S ribosomal protein L14

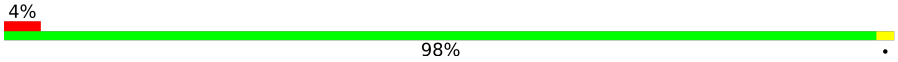
Chain 1O:

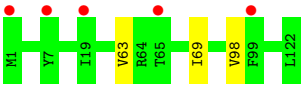




• Molecule 10: 50S ribosomal protein L14

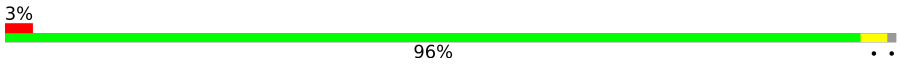
Chain 2O:

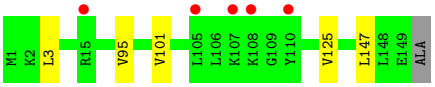




• Molecule 11: 50S ribosomal protein L15

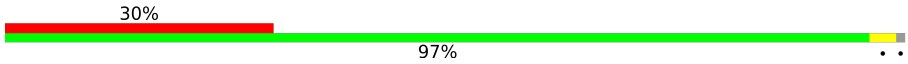
Chain 1P:

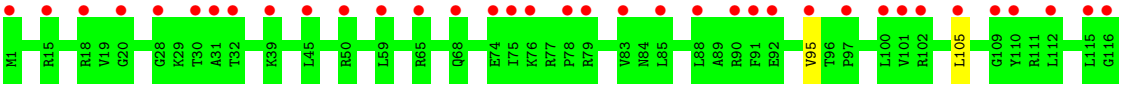


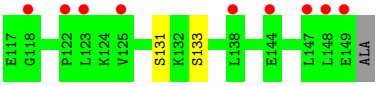


• Molecule 11: 50S ribosomal protein L15

Chain 2P:

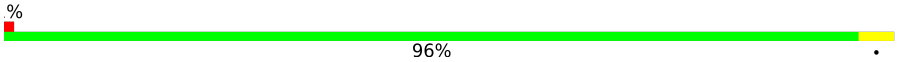


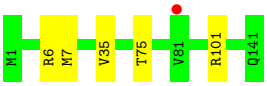




• Molecule 12: 50S ribosomal protein L16

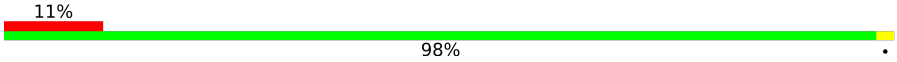
Chain 1Q:

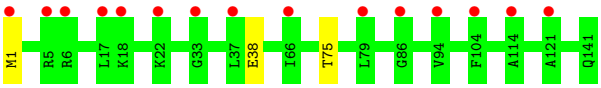




• Molecule 12: 50S ribosomal protein L16

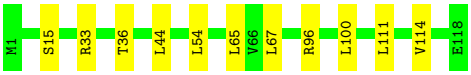
Chain 2Q:





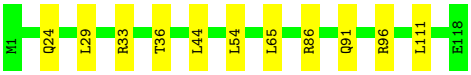
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



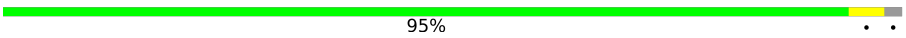
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



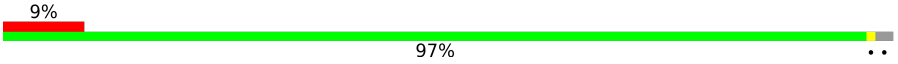
• Molecule 14: 50S ribosomal protein L18

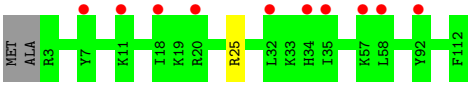
Chain 1S:



• Molecule 14: 50S ribosomal protein L18

Chain 2S:



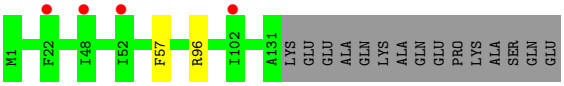


• Molecule 15: 50S ribosomal protein L19

Chain 1T:

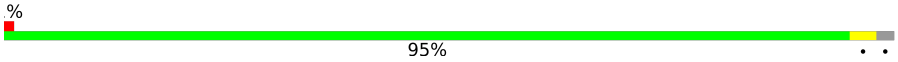
• Molecule 15: 50S ribosomal protein L19

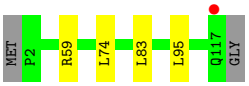
Chain 2T:



• Molecule 16: 50S ribosomal protein L20

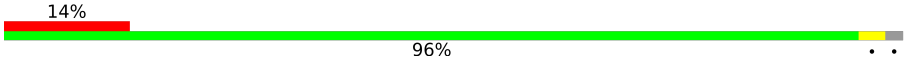
Chain 1U:

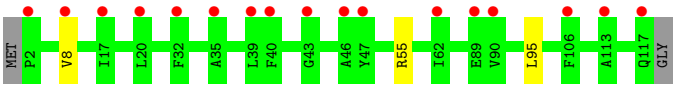




• Molecule 16: 50S ribosomal protein L20

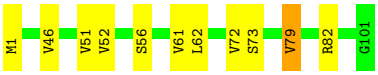
Chain 2U:





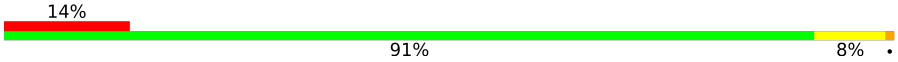
• Molecule 17: 50S ribosomal protein L21

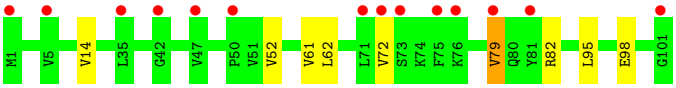
Chain 1V:



• Molecule 17: 50S ribosomal protein L21

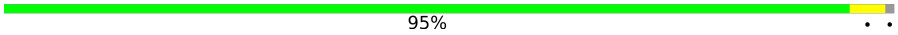
Chain 2V:

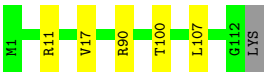




• Molecule 18: 50S ribosomal protein L22

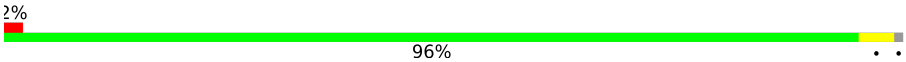
Chain 1W:

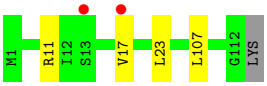




• Molecule 18: 50S ribosomal protein L22

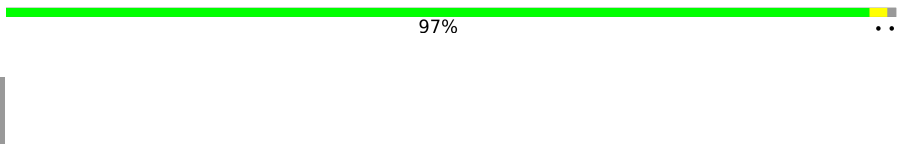
Chain 2W:





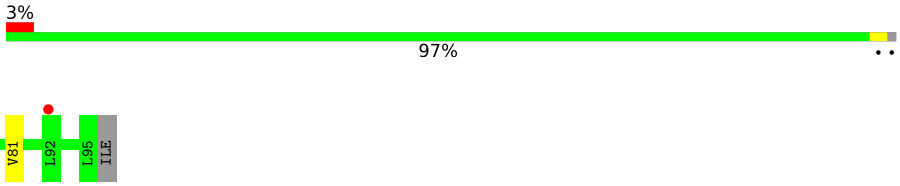
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



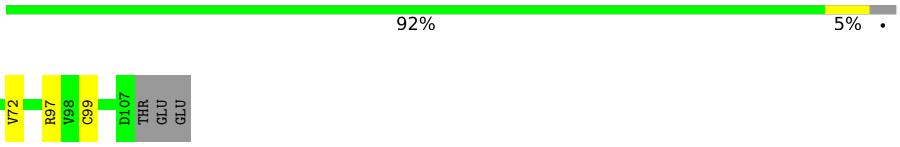
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



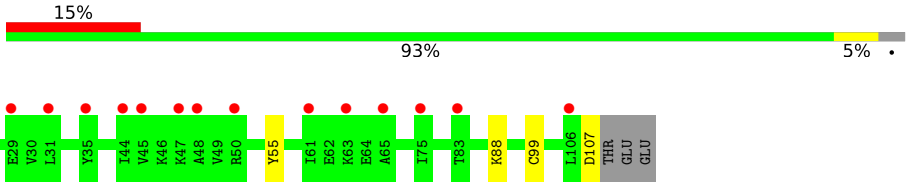
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



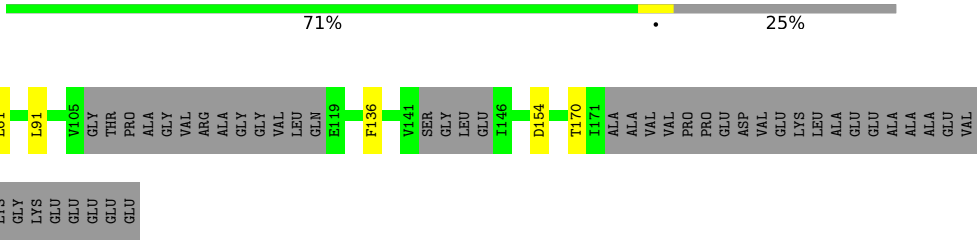
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



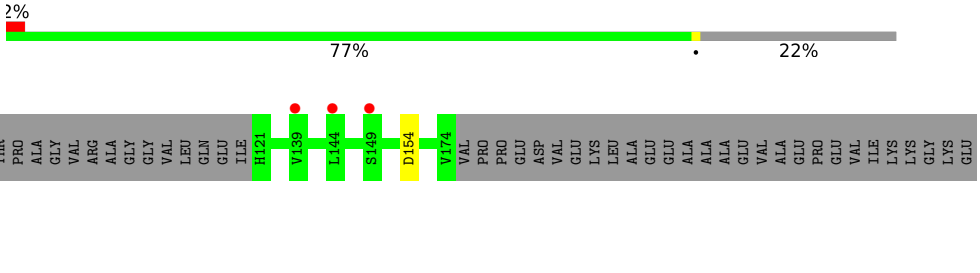
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



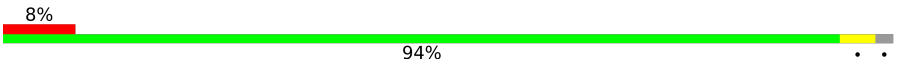
• Molecule 21: 50S ribosomal protein L25

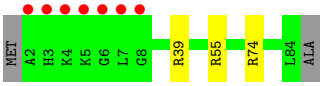
Chain 2Z:



• Molecule 22: 50S ribosomal protein L27

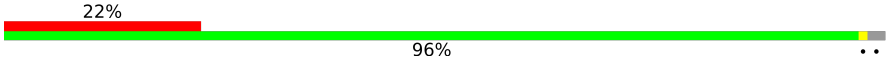
Chain 10:

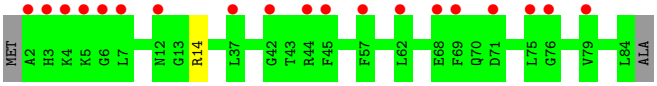




• Molecule 22: 50S ribosomal protein L27

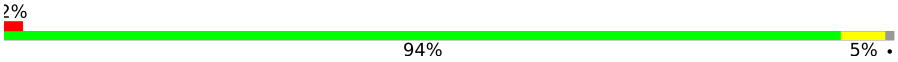
Chain 20:





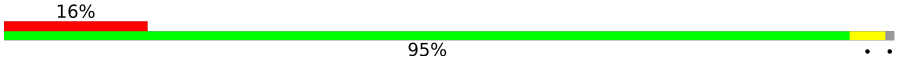
• Molecule 23: 50S ribosomal protein L28

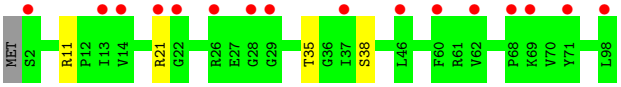
Chain 11:



• Molecule 23: 50S ribosomal protein L28

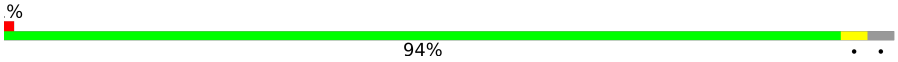
Chain 21:

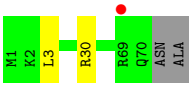




• Molecule 24: 50S ribosomal protein L29

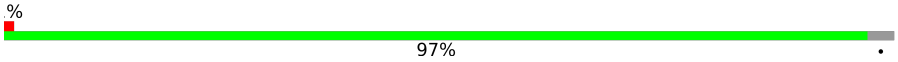
Chain 12:

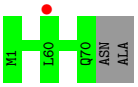




• Molecule 24: 50S ribosomal protein L29

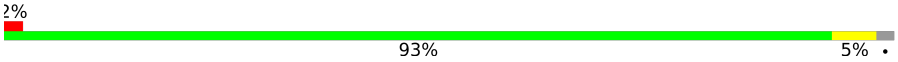
Chain 22:

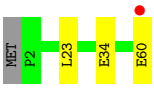




• Molecule 25: 50S ribosomal protein L30

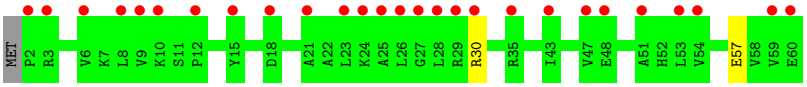
Chain 13:





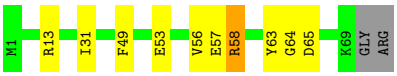
• Molecule 25: 50S ribosomal protein L30

Chain 23: 45% 95%



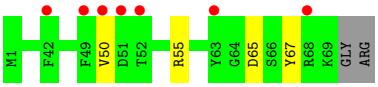
• Molecule 26: 50S ribosomal protein L31

Chain 14: 83% 13%



• Molecule 26: 50S ribosomal protein L31

Chain 24: 10% 92% 6%

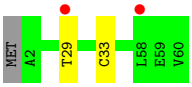


• Molecule 27: 50S ribosomal protein L32

Chain 15: 2% 93% 5%

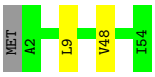
• Molecule 27: 50S ribosomal protein L32

Chain 25: 3% 95%



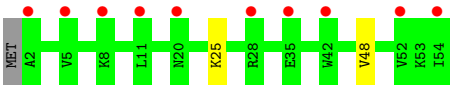
• Molecule 28: 50S ribosomal protein L33

Chain 16: 94%



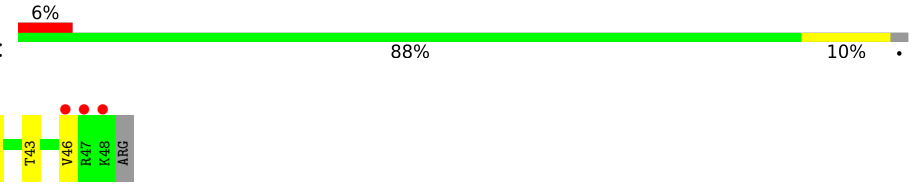
• Molecule 28: 50S ribosomal protein L33

Chain 26: 19% 94%



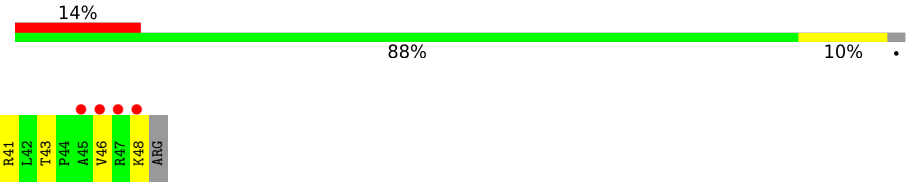
• Molecule 29: 50S ribosomal protein L34

Chain 17:



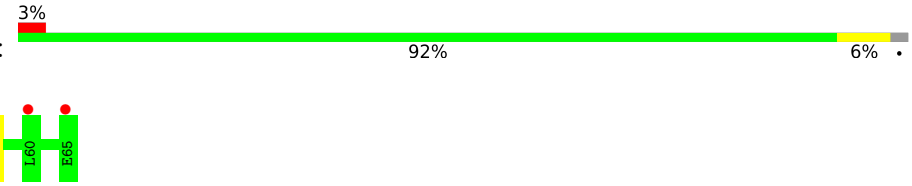
• Molecule 29: 50S ribosomal protein L34

Chain 27:



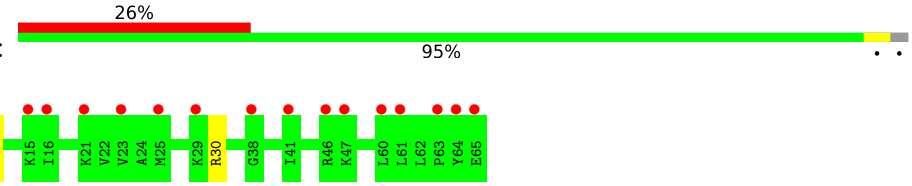
• Molecule 30: 50S ribosomal protein L35

Chain 18:



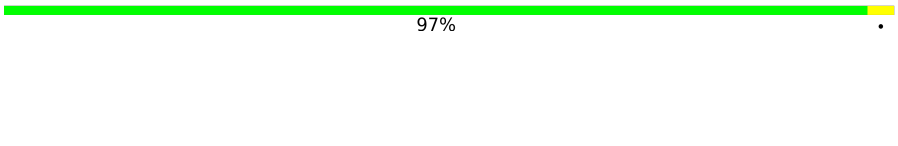
• Molecule 30: 50S ribosomal protein L35

Chain 28:



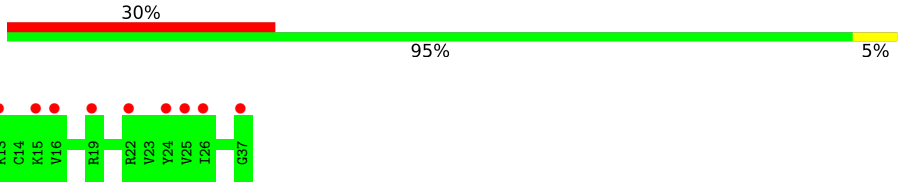
• Molecule 31: 50S ribosomal protein L36

Chain 19:



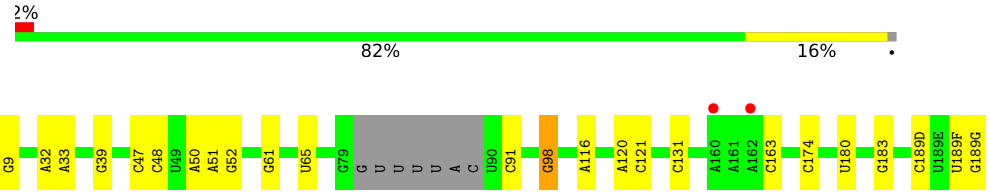
• Molecule 31: 50S ribosomal protein L36

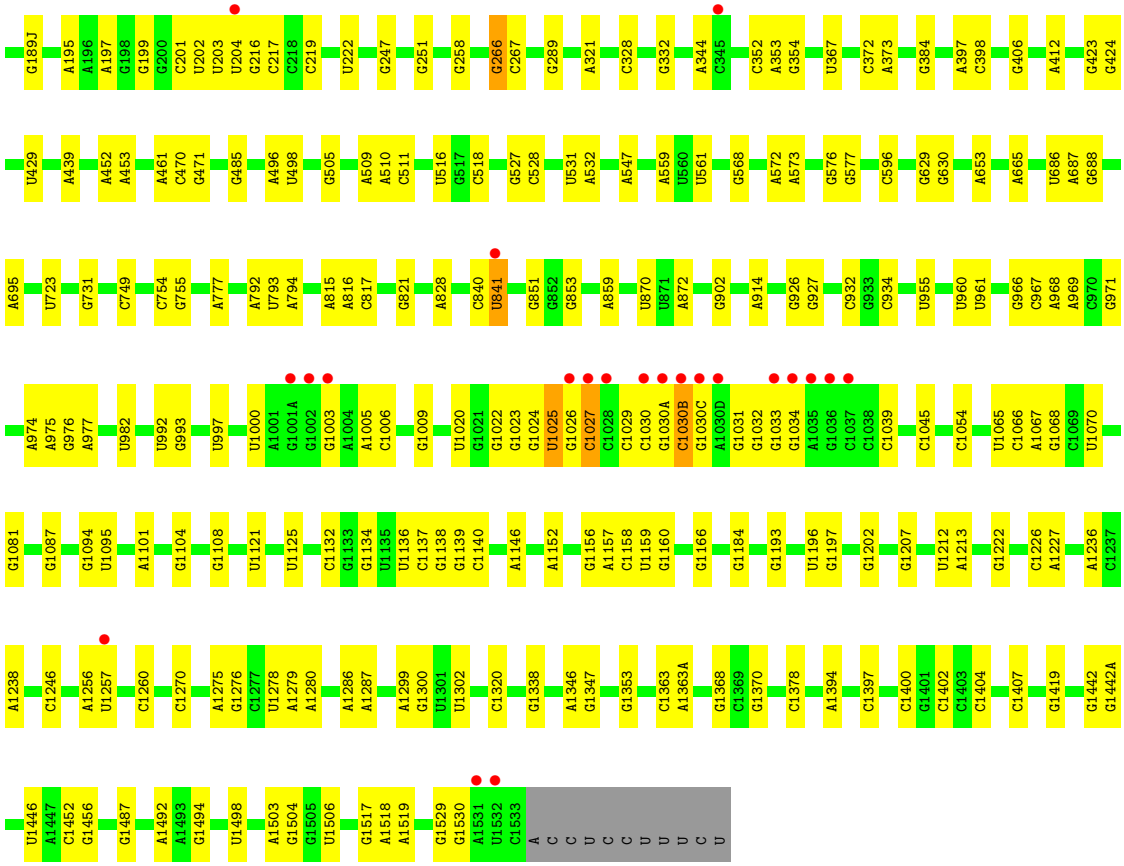
Chain 29:



• Molecule 32: 16S Ribosomal RNA

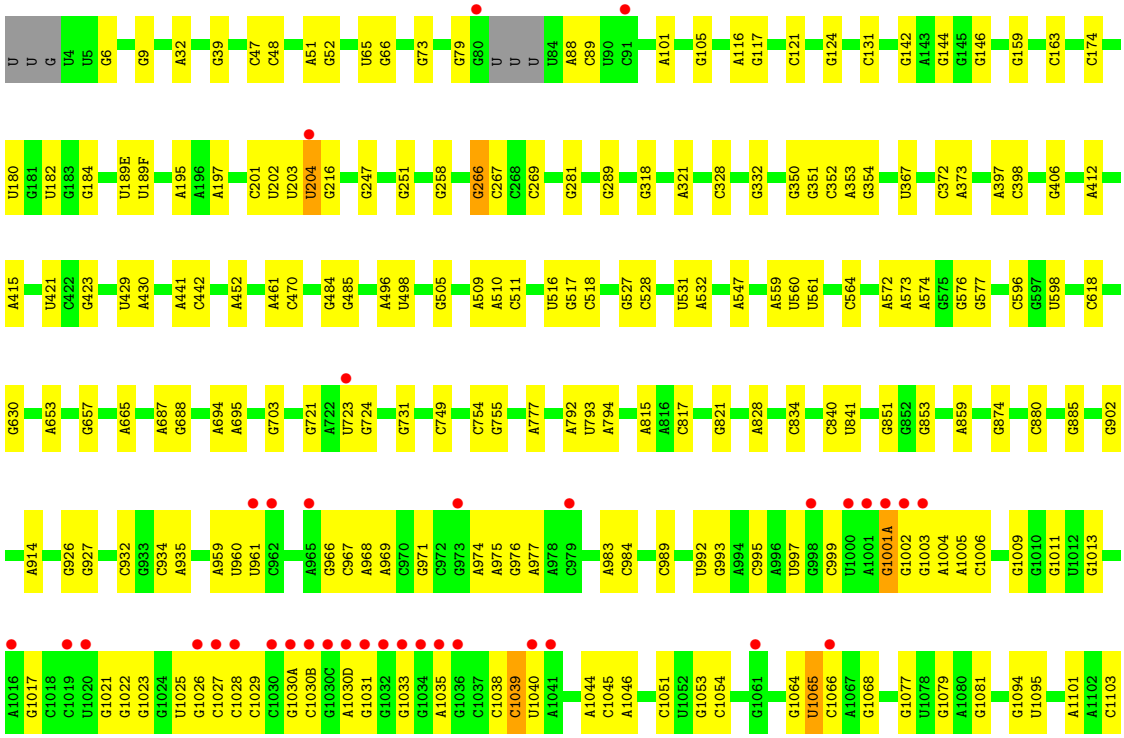
Chain 1a:

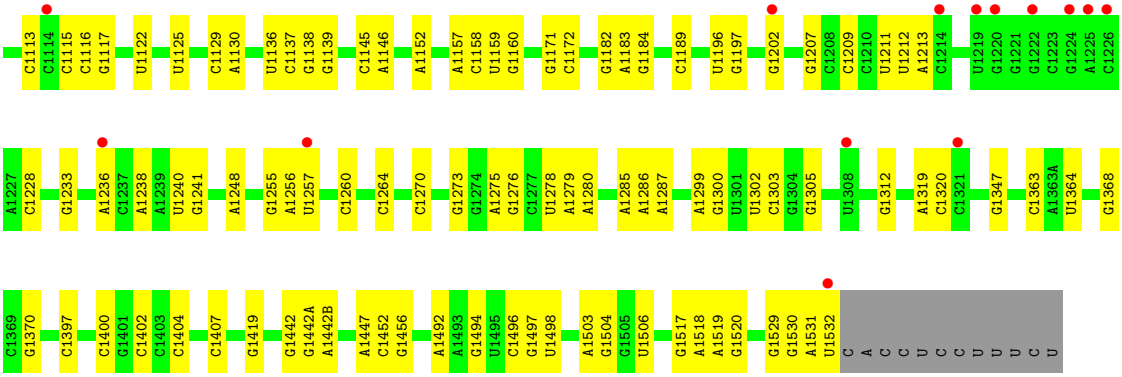




- Molecule 32: 16S Ribosomal RNA

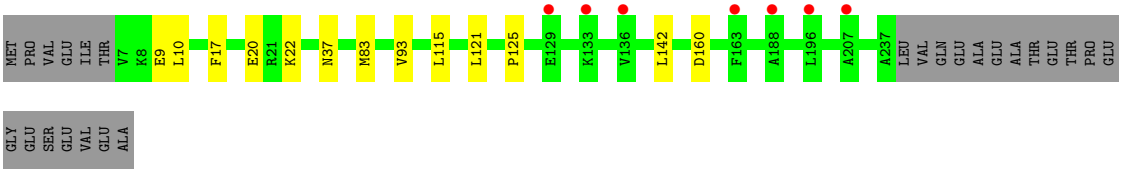
Chain 2a:





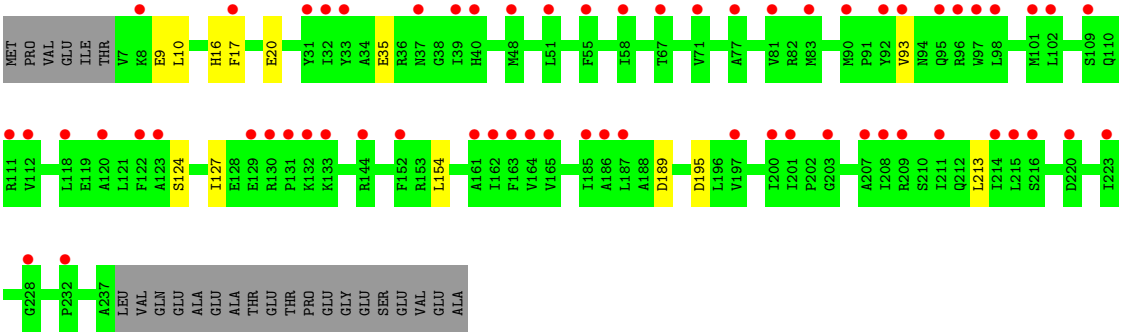
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



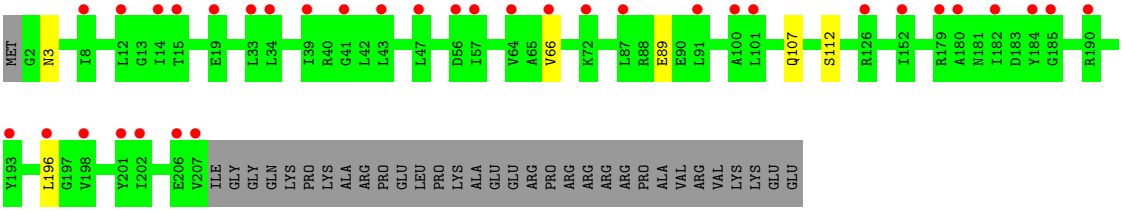
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



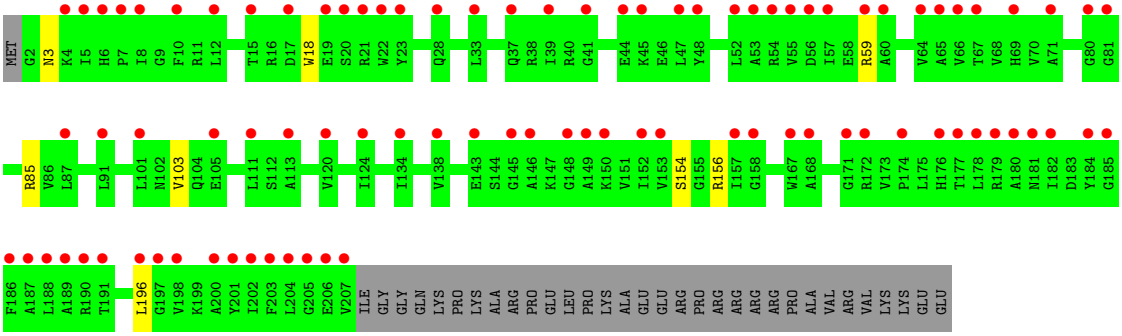
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



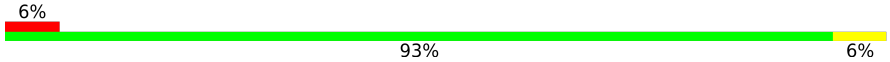
• Molecule 34: 30S ribosomal protein S3

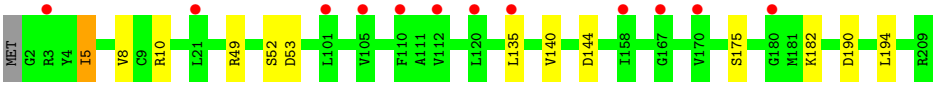
Chain 2c:



- Molecule 35: 30S ribosomal protein S4

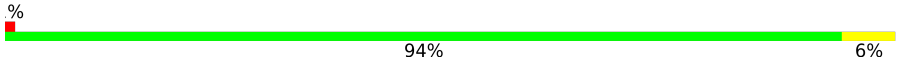
Chain 1d:

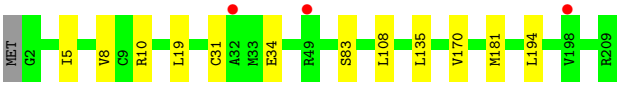




- Molecule 35: 30S ribosomal protein S4

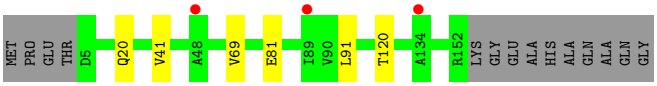
Chain 2d:





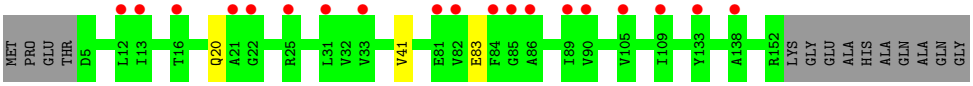
- Molecule 36: 30S ribosomal protein S5

Chain 1e:



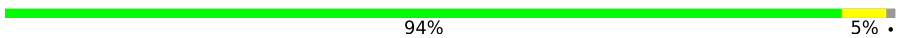
- Molecule 36: 30S ribosomal protein S5

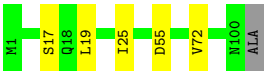
Chain 2e:



- Molecule 37: 30S ribosomal protein S6

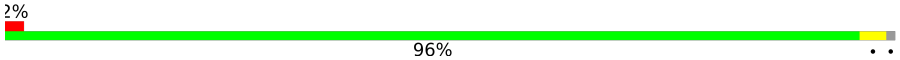
Chain 1f:

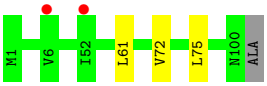




- Molecule 37: 30S ribosomal protein S6

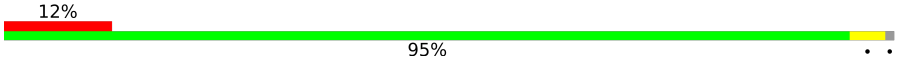
Chain 2f:

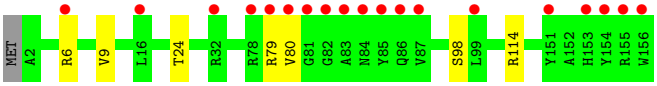




• Molecule 38: 30S ribosomal protein S7

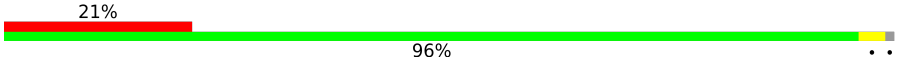
Chain 1g:

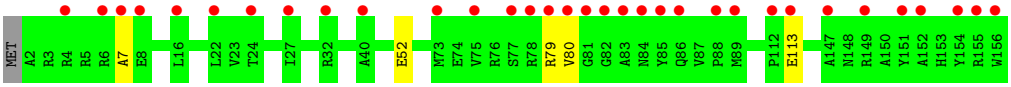




• Molecule 38: 30S ribosomal protein S7

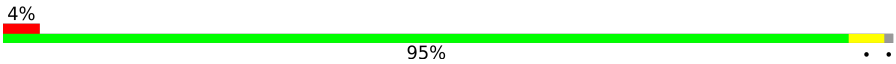
Chain 2g:





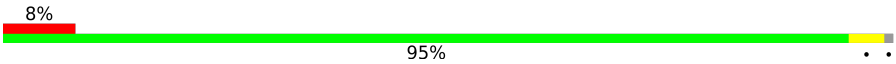
• Molecule 39: 30S ribosomal protein S8

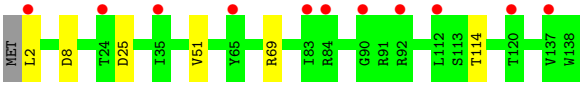
Chain 1h:



• Molecule 39: 30S ribosomal protein S8

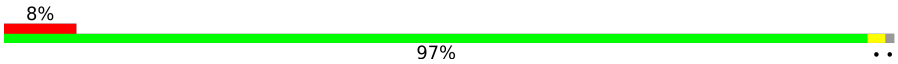
Chain 2h:





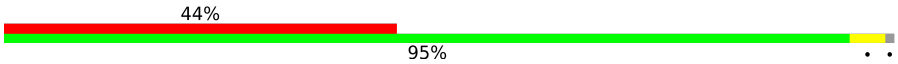
• Molecule 40: 30S ribosomal protein S9

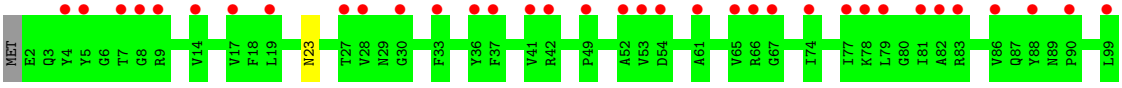
Chain 1i:

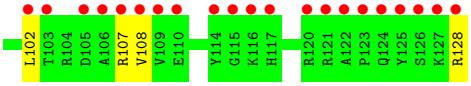


• Molecule 40: 30S ribosomal protein S9

Chain 2i:

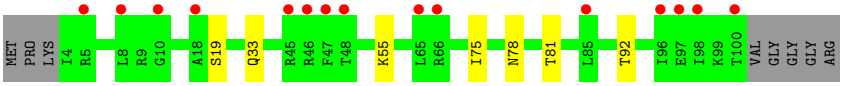






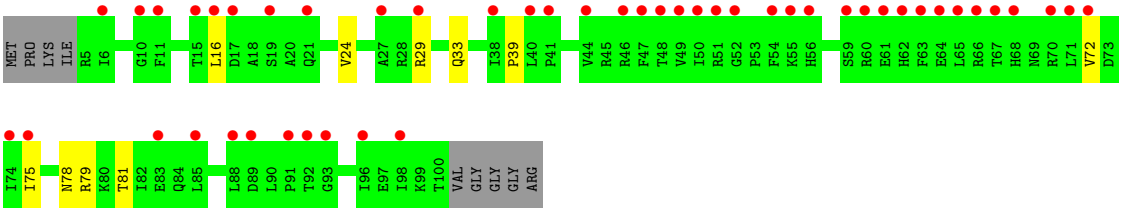
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



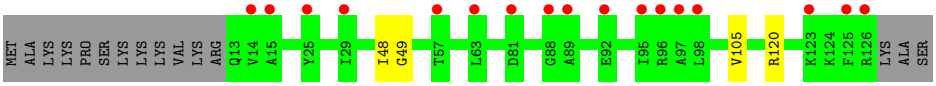
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



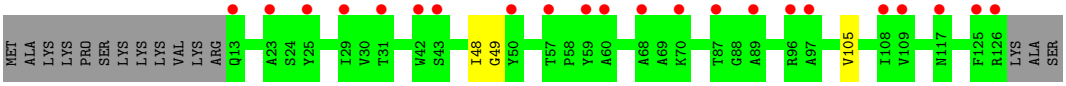
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



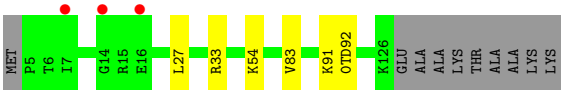
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



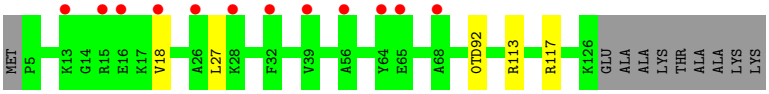
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



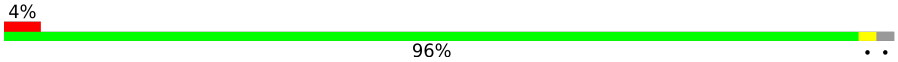
• Molecule 43: 30S ribosomal protein S12

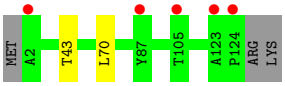
Chain 2l:



• Molecule 44: 30S ribosomal protein S13

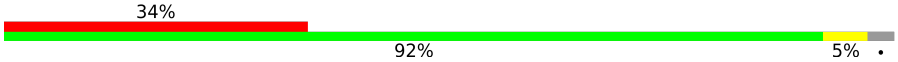
Chain 1m:

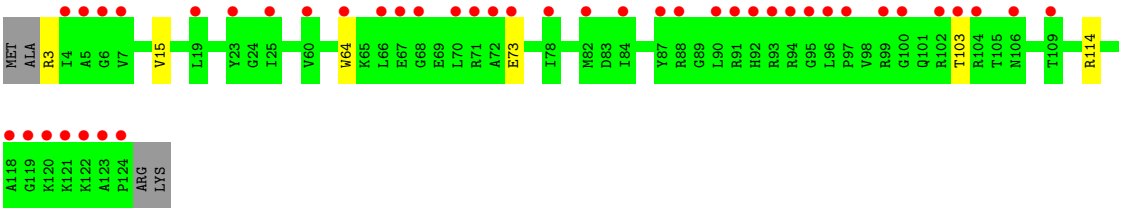




• Molecule 44: 30S ribosomal protein S13

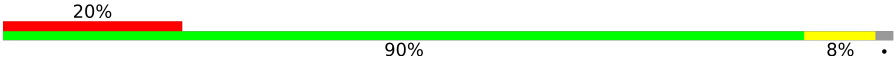
Chain 2m:

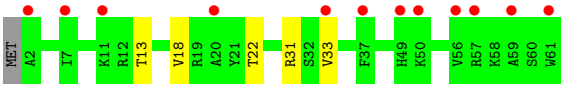




• Molecule 45: 30S ribosomal protein S14 type Z

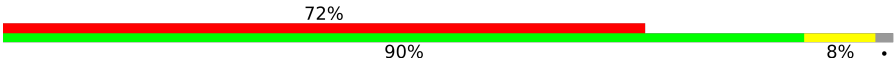
Chain 1n:

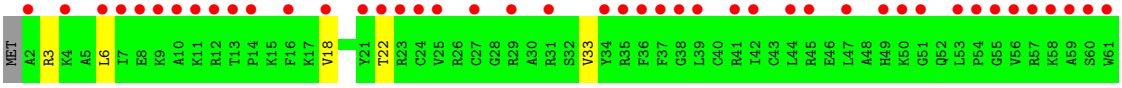




• Molecule 45: 30S ribosomal protein S14 type Z

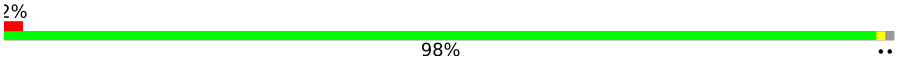
Chain 2n:

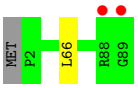




• Molecule 46: 30S ribosomal protein S15

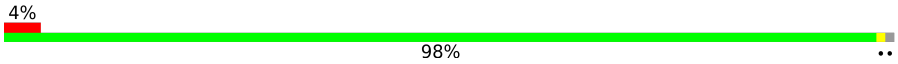
Chain 1o:

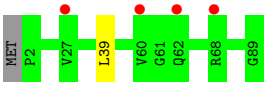




• Molecule 46: 30S ribosomal protein S15

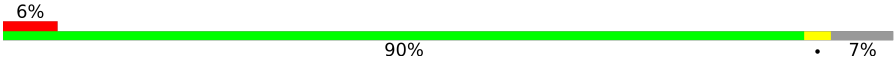
Chain 2o:

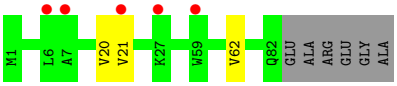




• Molecule 47: 30S ribosomal protein S16

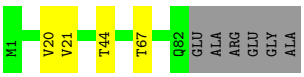
Chain 1p:





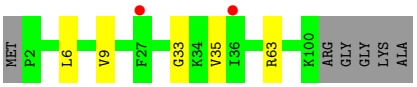
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



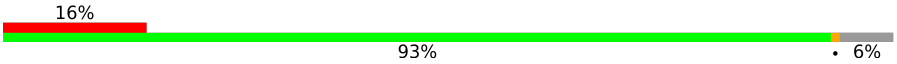
• Molecule 48: 30S ribosomal protein S17

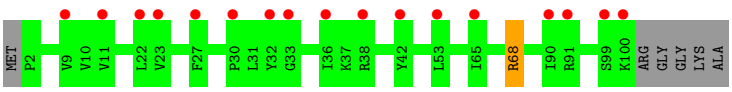
Chain 1q:



• Molecule 48: 30S ribosomal protein S17

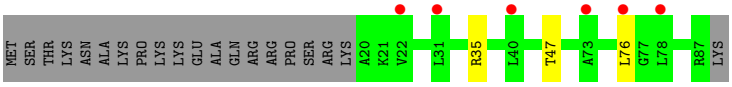
Chain 2q:





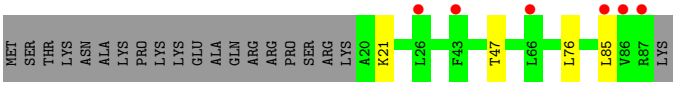
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



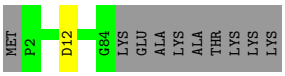
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



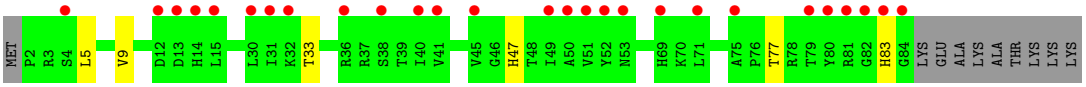
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



• Molecule 50: 30S ribosomal protein S19

Chain 2s:

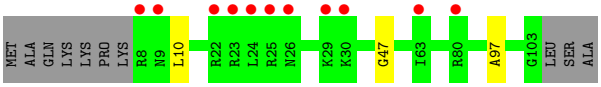


• Molecule 51: 30S ribosomal protein S20

Chain 1t:

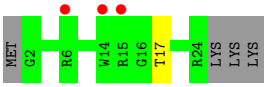
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



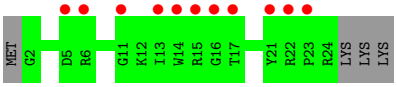
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



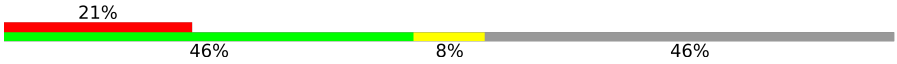
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



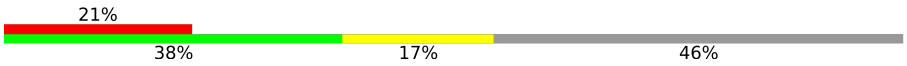
• Molecule 53: mRNA

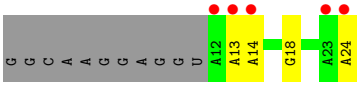
Chain 1v:



- Molecule 53: mRNA

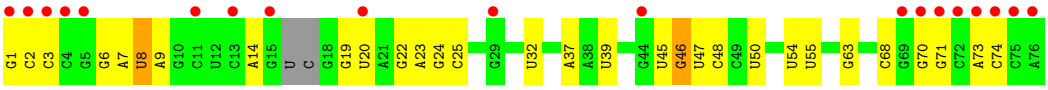
Chain 2v:





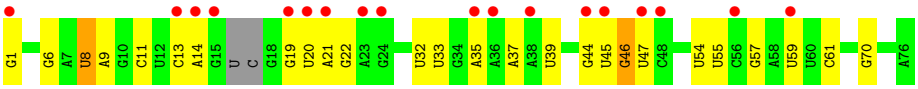
- Molecule 54: A-site and E-site tRNAs

Chain 1w:



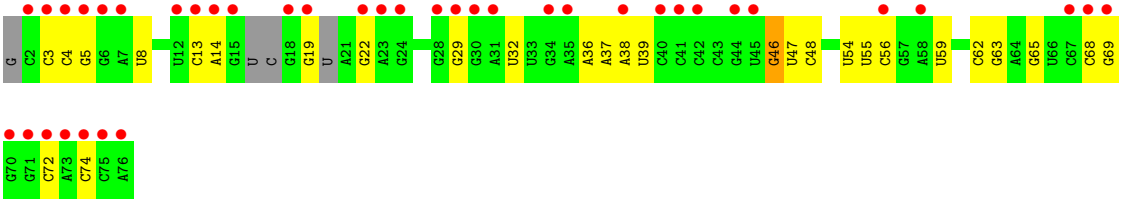
- Molecule 54: A-site and E-site tRNAs

Chain 1y:



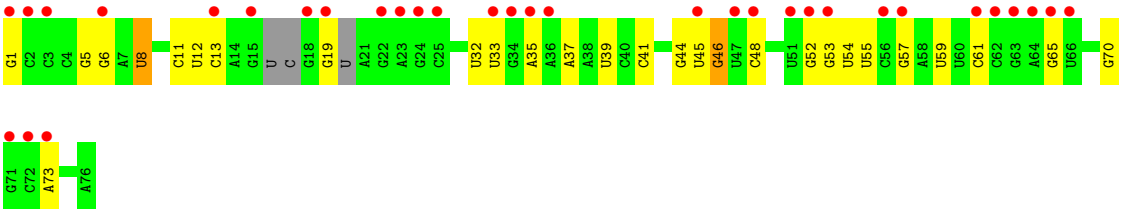
- Molecule 54: A-site and E-site tRNAs

Chain 2w:



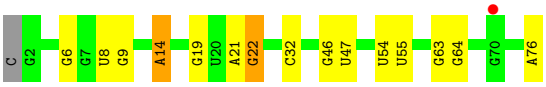
- Molecule 54: A-site and E-site tRNAs

Chain 2y:



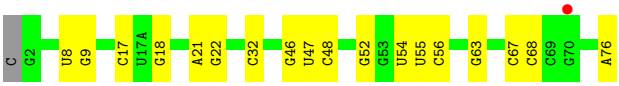
- Molecule 55: P-site tRNA

Chain 1x:



• Molecule 55: P-site tRNA

Chain 2x:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.99Å 448.29Å 618.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.28 – 2.60 254.56 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (127.28-2.60) 98.7 (254.56-2.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.229 , 0.276 0.230 , 0.277	Depositor DCC
R_{free} test set	86986 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	300833	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, K, PSU, OMG, MA6, 2MU, ZN, 7MG, 0TD, 5MU, CLM, 2MG, 4OC, SF4, 5MC, MIA, 2MA, M2G, UR3, MG

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	0.33	0/69009	0.82	39/107712 (0.0%)
1	2A	0.26	0/67293	0.78	15/105034 (0.0%)
2	1B	0.32	1/2882 (0.0%)	0.74	0/4494
2	2B	0.30	1/2879 (0.0%)	0.80	1/4487 (0.0%)
3	1D	0.32	0/2186	0.53	0/2944
3	2D	0.28	0/2186	0.49	0/2944
4	1E	0.28	0/1592	0.49	0/2149
4	2E	0.26	0/1592	0.48	0/2149
5	1F	0.27	0/1619	0.47	0/2193
5	2F	0.26	0/1615	0.44	0/2188
6	1G	0.27	0/1448	0.45	0/1957
6	2G	0.25	0/1453	0.45	0/1963
7	1H	0.27	0/1356	0.45	0/1834
7	2H	0.25	0/1356	0.44	0/1834
8	1I	0.25	0/1112	0.44	0/1514
8	2I	0.25	0/1079	0.47	0/1475
9	1N	0.28	0/1144	0.46	0/1543
9	2N	0.25	0/1144	0.43	0/1543
10	1O	0.30	0/943	0.49	0/1269
10	2O	0.28	0/943	0.48	0/1269
11	1P	0.27	0/1152	0.49	0/1533
11	2P	0.27	0/1152	0.48	0/1533
12	1Q	0.29	0/1143	0.46	0/1527
12	2Q	0.26	0/1143	0.45	0/1527
13	1R	0.26	0/982	0.47	0/1312
13	2R	0.24	0/982	0.44	0/1312
14	1S	0.27	0/883	0.48	0/1176
14	2S	0.25	0/880	0.43	0/1172
15	1T	0.26	0/1105	0.45	0/1477
15	2T	0.24	0/1097	0.44	0/1468
16	1U	0.29	0/977	0.44	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.25	0/977	0.39	0/1301
17	1V	0.30	0/782	0.52	0/1049
17	2V	0.27	0/782	0.49	0/1049
18	1W	0.28	0/897	0.47	0/1205
18	2W	0.26	0/897	0.42	0/1205
19	1X	0.30	0/764	0.50	0/1025
19	2X	0.25	0/764	0.45	0/1025
20	1Y	0.29	0/819	0.48	0/1095
20	2Y	0.27	0/819	0.49	0/1095
21	1Z	0.27	0/1267	0.48	0/1717
21	2Z	0.26	0/1299	0.48	0/1763
22	10	0.29	0/662	0.48	0/881
22	20	0.27	0/662	0.49	0/881
23	11	0.27	0/762	0.47	0/1014
23	21	0.26	0/762	0.46	0/1014
24	12	0.26	0/590	0.41	0/781
24	22	0.24	0/590	0.36	0/781
25	13	0.27	0/474	0.45	0/635
25	23	0.25	0/469	0.41	0/630
26	14	0.29	0/565	0.53	0/761
26	24	0.29	0/545	0.49	0/737
27	15	0.27	0/469	0.52	0/635
27	25	0.27	0/469	0.44	0/635
28	16	0.28	0/460	0.48	0/613
28	26	0.26	0/456	0.44	0/608
29	17	0.26	0/426	0.45	0/561
29	27	0.24	0/426	0.45	0/561
30	18	0.28	0/525	0.49	0/691
30	28	0.25	0/525	0.44	0/691
31	19	0.27	0/310	0.48	0/407
31	29	0.26	0/310	0.50	0/407
32	1a	0.26	0/35795	0.81	24/55864 (0.0%)
32	2a	0.25	0/35886	0.81	20/56005 (0.0%)
33	1b	0.25	0/1881	0.45	0/2542
33	2b	0.26	0/1860	0.45	0/2518
34	1c	0.25	0/1572	0.43	0/2126
34	2c	0.25	0/1566	0.45	0/2119
35	1d	0.25	0/1685	0.42	0/2262
35	2d	0.25	0/1704	0.43	0/2284
36	1e	0.26	0/1145	0.48	0/1543
36	2e	0.25	0/1149	0.47	0/1548
37	1f	0.26	0/823	0.45	0/1115
37	2f	0.26	0/829	0.44	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.24	0/1250	0.41	0/1679
38	2g	0.24	0/1254	0.41	0/1683
39	1h	0.25	0/1108	0.44	0/1494
39	2h	0.24	0/1108	0.43	0/1494
40	1i	0.27	0/1002	0.47	0/1346
40	2i	0.26	0/997	0.47	0/1343
41	1j	0.24	0/722	0.48	0/982
41	2j	0.25	0/727	0.48	0/988
42	1k	0.25	0/844	0.45	0/1145
42	2k	0.25	0/848	0.44	0/1149
43	1l	0.26	0/937	0.49	0/1260
43	2l	0.25	0/937	0.47	0/1260
44	1m	0.26	0/969	0.43	0/1302
44	2m	0.26	0/961	0.47	0/1291
45	1n	0.25	0/501	0.41	0/664
45	2n	0.25	0/501	0.40	0/664
46	1o	0.24	0/739	0.42	0/985
46	2o	0.23	0/739	0.39	0/985
47	1p	0.24	0/697	0.44	0/939
47	2p	0.26	0/693	0.47	0/935
48	1q	0.25	0/836	0.44	0/1117
48	2q	0.25	0/836	0.44	0/1117
49	1r	0.25	0/560	0.42	0/746
49	2r	0.24	0/560	0.42	0/746
50	1s	0.25	0/667	0.50	0/900
50	2s	0.27	0/661	0.53	0/893
51	1t	0.24	0/730	0.41	0/965
51	2t	0.24	0/729	0.40	0/965
52	1u	0.24	0/203	0.44	0/266
52	2u	0.27	0/203	0.46	0/266
53	1v	0.34	0/310	0.88	0/480
53	2v	0.38	0/310	0.89	0/480
54	1w	0.43	1/1606 (0.1%)	1.04	1/2497 (0.0%)
54	1y	0.41	1/1606 (0.1%)	1.00	4/2497 (0.2%)
54	2w	0.34	0/1556	0.99	0/2418
54	2y	0.41	1/1583 (0.1%)	0.98	3/2459 (0.1%)
55	1x	0.39	0/1725	1.02	10/2689 (0.4%)
55	2x	0.31	0/1725	0.92	1/2689 (0.0%)
All	All	0.28	5/316686 (0.0%)	0.73	118/474113 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	14	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	1	G	OP3-P	-10.51	1.48	1.61
54	1w	1	G	OP3-P	-10.46	1.48	1.61
2	2B	1	U	OP3-P	-10.40	1.48	1.61
54	2y	1	G	OP3-P	-10.33	1.48	1.61
2	1B	1	U	OP3-P	-10.31	1.48	1.61

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1075	C	N1-C2-O2	10.47	125.18	118.90
1	1A	801	G	O5'-P-OP2	-9.90	96.79	105.70
1	1A	975	C	N1-C2-O2	-9.05	113.47	118.90
2	2B	80	U	O4'-C1'-N1	8.59	115.07	108.20
1	2A	2473	U	C2-N1-C1'	7.86	127.13	117.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	57	GLU	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	261 (96%)	11 (4%)	1 (0%)	34	57
3	2D	273/276 (99%)	261 (96%)	11 (4%)	1 (0%)	34	57
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	52
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	52
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	29	52
5	2F	201/210 (96%)	197 (98%)	1 (0%)	3 (2%)	10	21
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	25	47
6	2G	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	14	30
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	25	47
7	2H	172/180 (96%)	160 (93%)	10 (6%)	2 (1%)	13	27
8	1I	144/148 (97%)	137 (95%)	7 (5%)	0	100	100
8	2I	144/148 (97%)	134 (93%)	10 (7%)	0	100	100
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
12	1Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	32
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	32
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
20	2Y	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	1Z	148/206 (72%)	140 (95%)	8 (5%)	0	100	100
21	2Z	156/206 (76%)	142 (91%)	14 (9%)	0	100	100
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	30
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	57 (85%)	7 (10%)	3 (4%)	2	3
26	24	67/71 (94%)	54 (81%)	11 (16%)	2 (3%)	4	7
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	51 (100%)	0	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	4	6
33	2b	229/256 (90%)	203 (89%)	20 (9%)	6 (3%)	5	9
34	1c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	15	32
34	2c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	15	32
35	1d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	193 (94%)	11 (5%)	2 (1%)	15	32
36	1e	146/162 (90%)	140 (96%)	5 (3%)	1 (1%)	22	43
36	2e	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	12	24
38	2g	153/156 (98%)	140 (92%)	11 (7%)	2 (1%)	12	24
39	1h	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
40	2i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
41	1j	95/105 (90%)	85 (90%)	6 (6%)	4 (4%)	3	3
41	2j	94/105 (90%)	81 (86%)	6 (6%)	7 (7%)	1	1
42	1k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	8	16
42	2k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	8	16
43	1l	119/132 (90%)	112 (94%)	6 (5%)	1 (1%)	19	39
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100	100
44	2m	120/126 (95%)	111 (92%)	9 (8%)	0	100	100
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
47	2p	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
48	1q	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	15	32
48	2q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	15	32
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	13	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	4 6
51	2t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	4 6
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%)	10749 (94%)	549 (5%)	72 (1%)	25 47

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
23	11	3	LYS
26	14	58	ARG
33	1b	10	LEU

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%)	200 (93%)	15 (7%)	15 30
3	2D	215/218 (99%)	201 (94%)	14 (6%)	17 34
4	1E	164/166 (99%)	151 (92%)	13 (8%)	12 24
4	2E	164/166 (99%)	156 (95%)	8 (5%)	25 48
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11 23
5	2F	159/166 (96%)	147 (92%)	12 (8%)	13 27
6	1G	143/156 (92%)	136 (95%)	7 (5%)	25 48
6	2G	143/156 (92%)	129 (90%)	14 (10%)	8 15
7	1H	144/148 (97%)	137 (95%)	7 (5%)	25 48
7	2H	144/148 (97%)	140 (97%)	4 (3%)	43 69
8	1I	113/124 (91%)	108 (96%)	5 (4%)	28 53
8	2I	105/124 (85%)	96 (91%)	9 (9%)	10 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	1N	118/119 (99%)	111 (94%)	7 (6%)	19	39
9	2N	118/119 (99%)	114 (97%)	4 (3%)	37	63
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	67
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	67
11	1P	115/116 (99%)	110 (96%)	5 (4%)	29	54
11	2P	115/116 (99%)	111 (96%)	4 (4%)	36	62
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	27	52
12	2Q	111/111 (100%)	108 (97%)	3 (3%)	44	71
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	11
13	2R	101/101 (100%)	90 (89%)	11 (11%)	6	11
14	1S	86/88 (98%)	82 (95%)	4 (5%)	26	50
14	2S	85/88 (97%)	84 (99%)	1 (1%)	71	87
15	1T	115/127 (91%)	111 (96%)	4 (4%)	36	62
15	2T	113/127 (89%)	111 (98%)	2 (2%)	59	80
16	1U	93/94 (99%)	89 (96%)	4 (4%)	29	54
16	2U	93/94 (99%)	90 (97%)	3 (3%)	39	65
17	1V	80/82 (98%)	69 (86%)	11 (14%)	3	6
17	2V	80/82 (98%)	71 (89%)	9 (11%)	6	10
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21	42
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	53
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	72
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	72
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	14	29
20	2Y	85/91 (93%)	80 (94%)	5 (6%)	19	39
21	1Z	135/179 (75%)	127 (94%)	8 (6%)	19	39
21	2Z	137/179 (76%)	135 (98%)	2 (2%)	65	83
22	10	65/67 (97%)	62 (95%)	3 (5%)	27	51
22	20	65/67 (97%)	64 (98%)	1 (2%)	65	83
23	11	80/83 (96%)	76 (95%)	4 (5%)	24	47
23	21	80/83 (96%)	76 (95%)	4 (5%)	24	47
24	12	65/67 (97%)	63 (97%)	2 (3%)	40	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	39
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	57
26	14	59/63 (94%)	52 (88%)	7 (12%)	5	9
26	24	53/63 (84%)	51 (96%)	2 (4%)	33	59
27	15	50/52 (96%)	47 (94%)	3 (6%)	19	39
27	25	50/52 (96%)	48 (96%)	2 (4%)	31	57
28	16	51/52 (98%)	49 (96%)	2 (4%)	32	58
28	26	50/52 (96%)	48 (96%)	2 (4%)	31	57
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	9
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	9
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	28
30	28	54/55 (98%)	52 (96%)	2 (4%)	34	60
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	68
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	39
33	1b	192/220 (87%)	186 (97%)	6 (3%)	40	66
33	2b	187/220 (85%)	180 (96%)	7 (4%)	34	60
34	1c	142/188 (76%)	138 (97%)	4 (3%)	43	69
34	2c	140/188 (74%)	134 (96%)	6 (4%)	29	54
35	1d	169/181 (93%)	156 (92%)	13 (8%)	13	25
35	2d	173/181 (96%)	163 (94%)	10 (6%)	20	40
36	1e	113/123 (92%)	108 (96%)	5 (4%)	28	53
36	2e	114/123 (93%)	111 (97%)	3 (3%)	46	72
37	1f	84/90 (93%)	79 (94%)	5 (6%)	19	39
37	2f	85/90 (94%)	82 (96%)	3 (4%)	36	62
38	1g	119/127 (94%)	114 (96%)	5 (4%)	30	55
38	2g	120/127 (94%)	117 (98%)	3 (2%)	47	73
39	1h	114/119 (96%)	108 (95%)	6 (5%)	22	45
39	2h	114/119 (96%)	108 (95%)	6 (5%)	22	45
40	1i	90/99 (91%)	87 (97%)	3 (3%)	38	64
40	2i	89/99 (90%)	84 (94%)	5 (6%)	21	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	1j	66/92 (72%)	63 (96%)	3 (4%)	27	52
41	2j	69/92 (75%)	66 (96%)	3 (4%)	29	54
42	1k	82/99 (83%)	80 (98%)	2 (2%)	49	74
42	2k	83/99 (84%)	82 (99%)	1 (1%)	71	87
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	55
43	2l	96/108 (89%)	92 (96%)	4 (4%)	30	55
44	1m	93/101 (92%)	91 (98%)	2 (2%)	52	76
44	2m	92/101 (91%)	86 (94%)	6 (6%)	17	34
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	14
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	14
46	1o	78/80 (98%)	77 (99%)	1 (1%)	69	86
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69	86
47	1p	69/74 (93%)	66 (96%)	3 (4%)	29	54
47	2p	68/74 (92%)	64 (94%)	4 (6%)	19	39
48	1q	94/97 (97%)	90 (96%)	4 (4%)	29	54
48	2q	94/97 (97%)	93 (99%)	1 (1%)	73	88
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24	46
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16	32
50	1s	69/80 (86%)	68 (99%)	1 (1%)	67	85
50	2s	67/80 (84%)	62 (92%)	5 (8%)	13	27
51	1t	70/82 (85%)	66 (94%)	4 (6%)	20	41
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	42
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8841 (95%)	462 (5%)	24	47

5 of 462 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	1n	33	VAL
45	2n	6	LEU
6	2G	31	VAL
44	2m	64	TRP
35	2d	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
33	2b	40	HIS
38	2g	86	GLN
33	2b	94	ASN
36	2e	78	HIS
40	2i	3	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	431 (15%)	29 (1%)
1	2A	2788/2915 (95%)	482 (17%)	24 (0%)
2	1B	120/121 (99%)	11 (9%)	1 (0%)
2	2B	118/121 (97%)	33 (27%)	0
32	1a	1494/1521 (98%)	238 (15%)	0
32	2a	1498/1521 (98%)	284 (18%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1w	71/76 (93%)	23 (32%)	0
54	1y	71/76 (93%)	19 (26%)	0
54	2w	68/76 (89%)	22 (32%)	0
54	2y	69/76 (90%)	21 (30%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	13 (17%)	0
All	All	9332/9620 (97%)	1593 (17%)	54 (0%)

5 of 1593 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	9	U
1	1A	12	U
1	1A	13	A
1	1A	27	G
1	1A	34	C

5 of 54 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2756	U
1	2A	277	C
1	2A	1992	G

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Mol	Chain	Res	Type
2	1B	1	U
1	2A	266	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	4OC	1a	1402	32	20,23,24	0.77	0	26,32,35	0.94	1 (3%)
32	MA6	2a	1518	32	19,26,27	0.97	1 (5%)	18,38,41	1.67	4 (22%)
1	2MU	1A	2552	56,1	19,22,24	1.18	2 (10%)	26,31,36	1.89	6 (23%)
32	5MC	2a	967	32	18,22,23	0.98	2 (11%)	26,32,35	1.13	3 (11%)
1	2MU	2A	2552	56,1	19,22,24	1.29	3 (15%)	26,31,36	1.80	6 (23%)
32	5MC	1a	1404	32	18,22,23	0.98	2 (11%)	26,32,35	1.14	3 (11%)
54	PSU	1w	39	54	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
54	4SU	1y	8	54	18,21,22	1.67	3 (16%)	26,30,33	1.95	4 (15%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	5MU	1A	1939	56,1	19,22,23	1.40	6 (31%)	28,32,35	2.14	6 (21%)
54	MIA	1w	37	54	24,31,32	2.21	4 (16%)	26,44,47	2.59	10 (38%)
1	PSU	2A	2605	1	18,21,22	1.36	3 (16%)	22,30,33	1.88	4 (18%)
32	MA6	2a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	1.58	3 (16%)
32	7MG	1a	527	32,56	22,26,27	1.38	4 (18%)	29,39,42	2.49	8 (27%)
54	PSU	2w	39	54	18,21,22	1.34	2 (11%)	22,30,33	1.70	3 (13%)
1	PSU	1A	1917	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
55	4SU	2x	8	55,56	18,21,22	1.95	5 (27%)	26,30,33	1.75	7 (26%)
1	5MC	2A	1942	1	18,22,23	0.97	2 (11%)	26,32,35	1.12	2 (7%)
54	PSU	2y	55	54	18,21,22	1.32	2 (11%)	22,30,33	1.88	4 (18%)
54	PSU	1y	55	54	18,21,22	1.32	2 (11%)	22,30,33	1.88	3 (13%)
32	5MC	1a	1407	32	18,22,23	0.94	2 (11%)	26,32,35	1.14	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	5MU	1w	54	54	19,22,23	1.37	5 (26%)	28,32,35	2.14	8 (28%)
32	5MC	2a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.10	2 (7%)
32	5MC	1a	967	32	18,22,23	0.95	2 (11%)	26,32,35	1.14	2 (7%)
54	7MG	1w	46	54	22,26,27	1.44	4 (18%)	29,39,42	2.44	6 (20%)
55	5MU	2x	54	55	19,22,23	1.41	6 (31%)	28,32,35	2.01	6 (21%)
32	PSU	1a	516	32	18,21,22	1.34	2 (11%)	22,30,33	1.81	3 (13%)
54	PSU	2y	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
32	2MG	2a	1207	32	18,26,27	0.92	1 (5%)	16,38,41	1.06	1 (6%)
1	5MC	1A	1962	56,1	18,22,23	0.90	2 (11%)	26,32,35	1.11	2 (7%)
32	7MG	2a	527	32,56	22,26,27	1.34	4 (18%)	29,39,42	2.51	7 (24%)
54	7MG	2w	46	54	22,26,27	1.38	4 (18%)	29,39,42	2.44	7 (24%)
54	MIA	2y	37	54	18,24,32	1.11	2 (11%)	18,35,47	1.26	2 (11%)
54	PSU	1w	55	54	18,21,22	1.40	2 (11%)	22,30,33	1.96	3 (13%)
32	5MC	2a	1407	32	18,22,23	0.93	2 (11%)	26,32,35	1.10	2 (7%)
54	4SU	1w	8	54	18,21,22	1.72	5 (27%)	26,30,33	1.84	5 (19%)
55	5MC	1x	32	55	18,22,23	0.99	2 (11%)	26,32,35	1.22	2 (7%)
1	5MU	1A	1915	1	19,22,23	1.44	5 (26%)	28,32,35	2.06	5 (17%)
32	2MG	1a	1207	32	18,26,27	0.92	1 (5%)	16,38,41	1.10	2 (12%)
54	5MU	1y	54	54	19,22,23	1.41	5 (26%)	28,32,35	2.10	6 (21%)
32	5MC	2a	1404	32	18,22,23	1.01	2 (11%)	26,32,35	1.19	3 (11%)
54	PSU	2w	55	54	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
54	PSU	1w	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.79	3 (13%)
1	OMG	2A	2251	56,55,1	18,26,27	0.95	1 (5%)	19,38,41	1.05	2 (10%)
54	7MG	2y	46	54	22,26,27	1.34	3 (13%)	29,39,42	2.62	6 (20%)
1	2MA	1A	2503	56,1	17,25,26	0.99	1 (5%)	17,37,40	1.00	2 (11%)
32	MA6	1a	1518	32	19,26,27	0.96	1 (5%)	18,38,41	1.69	5 (27%)
1	2MA	2A	2503	56,1	17,25,26	1.04	1 (5%)	17,37,40	0.93	2 (11%)
1	PSU	2A	1911	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
54	4SU	2y	8	54	18,21,22	1.78	5 (27%)	26,30,33	1.98	5 (19%)
55	PSU	1x	55	55,56	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	5MU	2A	1915	1	19,22,23	1.44	5 (26%)	28,32,35	2.03	6 (21%)
55	5MU	1x	54	55,56	19,22,23	1.42	5 (26%)	28,32,35	1.96	6 (21%)
43	0TD	2l	92	43	7,9,10	4.71	1 (14%)	6,11,13	3.45	3 (50%)
1	5MU	2A	1939	56,1	19,22,23	1.42	5 (26%)	28,32,35	2.22	6 (21%)
1	4OC	2A	1920	1	19,22,24	0.81	0	26,31,35	0.88	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	5MU	2w	54	54	19,22,23	1.37	6 (31%)	28,32,35	1.84	7 (25%)
54	5MU	2y	54	54	19,22,23	1.43	6 (31%)	28,32,35	1.83	6 (21%)
54	7MG	1y	46	54	22,26,27	1.34	4 (18%)	29,39,42	2.50	6 (20%)
54	PSU	1y	39	54	18,21,22	1.31	2 (11%)	22,30,33	1.91	3 (13%)
32	M2G	2a	966	32	20,27,28	1.46	3 (15%)	22,40,43	0.96	2 (9%)
54	4SU	2w	8	54	18,21,22	1.70	4 (22%)	26,30,33	2.57	6 (23%)
1	PSU	1A	2605	56,1	18,21,22	1.35	2 (11%)	22,30,33	1.78	3 (13%)
55	4SU	1x	8	55	18,21,22	2.05	6 (33%)	26,30,33	1.59	5 (19%)
32	5MC	1a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.13	3 (11%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	1A	2251	56,55,1	18,26,27	0.89	1 (5%)	19,38,41	1.13	3 (15%)
54	PSU	2w	32	54	18,21,22	1.33	2 (11%)	22,30,33	1.84	3 (13%)
54	MIA	2w	37	54	20,27,32	1.75	3 (15%)	22,39,47	1.80	7 (31%)
55	5MC	2x	32	55	18,22,23	0.98	2 (11%)	26,32,35	1.16	3 (11%)
54	PSU	2y	39	54	18,21,22	1.32	2 (11%)	22,30,33	1.85	4 (18%)
43	0TD	1l	92	43	7,9,10	4.77	1 (14%)	6,11,13	4.79	3 (50%)
32	M2G	1a	966	32	20,27,28	1.41	3 (15%)	22,40,43	0.89	2 (9%)
1	5MC	1A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.13	2 (7%)
54	PSU	1y	32	54	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
54	MIA	1y	37	54	18,24,32	1.11	2 (11%)	18,35,47	1.28	2 (11%)
32	UR3	2a	1498	32	19,22,23	1.04	2 (10%)	26,32,35	1.48	2 (7%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	22,30,33	1.77	3 (13%)
32	4OC	2a	1402	32,56	20,23,24	0.78	0	26,32,35	0.96	1 (3%)
32	MA6	1a	1519	32	19,26,27	1.01	1 (5%)	18,38,41	1.63	4 (22%)
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
32	UR3	1a	1498	32	19,22,23	1.01	1 (5%)	26,32,35	1.44	2 (7%)
1	5MC	2A	1962	56,1	18,22,23	0.94	2 (11%)	26,32,35	1.13	2 (7%)
1	4OC	1A	1920	1	19,22,24	0.82	0	26,31,35	0.92	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1518	32	-	2/7/29/30	0/3/3/3
1	2MU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	56,1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	6/7/29/30	0/3/3/3
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
54	PSU	2w	39	54	-	2/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	1/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	1/7/37/38	0/3/3/3
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
54	MIA	2y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
54	5MU	1y	54	54	-	1/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	56,55,1	-	1/5/27/28	0/3/3/3
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
1	2MA	1A	2503	56,1	-	2/3/25/26	0/3/3/3
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
1	2MA	2A	2503	56,1	-	1/3/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	2/7/25/26	0/2/2/2
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
1	5MU	2A	1939	56,1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	3/7/37/38	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	56,55,1	-	0/5/27/28	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	56,1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	1/9/27/30	0/2/2/2

The worst 5 of 215 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.32	1.69	1.82
43	2l	92	0TD	CB-SB	-12.18	1.69	1.82
54	1w	37	MIA	C13-C14	7.14	1.52	1.32
54	1w	37	MIA	C2-S10	-6.54	1.70	1.75
54	2w	37	MIA	C2-S10	-6.28	1.70	1.75

The worst 5 of 315 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-10.98	82.57	102.44
54	2y	46	7MG	N9-C4-N3	9.61	139.84	125.47
54	1y	46	7MG	N9-C4-N3	9.00	138.94	125.47
32	2a	527	7MG	N9-C4-N3	8.90	138.78	125.47
32	1a	527	7MG	N9-C4-N3	8.71	138.49	125.47

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2840 ligands modelled in this entry, 2836 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	$\#\|Z\| > 2$
57	CLM	2A	3888	-	19,20,20	0.94	2 (10%)	23,27,27	1.01	1 (4%)
57	CLM	1A	4102	-	19,20,20	0.92	1 (5%)	23,27,27	0.75	0
60	SF4	2d	302	35	0,12,12	-	-	-		
60	SF4	1d	302	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CLM	2A	3888	-	-	6/20/22/22	0/1/1/1
57	CLM	1A	4102	-	-	7/20/22/22	0/1/1/1
60	SF4	2d	302	35	-	-	0/6/5/5
60	SF4	1d	302	35	-	-	0/6/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3888	CLM	C6-C5	-2.42	1.48	1.51
57	1A	4102	CLM	C6-C5	-2.10	1.48	1.51
57	2A	3888	CLM	C9-N9	-2.09	1.40	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	2A	3888	CLM	C6-C5-C3	-2.83	106.66	111.64

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

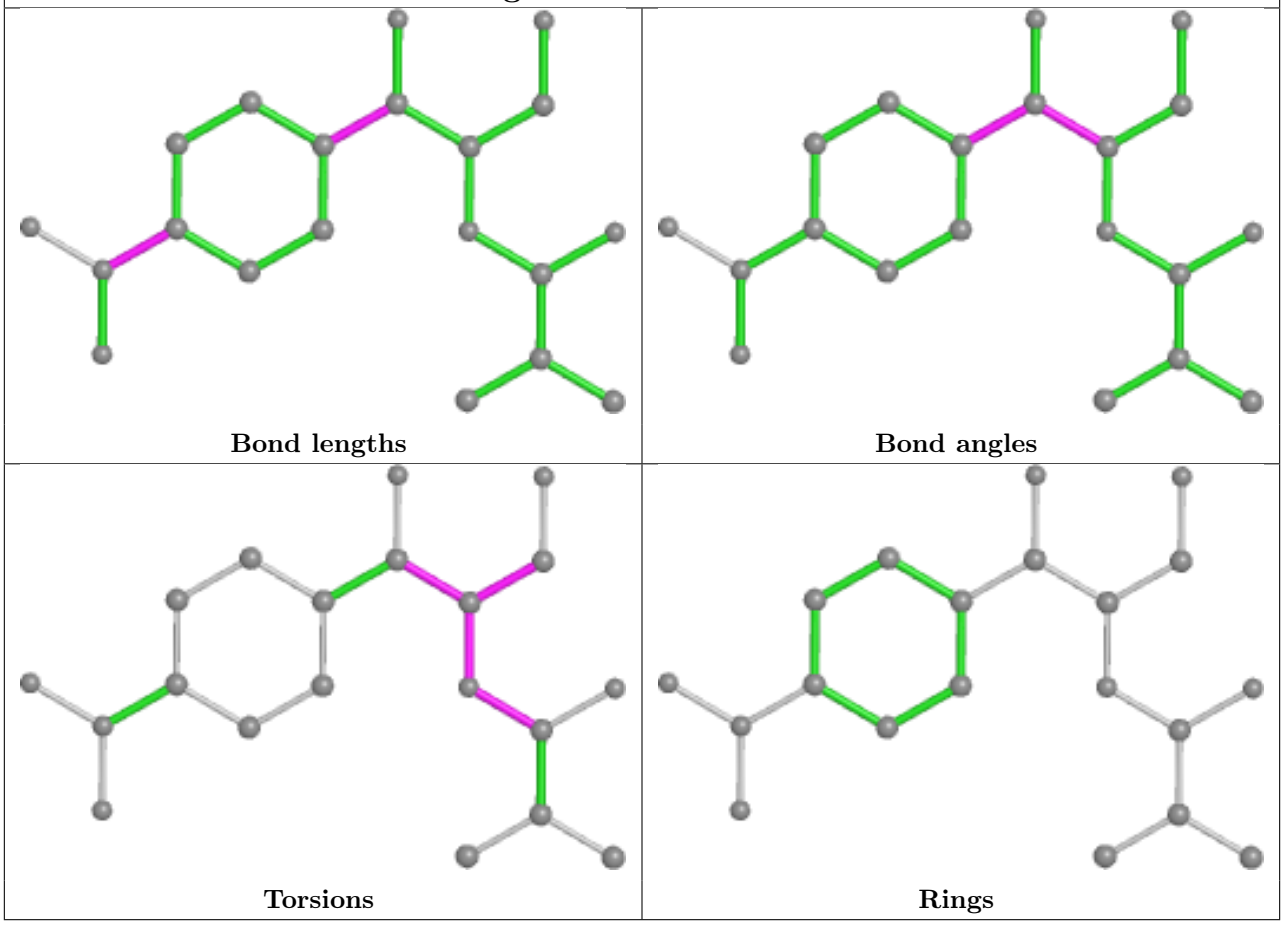
Mol	Chain	Res	Type	Atoms
57	2A	3888	CLM	C1-C2-N2-C3
57	2A	3888	CLM	O2-C2-N2-C3
57	2A	3888	CLM	C4-C3-N2-C2
57	2A	3888	CLM	N2-C3-C4-O4
57	2A	3888	CLM	C5-C3-C4-O4

There are no ring outliers.

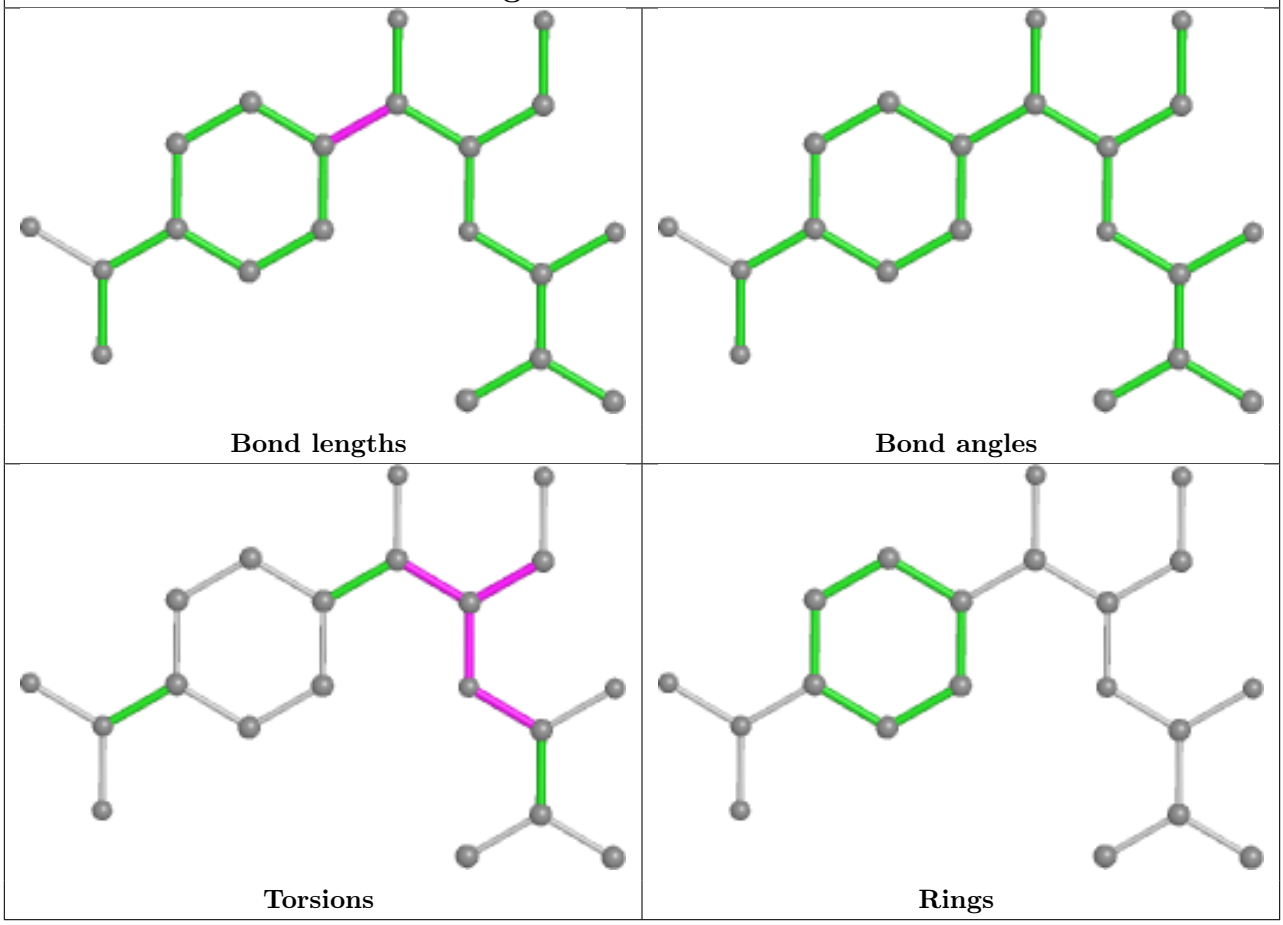
No monomer is involved in short contacts.

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

Ligand CLM 2A 3888



Ligand CLM 1A 4102



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%)	0.40	45 (1%)	72	68	17, 34, 87, 101	0
1	2A	2789/2915 (95%)	0.16	58 (2%)	63	58	34, 57, 87, 102	0
2	1B	120/121 (99%)	0.09	0	100	100	27, 48, 58, 79	0
2	2B	120/121 (99%)	-0.34	0	100	100	58, 78, 85, 87	0
3	1D	275/276 (99%)	0.48	5 (1%)	68	64	20, 35, 50, 73	0
3	2D	275/276 (99%)	0.70	12 (4%)	34	27	33, 51, 62, 73	0
4	1E	204/206 (99%)	0.53	2 (0%)	82	80	18, 40, 57, 73	0
4	2E	204/206 (99%)	0.45	7 (3%)	45	38	35, 58, 69, 79	0
5	1F	203/210 (96%)	0.36	0	100	100	16, 41, 63, 80	0
5	2F	203/210 (96%)	0.57	7 (3%)	45	38	37, 64, 77, 83	0
6	1G	181/182 (99%)	0.15	1 (0%)	89	88	39, 56, 69, 78	0
6	2G	181/182 (99%)	0.73	23 (12%)	3	2	68, 77, 85, 93	0
7	1H	174/180 (96%)	0.12	0	100	100	37, 50, 62, 71	0
7	2H	174/180 (96%)	1.38	47 (27%)	0	0	67, 78, 84, 91	0
8	1I	146/148 (98%)	0.05	2 (1%)	75	71	45, 70, 77, 81	0
8	2I	146/148 (98%)	0.33	11 (7%)	14	10	53, 70, 80, 85	0
9	1N	140/140 (100%)	0.37	1 (0%)	87	86	26, 38, 54, 72	0
9	2N	140/140 (100%)	1.15	29 (20%)	1	0	46, 64, 75, 80	0
10	1O	122/122 (100%)	0.46	0	100	100	26, 40, 55, 61	0
10	2O	122/122 (100%)	0.59	5 (4%)	37	30	44, 57, 68, 73	0
11	1P	149/150 (99%)	0.72	5 (3%)	45	38	17, 44, 64, 72	0
11	2P	149/150 (99%)	1.50	45 (30%)	0	0	38, 64, 77, 83	0
12	1Q	141/141 (100%)	0.38	1 (0%)	87	86	27, 41, 54, 74	0
12	2Q	141/141 (100%)	0.79	15 (10%)	6	4	52, 65, 74, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.41	0	100	100	22, 34, 47, 55	0
13	2R	118/118 (100%)	0.36	0	100	100	38, 51, 59, 67	0
14	1S	110/112 (98%)	0.16	0	100	100	37, 49, 61, 65	0
14	2S	110/112 (98%)	0.55	10 (9%)	9	6	63, 73, 80, 84	0
15	1T	131/146 (89%)	0.47	0	100	100	33, 43, 64, 70	0
15	2T	131/146 (89%)	0.35	4 (3%)	49	42	49, 59, 74, 79	0
16	1U	116/118 (98%)	0.48	1 (0%)	84	82	20, 29, 47, 60	0
16	2U	116/118 (98%)	1.01	17 (14%)	2	1	47, 61, 74, 80	0
17	1V	101/101 (100%)	0.35	0	100	100	20, 39, 56, 69	0
17	2V	101/101 (100%)	0.95	14 (13%)	2	1	42, 68, 76, 82	0
18	1W	112/113 (99%)	0.40	0	100	100	21, 30, 46, 75	0
18	2W	112/113 (99%)	0.56	2 (1%)	68	64	38, 50, 66, 88	0
19	1X	95/96 (98%)	0.30	0	100	100	24, 36, 55, 72	0
19	2X	95/96 (98%)	0.31	3 (3%)	47	40	44, 58, 70, 81	0
20	1Y	107/110 (97%)	0.28	0	100	100	33, 48, 66, 74	0
20	2Y	107/110 (97%)	1.02	17 (15%)	1	1	59, 68, 75, 84	0
21	1Z	154/206 (74%)	0.13	1 (0%)	89	88	41, 60, 77, 85	0
21	2Z	160/206 (77%)	0.44	4 (2%)	57	51	66, 78, 86, 88	0
22	10	83/85 (97%)	0.80	7 (8%)	11	7	27, 37, 60, 72	0
22	20	83/85 (97%)	1.50	19 (22%)	0	0	53, 64, 74, 83	0
23	11	97/98 (98%)	0.51	2 (2%)	63	58	24, 43, 63, 68	0
23	21	97/98 (98%)	1.11	16 (16%)	1	1	40, 56, 71, 73	0
24	12	70/72 (97%)	0.20	1 (1%)	75	71	32, 46, 57, 65	0
24	22	70/72 (97%)	0.43	1 (1%)	75	71	54, 68, 73, 76	0
25	13	59/60 (98%)	0.40	1 (1%)	70	66	25, 36, 58, 78	0
25	23	59/60 (98%)	2.02	27 (45%)	0	0	53, 64, 77, 79	0
26	14	69/71 (97%)	-0.07	0	100	100	49, 71, 81, 85	0
26	24	69/71 (97%)	0.26	7 (10%)	7	4	76, 82, 88, 91	0
27	15	59/60 (98%)	0.44	1 (1%)	70	66	18, 29, 45, 63	0
27	25	59/60 (98%)	0.33	2 (3%)	45	38	38, 50, 63, 67	0
28	16	53/54 (98%)	0.58	0	100	100	30, 41, 55, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	1.21	10 (18%) 1 0	49, 61, 68, 75	0
29	17	48/49 (97%)	0.70	3 (6%) 20 15	18, 24, 52, 58	0
29	27	48/49 (97%)	1.07	7 (14%) 2 1	32, 41, 60, 68	0
30	18	64/65 (98%)	0.76	2 (3%) 49 42	26, 31, 38, 54	0
30	28	64/65 (98%)	1.55	17 (26%) 0 0	45, 54, 60, 71	0
31	19	37/37 (100%)	0.27	0 100 100	27, 38, 54, 57	0
31	29	37/37 (100%)	1.47	11 (29%) 0 0	59, 66, 73, 76	0
32	1a	1488/1521 (97%)	-0.02	24 (1%) 72 68	33, 65, 87, 100	0
32	2a	1491/1521 (98%)	0.10	50 (3%) 45 38	50, 75, 91, 99	0
33	1b	231/256 (90%)	0.21	7 (3%) 50 43	63, 74, 82, 87	0
33	2b	231/256 (90%)	1.42	63 (27%) 0 0	71, 83, 88, 92	0
34	1c	206/239 (86%)	0.94	35 (16%) 1 1	59, 70, 78, 83	0
34	2c	206/239 (86%)	1.89	90 (43%) 0 0	72, 82, 87, 91	0
35	1d	208/209 (99%)	0.51	12 (5%) 23 17	56, 69, 80, 84	0
35	2d	208/209 (99%)	0.27	3 (1%) 75 71	57, 67, 75, 82	0
36	1e	148/162 (91%)	0.40	3 (2%) 65 60	49, 63, 70, 76	0
36	2e	148/162 (91%)	0.76	19 (12%) 3 2	67, 76, 81, 88	0
37	1f	100/101 (99%)	0.21	0 100 100	50, 64, 70, 73	0
37	2f	100/101 (99%)	0.16	2 (2%) 65 60	60, 70, 77, 81	0
38	1g	155/156 (99%)	0.97	19 (12%) 4 2	50, 67, 76, 87	0
38	2g	155/156 (99%)	1.36	33 (21%) 0 0	66, 75, 82, 88	0
39	1h	137/138 (99%)	0.55	5 (3%) 42 35	56, 64, 71, 75	0
39	2h	137/138 (99%)	0.69	11 (8%) 12 9	67, 75, 80, 86	0
40	1i	127/128 (99%)	0.67	10 (7%) 12 9	52, 72, 77, 79	0
40	2i	127/128 (99%)	2.01	56 (44%) 0 0	68, 80, 86, 89	0
41	1j	97/105 (92%)	1.06	15 (15%) 2 1	58, 76, 83, 89	0
41	2j	96/105 (91%)	2.13	48 (50%) 0 0	71, 82, 88, 96	0
42	1k	114/129 (88%)	1.15	17 (14%) 2 1	38, 61, 70, 74	0
42	2k	114/129 (88%)	1.20	22 (19%) 1 0	56, 72, 77, 82	0
43	1l	121/132 (91%)	0.34	3 (2%) 57 51	42, 56, 66, 69	0
43	2l	121/132 (91%)	0.72	12 (9%) 7 5	58, 69, 76, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.06	5 (4%) 37 30	55, 67, 75, 81	0
44	2m	122/126 (96%)	1.72	43 (35%) 0 0	71, 79, 85, 88	0
45	1n	60/61 (98%)	1.16	12 (20%) 1 0	60, 68, 73, 76	0
45	2n	60/61 (98%)	3.35	44 (73%) 0 0	74, 82, 86, 90	0
46	1o	88/89 (98%)	0.34	2 (2%) 60 54	48, 60, 70, 74	0
46	2o	88/89 (98%)	0.54	4 (4%) 33 26	60, 70, 78, 82	0
47	1p	82/88 (93%)	0.85	5 (6%) 21 16	56, 70, 76, 79	0
47	2p	82/88 (93%)	0.22	0 100 100	58, 65, 74, 80	0
48	1q	99/105 (94%)	0.52	2 (2%) 65 60	50, 63, 71, 73	0
48	2q	99/105 (94%)	1.01	17 (17%) 1 0	62, 69, 77, 81	0
49	1r	68/88 (77%)	0.75	6 (8%) 10 7	55, 64, 73, 75	0
49	2r	68/88 (77%)	0.57	6 (8%) 10 7	62, 71, 78, 82	0
50	1s	83/93 (89%)	0.00	0 100 100	60, 70, 77, 80	0
50	2s	83/93 (89%)	1.58	27 (32%) 0 0	75, 82, 87, 91	0
51	1t	96/106 (90%)	0.41	6 (6%) 20 15	58, 68, 76, 81	0
51	2t	96/106 (90%)	0.68	11 (11%) 4 3	57, 69, 76, 79	0
52	1u	23/27 (85%)	0.85	3 (13%) 3 2	59, 64, 69, 71	0
52	2u	23/27 (85%)	2.05	11 (47%) 0 0	74, 77, 81, 85	0
53	1v	13/24 (54%)	1.28	5 (38%) 0 0	47, 66, 80, 86	0
53	2v	13/24 (54%)	1.67	5 (38%) 0 0	69, 82, 92, 92	0
54	1w	67/76 (88%)	1.66	19 (28%) 0 0	59, 87, 94, 98	0
54	1y	67/76 (88%)	1.36	18 (26%) 0 0	38, 86, 93, 96	0
54	2w	65/76 (85%)	2.95	39 (60%) 0 0	74, 91, 96, 101	0
54	2y	66/76 (86%)	1.92	33 (50%) 0 0	57, 92, 96, 99	0
55	1x	72/77 (93%)	0.22	1 (1%) 75 71	37, 62, 77, 85	0
55	2x	72/77 (93%)	0.15	1 (1%) 75 71	55, 78, 86, 89	0
All	All	20875/21748 (95%)	0.50	1412 (6%) 17 12	16, 62, 85, 102	0

The worst 5 of 1412 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	11.9
38	2g	80	VAL	11.5

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Mol	Chain	Res	Type	RSRZ
54	1w	71	G	10.9
38	1g	80	VAL	10.4
44	2m	6	GLY	9.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.69	0.47	90,96,107,107	0
54	PSU	2w	55	20/21	0.74	0.30	81,91,96,98	0
54	4SU	2w	8	20/21	0.74	0.21	83,93,104,117	0
54	7MG	2y	46	24/25	0.76	0.31	86,95,102,123	0
54	PSU	1y	55	20/21	0.76	0.26	80,89,98,103	0
54	7MG	1w	46	24/25	0.79	0.17	77,89,99,107	0
54	7MG	2w	46	24/25	0.79	0.23	80,93,101,121	0
54	5MU	2y	54	21/22	0.80	0.39	84,91,99,112	0
54	5MU	1y	54	21/22	0.82	0.30	79,85,91,97	0
54	4SU	1y	8	20/21	0.83	0.21	81,89,98,99	0
54	MIA	2y	37	22/30	0.83	0.26	75,87,99,109	0
54	PSU	2y	32	20/21	0.84	0.25	79,85,93,102	0
54	7MG	1y	46	24/25	0.85	0.32	79,90,98,101	0
54	PSU	2y	39	20/21	0.85	0.26	79,84,92,96	0
54	4SU	1w	8	20/21	0.86	0.17	80,85,93,94	0
54	4SU	2y	8	20/21	0.86	0.21	88,93,99,104	0
54	PSU	1y	32	20/21	0.86	0.29	78,82,87,88	0
55	4SU	2x	8	20/21	0.86	0.17	73,79,87,90	0
54	PSU	2w	39	20/21	0.87	0.42	81,86,88,92	0
54	MIA	2w	37	25/30	0.87	0.27	75,82,88,103	0
32	M2G	2a	966	25/26	0.87	0.24	60,69,84,86	0
54	PSU	2w	32	20/21	0.88	0.43	78,85,93,97	0
43	0TD	2l	92	10/11	0.89	0.21	67,71,72,79	0
1	5MU	2A	1915	21/22	0.89	0.17	74,78,84,94	0
32	2MG	2a	1207	24/25	0.89	0.15	63,83,92,95	0
54	PSU	1w	55	20/21	0.89	0.17	74,83,92,95	0
54	PSU	1w	32	20/21	0.90	0.26	65,76,82,84	0
54	MIA	1y	37	22/30	0.91	0.26	74,78,84,85	0
54	5MU	2w	54	21/22	0.91	0.21	67,82,87,93	0
32	PSU	2a	516	20/21	0.91	0.15	70,77,83,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
43	0TD	1l	92	10/11	0.91	0.19	47,55,60,75	0
55	5MU	2x	54	21/22	0.91	0.21	68,77,82,94	0
55	PSU	2x	55	20/21	0.91	0.17	72,80,82,85	0
54	MIA	1w	37	29/30	0.92	0.22	56,65,72,74	0
1	PSU	2A	1917	20/21	0.92	0.16	62,71,81,87	0
32	5MC	2a	967	21/22	0.92	0.18	61,70,78,82	0
1	PSU	2A	1911	20/21	0.92	0.17	60,66,73,75	0
54	PSU	1w	39	20/21	0.93	0.25	67,74,85,85	0
54	PSU	1y	39	20/21	0.93	0.21	74,76,80,80	0
1	4OC	2A	1920	21/23	0.94	0.20	61,65,67,71	0
32	5MC	2a	1404	21/22	0.94	0.19	56,60,65,68	0
32	5MC	1a	967	21/22	0.94	0.21	52,59,63,64	0
55	5MC	2x	32	21/22	0.94	0.20	60,73,78,82	0
1	5MU	1A	1915	21/22	0.94	0.17	56,61,68,71	0
54	5MU	1w	54	21/22	0.94	0.17	64,72,79,82	0
32	PSU	1a	516	20/21	0.95	0.12	60,66,71,71	0
32	5MC	2a	1400	21/22	0.95	0.17	60,69,76,83	0
1	PSU	1A	1917	20/21	0.95	0.19	48,57,62,63	0
55	4SU	1x	8	20/21	0.95	0.17	51,59,65,71	0
32	4OC	2a	1402	22/23	0.95	0.16	53,65,69,70	0
32	2MG	1a	1207	24/25	0.95	0.14	59,67,73,75	0
55	5MU	1x	54	21/22	0.95	0.15	51,64,70,76	0
32	5MC	2a	1407	21/22	0.95	0.17	53,59,63,64	0
55	PSU	1x	55	20/21	0.95	0.18	49,63,70,73	0
32	UR3	2a	1498	21/22	0.95	0.20	55,61,65,66	0
32	7MG	2a	527	24/25	0.96	0.15	63,66,72,76	0
32	MA6	2a	1518	24/25	0.96	0.24	55,65,68,71	0
55	5MC	1x	32	21/22	0.96	0.23	46,54,60,74	0
32	MA6	2a	1519	24/25	0.96	0.28	52,63,67,69	0
1	5MC	2A	1942	21/22	0.96	0.18	54,60,66,68	0
1	2MA	2A	2503	23/24	0.96	0.23	32,36,43,45	0
32	7MG	1a	527	24/25	0.96	0.19	42,49,57,58	0
1	4OC	1A	1920	21/23	0.96	0.22	37,44,48,53	0
1	5MU	2A	1939	21/22	0.97	0.23	36,44,49,51	0
32	M2G	1a	966	25/26	0.97	0.19	49,55,59,66	0
1	PSU	1A	1911	20/21	0.97	0.20	40,49,57,57	0
1	5MC	2A	1962	21/22	0.97	0.17	40,52,59,68	0
1	OMG	2A	2251	24/25	0.97	0.24	42,45,51,56	0
32	5MC	1a	1400	21/22	0.97	0.20	39,50,54,59	0
1	5MC	1A	1942	21/22	0.97	0.20	31,40,43,49	0
1	2MU	2A	2552	21/23	0.97	0.23	35,42,46,62	0
32	4OC	1a	1402	22/23	0.97	0.21	37,45,51,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	5MC	1a	1407	21/22	0.97	0.22	36,41,43,45	0
32	MA6	1a	1519	24/25	0.97	0.21	38,42,47,50	0
1	2MA	1A	2503	23/24	0.98	0.22	14,21,24,31	0
1	2MU	1A	2552	21/23	0.98	0.20	21,29,33,39	0
32	UR3	1a	1498	21/22	0.98	0.21	39,43,46,48	0
1	PSU	1A	2605	20/21	0.98	0.21	19,26,35,35	0
1	PSU	2A	2605	20/21	0.98	0.18	34,42,47,47	0
32	MA6	1a	1518	24/25	0.98	0.23	34,41,45,49	0
1	5MU	1A	1939	21/22	0.98	0.21	23,29,33,40	0
32	5MC	1a	1404	21/22	0.98	0.19	35,41,44,44	0
1	5MC	1A	1962	21/22	0.98	0.21	29,36,41,44	0
1	OMG	1A	2251	24/25	0.98	0.22	19,25,28,29	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3819	1/1	0.09	0.29	69,69,69,69	0
56	MG	1A	3982	1/1	0.14	0.30	77,77,77,77	0
56	MG	2a	3173	1/1	0.20	0.21	70,70,70,70	0
56	MG	2a	3136	1/1	0.28	0.30	78,78,78,78	0
56	MG	1a	1807	1/1	0.33	0.12	66,66,66,66	0
56	MG	1A	4000	1/1	0.33	0.17	62,62,62,62	0
56	MG	1A	4043	1/1	0.34	0.34	66,66,66,66	0
56	MG	2A	3817	1/1	0.40	0.29	75,75,75,75	0
56	MG	1A	3979	1/1	0.40	0.23	69,69,69,69	0
56	MG	1A	4061	1/1	0.41	0.14	68,68,68,68	0
56	MG	1a	1790	1/1	0.42	0.12	74,74,74,74	0
56	MG	1a	1784	1/1	0.43	0.21	56,56,56,56	0
56	MG	1A	3801	1/1	0.44	0.13	53,53,53,53	0
56	MG	1A	3924	1/1	0.46	0.14	71,71,71,71	0
56	MG	2A	3828	1/1	0.46	0.10	59,59,59,59	0
56	MG	2A	3864	1/1	0.47	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	2a	3070	1/1	0.48	0.25	68,68,68,68	0
56	MG	2A	3855	1/1	0.48	0.20	74,74,74,74	0
56	MG	1a	1793	1/1	0.48	0.11	78,78,78,78	0
56	MG	1A	3771	1/1	0.49	0.17	19,19,19,19	0
56	MG	1a	1655	1/1	0.49	0.19	76,76,76,76	0
56	MG	1A	4067	1/1	0.50	0.14	55,55,55,55	0
56	MG	2A	3040	1/1	0.50	0.57	88,88,88,88	0
56	MG	2a	3101	1/1	0.52	0.16	68,68,68,68	0
56	MG	2A	3532	1/1	0.53	0.14	61,61,61,61	0
56	MG	2A	3285	1/1	0.53	0.23	62,62,62,62	0
56	MG	2a	3167	1/1	0.54	0.07	75,75,75,75	0
56	MG	1A	3980	1/1	0.54	0.11	62,62,62,62	0
56	MG	1a	1731	1/1	0.56	0.21	69,69,69,69	0
56	MG	2A	3830	1/1	0.56	0.17	77,77,77,77	0
56	MG	2A	3650	1/1	0.56	0.21	67,67,67,67	0
56	MG	2a	3178	1/1	0.56	0.38	91,91,91,91	0
56	MG	2a	3149	1/1	0.57	0.07	76,76,76,76	0
56	MG	1a	1812	1/1	0.57	0.13	62,62,62,62	0
56	MG	1A	4056	1/1	0.58	0.14	45,45,45,45	0
56	MG	2A	3640	1/1	0.58	0.18	64,64,64,64	0
56	MG	2a	3188	1/1	0.58	0.14	59,59,59,59	0
56	MG	2a	3196	1/1	0.58	0.12	76,76,76,76	0
56	MG	2a	3176	1/1	0.59	0.12	72,72,72,72	0
56	MG	1A	3985	1/1	0.59	0.17	61,61,61,61	0
56	MG	2a	3182	1/1	0.59	0.07	83,83,83,83	0
56	MG	1A	3332	1/1	0.59	0.20	57,57,57,57	0
56	MG	1A	4083	1/1	0.59	0.17	51,51,51,51	0
56	MG	2a	3199	1/1	0.59	0.12	70,70,70,70	0
56	MG	1A	3998	1/1	0.60	0.25	67,67,67,67	0
56	MG	1a	1714	1/1	0.60	0.22	62,62,62,62	0
56	MG	2a	3142	1/1	0.60	0.08	68,68,68,68	0
56	MG	2a	3031	1/1	0.61	0.60	69,69,69,69	0
56	MG	1a	1766	1/1	0.61	0.13	61,61,61,61	0
56	MG	1A	3661	1/1	0.62	0.18	29,29,29,29	0
56	MG	2D	308	1/1	0.62	0.12	39,39,39,39	0
56	MG	1a	1824	1/1	0.62	0.10	60,60,60,60	0
56	MG	1a	1789	1/1	0.62	0.20	77,77,77,77	0
56	MG	1A	3784	1/1	0.62	0.09	66,66,66,66	0
56	MG	1A	4032	1/1	0.62	0.36	57,57,57,57	0
56	MG	2A	3844	1/1	0.62	0.18	72,72,72,72	0
56	MG	1A	3996	1/1	0.62	0.16	51,51,51,51	0
56	MG	1A	3844	1/1	0.64	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3779	1/1	0.64	0.11	71,71,71,71	0
56	MG	2A	3321	1/1	0.64	0.32	65,65,65,65	0
56	MG	1a	1800	1/1	0.64	0.09	50,50,50,50	0
56	MG	2A	3570	1/1	0.64	0.11	48,48,48,48	0
56	MG	1A	4081	1/1	0.64	0.10	44,44,44,44	0
56	MG	1A	3697	1/1	0.65	0.21	38,38,38,38	0
56	MG	1A	4049	1/1	0.65	0.18	54,54,54,54	0
56	MG	2A	3029	1/1	0.65	0.19	62,62,62,62	0
56	MG	1A	4052	1/1	0.65	0.23	48,48,48,48	0
56	MG	2A	3734	1/1	0.65	0.16	52,52,52,52	0
56	MG	2a	3193	1/1	0.65	0.16	82,82,82,82	0
56	MG	1a	1803	1/1	0.65	0.09	61,61,61,61	0
56	MG	1A	4068	1/1	0.65	0.18	61,61,61,61	0
56	MG	2A	3859	1/1	0.66	0.14	60,60,60,60	0
56	MG	2A	3048	1/1	0.66	0.19	65,65,65,65	0
56	MG	2A	3618	1/1	0.66	0.10	49,49,49,49	0
56	MG	2a	3120	1/1	0.66	0.20	66,66,66,66	0
56	MG	2w	102	1/1	0.66	0.16	72,72,72,72	0
56	MG	2A	3833	1/1	0.67	0.10	53,53,53,53	0
56	MG	2a	3180	1/1	0.67	0.10	71,71,71,71	0
56	MG	1a	1660	1/1	0.68	0.14	72,72,72,72	0
56	MG	1a	1753	1/1	0.68	0.18	53,53,53,53	0
56	MG	1A	3292	1/1	0.68	0.15	57,57,57,57	0
56	MG	2A	3214	1/1	0.68	0.14	62,62,62,62	0
56	MG	2A	3798	1/1	0.68	0.10	51,51,51,51	0
56	MG	2A	3848	1/1	0.68	0.09	74,74,74,74	0
56	MG	2A	3247	1/1	0.68	0.35	70,70,70,70	0
56	MG	1A	3411	1/1	0.69	0.52	57,57,57,57	0
56	MG	2a	3015	1/1	0.69	0.18	69,69,69,69	0
56	MG	1A	3512	1/1	0.69	0.26	60,60,60,60	0
56	MG	2a	3052	1/1	0.69	0.16	56,56,56,56	0
56	MG	1A	4033	1/1	0.69	0.16	55,55,55,55	0
56	MG	2A	3780	1/1	0.69	0.09	69,69,69,69	0
56	MG	1e	201	1/1	0.69	0.17	73,73,73,73	0
56	MG	2A	3812	1/1	0.69	0.42	76,76,76,76	0
56	MG	2A	3637	1/1	0.69	0.18	47,47,47,47	0
56	MG	1A	3300	1/1	0.69	0.16	44,44,44,44	0
56	MG	2a	3165	1/1	0.69	0.08	78,78,78,78	0
56	MG	1A	3767	1/1	0.70	0.22	30,30,30,30	0
56	MG	1A	3928	1/1	0.70	0.22	69,69,69,69	0
56	MG	2A	3805	1/1	0.70	0.09	67,67,67,67	0
56	MG	1a	1798	1/1	0.70	0.16	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3165	1/1	0.70	0.33	39,39,39,39	0
56	MG	1A	3605	1/1	0.70	0.22	37,37,37,37	0
56	MG	1A	3329	1/1	0.70	0.29	51,51,51,51	0
56	MG	1A	3494	1/1	0.70	0.20	56,56,56,56	0
56	MG	1A	3901	1/1	0.70	0.14	53,53,53,53	0
56	MG	2A	3467	1/1	0.71	0.19	74,74,74,74	0
56	MG	1a	1806	1/1	0.71	0.12	59,59,59,59	0
56	MG	1P	206	1/1	0.71	0.32	62,62,62,62	0
56	MG	2a	3095	1/1	0.71	0.17	79,79,79,79	0
56	MG	2A	3869	1/1	0.71	0.12	45,45,45,45	0
56	MG	1a	1772	1/1	0.71	0.21	60,60,60,60	0
56	MG	2a	3225	1/1	0.71	0.23	73,73,73,73	0
56	MG	1A	3968	1/1	0.71	0.36	43,43,43,43	0
56	MG	1A	3987	1/1	0.72	0.09	50,50,50,50	0
56	MG	2a	3170	1/1	0.72	0.18	73,73,73,73	0
56	MG	1A	4059	1/1	0.72	0.20	27,27,27,27	0
56	MG	2A	3291	1/1	0.72	0.34	57,57,57,57	0
56	MG	1A	3360	1/1	0.72	0.16	65,65,65,65	0
56	MG	1A	3342	1/1	0.72	0.21	60,60,60,60	0
56	MG	2A	3762	1/1	0.72	0.15	59,59,59,59	0
56	MG	2A	3474	1/1	0.72	0.20	61,61,61,61	0
56	MG	1a	1746	1/1	0.72	0.12	59,59,59,59	0
56	MG	2A	3793	1/1	0.72	0.23	77,77,77,77	0
56	MG	2A	3543	1/1	0.72	0.13	45,45,45,45	0
56	MG	2a	3201	1/1	0.72	0.16	60,60,60,60	0
56	MG	1a	1609	1/1	0.72	0.11	65,65,65,65	0
56	MG	2v	101	1/1	0.72	0.12	78,78,78,78	0
56	MG	2A	3806	1/1	0.72	0.17	50,50,50,50	0
56	MG	1A	3742	1/1	0.73	0.24	17,17,17,17	0
56	MG	2A	3596	1/1	0.73	0.14	40,40,40,40	0
56	MG	1A	3392	1/1	0.73	0.27	45,45,45,45	0
56	MG	2A	3875	1/1	0.73	0.14	74,74,74,74	0
56	MG	1a	1818	1/1	0.73	0.16	71,71,71,71	0
56	MG	2A	3334	1/1	0.73	0.17	74,74,74,74	0
56	MG	2A	3169	1/1	0.73	0.31	57,57,57,57	0
56	MG	2a	3049	1/1	0.73	0.16	64,64,64,64	0
56	MG	2A	3711	1/1	0.73	0.18	54,54,54,54	0
56	MG	2A	3714	1/1	0.73	0.18	57,57,57,57	0
56	MG	2A	3207	1/1	0.73	0.15	64,64,64,64	0
56	MG	2A	3735	1/1	0.73	0.08	62,62,62,62	0
56	MG	2A	3838	1/1	0.73	0.17	43,43,43,43	0
56	MG	1A	3247	1/1	0.73	0.18	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	3561	1/1	0.73	0.34	62,62,62,62	0
56	MG	2A	3554	1/1	0.73	0.11	49,49,49,49	0
56	MG	2A	3405	1/1	0.74	0.20	64,64,64,64	0
56	MG	1a	1721	1/1	0.74	0.27	54,54,54,54	0
56	MG	1w	109	1/1	0.74	0.20	77,77,77,77	0
56	MG	2a	3041	1/1	0.74	0.21	66,66,66,66	0
56	MG	2A	3002	1/1	0.74	0.21	53,53,53,53	0
56	MG	2A	3804	1/1	0.74	0.17	53,53,53,53	0
56	MG	2a	3054	1/1	0.74	0.27	71,71,71,71	0
56	MG	1B	234	1/1	0.74	0.18	56,56,56,56	0
56	MG	1a	1780	1/1	0.74	0.15	58,58,58,58	0
56	MG	2A	3568	1/1	0.74	0.15	47,47,47,47	0
56	MG	2A	3860	1/1	0.74	0.16	73,73,73,73	0
56	MG	1A	3689	1/1	0.74	0.22	26,26,26,26	0
56	MG	1A	3869	1/1	0.74	0.18	45,45,45,45	0
56	MG	2a	3145	1/1	0.74	0.24	79,79,79,79	0
56	MG	2A	3820	1/1	0.74	0.12	73,73,73,73	0
56	MG	2a	3153	1/1	0.74	0.09	73,73,73,73	0
59	ZN	24	501	1/1	0.74	0.07	117,117,117,117	0
56	MG	2A	3320	1/1	0.75	0.14	54,54,54,54	0
56	MG	1B	228	1/1	0.75	0.18	42,42,42,42	0
56	MG	1A	3471	1/1	0.75	0.21	51,51,51,51	0
56	MG	2a	3003	1/1	0.75	0.14	63,63,63,63	0
56	MG	2A	3337	1/1	0.75	0.25	49,49,49,49	0
56	MG	2A	3353	1/1	0.75	0.16	71,71,71,71	0
56	MG	2A	3361	1/1	0.75	0.21	61,61,61,61	0
56	MG	2A	3382	1/1	0.75	0.52	47,47,47,47	0
56	MG	1a	1787	1/1	0.75	0.15	66,66,66,66	0
56	MG	2A	3063	1/1	0.75	0.21	58,58,58,58	0
56	MG	1A	3489	1/1	0.75	0.71	48,48,48,48	0
56	MG	2a	3082	1/1	0.75	0.11	65,65,65,65	0
56	MG	1A	3402	1/1	0.75	0.36	85,85,85,85	0
56	MG	1a	1620	1/1	0.75	0.27	55,55,55,55	0
56	MG	2A	3787	1/1	0.75	0.08	72,72,72,72	0
56	MG	1A	3341	1/1	0.75	0.21	50,50,50,50	0
56	MG	1A	3422	1/1	0.75	0.15	58,58,58,58	0
56	MG	1a	1801	1/1	0.75	0.12	64,64,64,64	0
56	MG	2a	3147	1/1	0.75	0.18	80,80,80,80	0
56	MG	2A	3740	1/1	0.76	0.07	67,67,67,67	0
56	MG	1A	4006	1/1	0.76	0.19	29,29,29,29	0
56	MG	1A	4012	1/1	0.76	0.09	68,68,68,68	0
56	MG	2A	3230	1/1	0.76	0.30	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3476	1/1	0.76	0.15	62,62,62,62	0
56	MG	2A	3243	1/1	0.76	0.67	64,64,64,64	0
56	MG	1A	3876	1/1	0.76	0.22	34,34,34,34	0
56	MG	1A	3224	1/1	0.76	0.15	45,45,45,45	0
56	MG	1A	3923	1/1	0.76	0.17	59,59,59,59	0
56	MG	2A	3308	1/1	0.76	0.12	56,56,56,56	0
56	MG	2A	3809	1/1	0.76	0.26	60,60,60,60	0
56	MG	1A	4089	1/1	0.76	0.21	65,65,65,65	0
56	MG	1A	3404	1/1	0.76	0.33	60,60,60,60	0
56	MG	2A	3333	1/1	0.76	0.31	65,65,65,65	0
56	MG	1A	3297	1/1	0.76	0.15	50,50,50,50	0
56	MG	1O	205	1/1	0.76	0.21	72,72,72,72	0
56	MG	2A	3674	1/1	0.76	0.15	63,63,63,63	0
56	MG	2A	3352	1/1	0.76	0.23	72,72,72,72	0
56	MG	1A	3019	1/1	0.76	0.18	41,41,41,41	0
56	MG	2A	3116	1/1	0.76	0.13	60,60,60,60	0
56	MG	2x	103	1/1	0.76	0.18	60,60,60,60	0
56	MG	1A	3871	1/1	0.76	0.11	32,32,32,32	0
56	MG	2A	3399	1/1	0.77	0.20	69,69,69,69	0
56	MG	2a	3174	1/1	0.77	0.19	75,75,75,75	0
56	MG	1A	3800	1/1	0.77	0.22	60,60,60,60	0
56	MG	2A	3452	1/1	0.77	0.17	70,70,70,70	0
56	MG	2a	3096	1/1	0.77	0.10	67,67,67,67	0
56	MG	1a	1698	1/1	0.77	0.28	62,62,62,62	0
56	MG	1A	3208	1/1	0.77	0.15	61,61,61,61	0
56	MG	2G	201	1/1	0.77	0.12	65,65,65,65	0
56	MG	2T	202	1/1	0.77	0.13	61,61,61,61	0
56	MG	2A	3255	1/1	0.77	0.32	69,69,69,69	0
56	MG	2A	3493	1/1	0.77	0.25	61,61,61,61	0
56	MG	2A	3802	1/1	0.77	0.12	57,57,57,57	0
56	MG	2j	201	1/1	0.77	0.14	76,76,76,76	0
56	MG	2A	3008	1/1	0.77	0.23	60,60,60,60	0
56	MG	1a	1822	1/1	0.77	0.10	69,69,69,69	0
56	MG	1A	3983	1/1	0.77	0.17	64,64,64,64	0
56	MG	2A	3217	1/1	0.77	0.38	67,67,67,67	0
56	MG	1A	3838	1/1	0.78	0.19	60,60,60,60	0
56	MG	1A	3053	1/1	0.78	0.14	62,62,62,62	0
56	MG	1a	1747	1/1	0.78	0.11	52,52,52,52	0
56	MG	1A	3382	1/1	0.78	0.25	46,46,46,46	0
56	MG	2A	3120	1/1	0.78	0.24	62,62,62,62	0
56	MG	2A	3397	1/1	0.78	0.18	72,72,72,72	0
56	MG	2a	3066	1/1	0.78	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	1A	3930	1/1	0.78	0.14	30,30,30,30	0
56	MG	2A	3585	1/1	0.78	0.13	77,77,77,77	0
56	MG	1a	1672	1/1	0.78	0.12	44,44,44,44	0
56	MG	2A	3599	1/1	0.78	0.20	68,68,68,68	0
56	MG	2A	3612	1/1	0.78	0.10	41,41,41,41	0
56	MG	2A	3421	1/1	0.78	0.19	69,69,69,69	0
56	MG	2A	3448	1/1	0.78	0.20	64,64,64,64	0
56	MG	1A	4035	1/1	0.78	0.06	64,64,64,64	0
56	MG	1A	4039	1/1	0.78	0.14	61,61,61,61	0
56	MG	1A	3962	1/1	0.78	0.12	48,48,48,48	0
56	MG	2A	3691	1/1	0.78	0.07	71,71,71,71	0
56	MG	2a	3151	1/1	0.78	0.15	91,91,91,91	0
56	MG	2A	3698	1/1	0.78	0.20	56,56,56,56	0
56	MG	2A	3883	1/1	0.79	0.24	68,68,68,68	0
56	MG	2A	3406	1/1	0.79	0.34	66,66,66,66	0
56	MG	1A	3338	1/1	0.79	0.20	48,48,48,48	0
56	MG	2R	201	1/1	0.79	0.16	65,65,65,65	0
56	MG	1A	4042	1/1	0.79	0.08	40,40,40,40	0
56	MG	2A	3661	1/1	0.79	0.32	59,59,59,59	0
56	MG	2a	3172	1/1	0.79	0.12	62,62,62,62	0
56	MG	2A	3071	1/1	0.79	0.14	40,40,40,40	0
56	MG	1A	3684	1/1	0.79	0.12	36,36,36,36	0
56	MG	1A	3503	1/1	0.79	0.40	57,57,57,57	0
56	MG	1A	3921	1/1	0.79	0.17	41,41,41,41	0
56	MG	1a	1703	1/1	0.79	0.25	60,60,60,60	0
56	MG	1B	229	1/1	0.79	0.14	38,38,38,38	0
56	MG	1A	3065	1/1	0.79	0.17	51,51,51,51	0
56	MG	1A	3726	1/1	0.79	0.10	53,53,53,53	0
56	MG	1A	3083	1/1	0.79	0.29	37,37,37,37	0
56	MG	2A	3381	1/1	0.79	0.13	57,57,57,57	0
56	MG	1a	1604	1/1	0.79	0.14	55,55,55,55	0
56	MG	2A	3856	1/1	0.79	0.06	58,58,58,58	0
56	MG	2A	3396	1/1	0.79	0.15	63,63,63,63	0
56	MG	2A	3789	1/1	0.79	0.09	44,44,44,44	0
56	MG	1A	3103	1/1	0.79	0.16	60,60,60,60	0
56	MG	2A	3271	1/1	0.79	0.13	58,58,58,58	0
56	MG	2A	3279	1/1	0.79	0.17	62,62,62,62	0
56	MG	2A	3315	1/1	0.80	0.11	62,62,62,62	0
56	MG	1A	4034	1/1	0.80	0.07	61,61,61,61	0
56	MG	1A	3317	1/1	0.80	0.18	65,65,65,65	0
56	MG	1a	1700	1/1	0.80	0.22	68,68,68,68	0
56	MG	1A	3148	1/1	0.80	0.31	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3086	1/1	0.80	0.18	66,66,66,66	0
56	MG	2A	3347	1/1	0.80	0.18	66,66,66,66	0
56	MG	2A	3094	1/1	0.80	0.14	62,62,62,62	0
56	MG	2A	3107	1/1	0.80	0.16	65,65,65,65	0
56	MG	1a	1711	1/1	0.80	0.19	39,39,39,39	0
56	MG	1A	4101	1/1	0.80	0.07	53,53,53,53	0
56	MG	1A	3002	1/1	0.80	0.15	51,51,51,51	0
56	MG	2A	3176	1/1	0.80	0.30	59,59,59,59	0
56	MG	1A	3004	1/1	0.80	0.21	22,22,22,22	0
56	MG	1A	4047	1/1	0.80	0.17	47,47,47,47	0
56	MG	2A	3402	1/1	0.80	0.12	65,65,65,65	0
56	MG	1a	1813	1/1	0.80	0.10	53,53,53,53	0
56	MG	1A	3933	1/1	0.80	0.10	49,49,49,49	0
56	MG	2A	3414	1/1	0.80	0.13	59,59,59,59	0
56	MG	1A	3577	1/1	0.80	0.33	47,47,47,47	0
56	MG	1A	3478	1/1	0.80	0.28	41,41,41,41	0
56	MG	1A	3639	1/1	0.80	0.18	36,36,36,36	0
56	MG	2A	3264	1/1	0.80	0.14	56,56,56,56	0
56	MG	1A	4016	1/1	0.80	0.20	25,25,25,25	0
56	MG	2W	203	1/1	0.80	0.26	51,51,51,51	0
56	MG	1x	109	1/1	0.80	0.12	61,61,61,61	0
56	MG	2a	3007	1/1	0.80	0.15	63,63,63,63	0
56	MG	2a	3014	1/1	0.80	0.16	63,63,63,63	0
56	MG	2A	3486	1/1	0.80	0.17	62,62,62,62	0
56	MG	1A	3058	1/1	0.80	0.18	32,32,32,32	0
56	MG	2A	3800	1/1	0.80	0.04	78,78,78,78	0
56	MG	1a	1656	1/1	0.80	0.11	62,62,62,62	0
56	MG	1A	3798	1/1	0.80	0.12	39,39,39,39	0
56	MG	2A	3551	1/1	0.80	0.12	43,43,43,43	0
56	MG	2a	3061	1/1	0.80	0.12	53,53,53,53	0
56	MG	1A	3537	1/1	0.81	0.17	61,61,61,61	0
56	MG	2a	3043	1/1	0.81	0.17	66,66,66,66	0
56	MG	2A	3242	1/1	0.81	0.18	64,64,64,64	0
56	MG	1A	3121	1/1	0.81	0.49	46,46,46,46	0
56	MG	2A	3808	1/1	0.81	0.24	63,63,63,63	0
56	MG	2A	3386	1/1	0.81	0.13	55,55,55,55	0
56	MG	1A	3992	1/1	0.81	0.18	25,25,25,25	0
56	MG	2A	3253	1/1	0.81	0.21	64,64,64,64	0
56	MG	2A	3818	1/1	0.81	0.15	64,64,64,64	0
56	MG	2A	3623	1/1	0.81	0.14	60,60,60,60	0
56	MG	2A	3072	1/1	0.81	0.21	61,61,61,61	0
56	MG	2a	3100	1/1	0.81	0.13	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3821	1/1	0.81	0.21	55,55,55,55	0
56	MG	2A	3823	1/1	0.81	0.10	50,50,50,50	0
56	MG	2A	3824	1/1	0.81	0.23	66,66,66,66	0
56	MG	2A	3077	1/1	0.81	0.27	57,57,57,57	0
56	MG	2A	3085	1/1	0.81	0.25	55,55,55,55	0
56	MG	1A	3394	1/1	0.81	0.25	50,50,50,50	0
56	MG	1A	3461	1/1	0.81	0.43	61,61,61,61	0
56	MG	2A	3684	1/1	0.81	0.12	56,56,56,56	0
56	MG	2A	3417	1/1	0.81	0.24	68,68,68,68	0
56	MG	2a	3157	1/1	0.81	0.10	57,57,57,57	0
56	MG	2A	3287	1/1	0.81	0.20	67,67,67,67	0
56	MG	2A	3703	1/1	0.81	0.07	59,59,59,59	0
56	MG	1A	3922	1/1	0.81	0.10	70,70,70,70	0
56	MG	1A	4060	1/1	0.81	0.46	52,52,52,52	0
56	MG	2A	3731	1/1	0.81	0.23	60,60,60,60	0
56	MG	1w	110	1/1	0.81	0.23	74,74,74,74	0
56	MG	2A	3145	1/1	0.81	0.11	66,66,66,66	0
56	MG	2A	3155	1/1	0.81	0.12	55,55,55,55	0
56	MG	2A	3759	1/1	0.81	0.11	62,62,62,62	0
56	MG	2A	3332	1/1	0.81	0.15	46,46,46,46	0
56	MG	2Q	202	1/1	0.81	0.13	53,53,53,53	0
56	MG	1a	1748	1/1	0.81	0.11	36,36,36,36	0
56	MG	2T	201	1/1	0.81	0.16	54,54,54,54	0
56	MG	2A	3494	1/1	0.81	0.09	67,67,67,67	0
56	MG	1A	4001	1/1	0.81	0.10	48,48,48,48	0
56	MG	2A	3538	1/1	0.81	0.15	38,38,38,38	0
56	MG	2f	202	1/1	0.81	0.13	65,65,65,65	0
56	MG	2a	3006	1/1	0.81	0.11	61,61,61,61	0
56	MG	1a	1760	1/1	0.81	0.15	56,56,56,56	0
56	MG	1G	203	1/1	0.81	0.10	63,63,63,63	0
56	MG	2A	3216	1/1	0.81	0.17	65,65,65,65	0
56	MG	2y	106	1/1	0.81	0.40	83,83,83,83	0
56	MG	1A	3934	1/1	0.81	0.11	55,55,55,55	0
56	MG	1A	3753	1/1	0.82	0.20	34,34,34,34	0
56	MG	1A	3765	1/1	0.82	0.18	43,43,43,43	0
56	MG	2A	3710	1/1	0.82	0.13	42,42,42,42	0
56	MG	1a	1611	1/1	0.82	0.13	68,68,68,68	0
56	MG	1A	3323	1/1	0.82	0.27	50,50,50,50	0
56	MG	1A	3497	1/1	0.82	0.22	50,50,50,50	0
56	MG	1A	3777	1/1	0.82	0.12	46,46,46,46	0
56	MG	1A	3340	1/1	0.82	0.15	50,50,50,50	0
56	MG	2A	3191	1/1	0.82	0.19	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3750	1/1	0.82	0.14	55,55,55,55	0
56	MG	1A	3665	1/1	0.82	0.12	30,30,30,30	0
56	MG	1a	1808	1/1	0.82	0.08	50,50,50,50	0
56	MG	1a	1673	1/1	0.82	0.13	63,63,63,63	0
56	MG	1a	1693	1/1	0.82	0.15	69,69,69,69	0
56	MG	2a	3053	1/1	0.82	0.14	70,70,70,70	0
56	MG	2A	3443	1/1	0.82	0.22	59,59,59,59	0
56	MG	2a	3060	1/1	0.82	0.21	71,71,71,71	0
56	MG	2A	3447	1/1	0.82	0.23	55,55,55,55	0
56	MG	2a	3062	1/1	0.82	0.14	71,71,71,71	0
56	MG	1a	1814	1/1	0.82	0.06	67,67,67,67	0
56	MG	2A	3239	1/1	0.82	0.39	56,56,56,56	0
56	MG	2A	3799	1/1	0.82	0.14	75,75,75,75	0
56	MG	2a	3086	1/1	0.82	0.15	63,63,63,63	0
56	MG	1A	4062	1/1	0.82	0.12	32,32,32,32	0
56	MG	1A	4004	1/1	0.82	0.11	51,51,51,51	0
56	MG	1A	3477	1/1	0.82	0.23	53,53,53,53	0
56	MG	2A	3250	1/1	0.82	0.73	64,64,64,64	0
56	MG	1a	1706	1/1	0.82	0.20	59,59,59,59	0
56	MG	1A	4074	1/1	0.82	0.12	48,48,48,48	0
56	MG	2A	3516	1/1	0.82	0.23	74,74,74,74	0
56	MG	2A	3522	1/1	0.82	0.09	41,41,41,41	0
56	MG	2A	3262	1/1	0.82	0.27	60,60,60,60	0
56	MG	1A	3418	1/1	0.82	0.23	55,55,55,55	0
56	MG	1A	3945	1/1	0.82	0.17	56,56,56,56	0
56	MG	2A	3546	1/1	0.82	0.17	65,65,65,65	0
56	MG	2a	3154	1/1	0.82	0.10	69,69,69,69	0
56	MG	1x	117	1/1	0.82	0.20	71,71,71,71	0
56	MG	1A	4024	1/1	0.82	0.16	70,70,70,70	0
56	MG	2a	3166	1/1	0.82	0.07	67,67,67,67	0
56	MG	1A	3948	1/1	0.82	0.19	36,36,36,36	0
56	MG	1B	207	1/1	0.82	0.25	70,70,70,70	0
56	MG	2A	3296	1/1	0.82	0.17	50,50,50,50	0
56	MG	2A	3033	1/1	0.82	0.13	36,36,36,36	0
56	MG	1B	215	1/1	0.82	0.07	55,55,55,55	0
56	MG	1A	3808	1/1	0.82	0.11	65,65,65,65	0
56	MG	2A	3614	1/1	0.82	0.15	45,45,45,45	0
56	MG	1A	3480	1/1	0.82	0.14	54,54,54,54	0
56	MG	2A	3622	1/1	0.82	0.10	38,38,38,38	0
56	MG	1A	3699	1/1	0.82	0.19	37,37,37,37	0
56	MG	1A	3703	1/1	0.82	0.18	48,48,48,48	0
56	MG	2A	3861	1/1	0.82	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	2a	3197	1/1	0.82	0.09	73,73,73,73	0
56	MG	1A	3564	1/1	0.82	0.17	49,49,49,49	0
56	MG	1A	3336	1/1	0.82	0.16	60,60,60,60	0
56	MG	2a	3209	1/1	0.82	0.24	73,73,73,73	0
56	MG	1U	201	1/1	0.82	0.28	51,51,51,51	0
56	MG	2A	3088	1/1	0.82	0.22	78,78,78,78	0
56	MG	2A	3886	1/1	0.82	0.12	71,71,71,71	0
56	MG	2B	202	1/1	0.82	0.15	63,63,63,63	0
56	MG	2A	3676	1/1	0.82	0.14	61,61,61,61	0
56	MG	11	104	1/1	0.82	0.12	48,48,48,48	0
56	MG	2O	8400	1/1	0.82	0.10	64,64,64,64	0
56	MG	2A	3099	1/1	0.82	0.23	68,68,68,68	0
56	MG	1A	3322	1/1	0.83	0.19	43,43,43,43	0
56	MG	2A	3323	1/1	0.83	0.14	57,57,57,57	0
56	MG	2A	3566	1/1	0.83	0.17	44,44,44,44	0
56	MG	2A	3123	1/1	0.83	0.11	59,59,59,59	0
56	MG	2A	3138	1/1	0.83	0.07	70,70,70,70	0
56	MG	1A	3706	1/1	0.83	0.24	53,53,53,53	0
56	MG	2A	3335	1/1	0.83	0.29	47,47,47,47	0
56	MG	1A	3937	1/1	0.83	0.10	60,60,60,60	0
56	MG	2a	3068	1/1	0.83	0.12	74,74,74,74	0
56	MG	2A	3162	1/1	0.83	0.21	64,64,64,64	0
56	MG	1d	301	1/1	0.83	0.23	48,48,48,48	0
56	MG	2A	3171	1/1	0.83	0.12	74,74,74,74	0
56	MG	1A	3346	1/1	0.83	0.21	52,52,52,52	0
56	MG	2A	3364	1/1	0.83	0.24	66,66,66,66	0
56	MG	1s	101	1/1	0.83	0.16	71,71,71,71	0
56	MG	2A	3203	1/1	0.83	0.13	48,48,48,48	0
56	MG	1A	3498	1/1	0.83	0.25	59,59,59,59	0
56	MG	2a	3127	1/1	0.83	0.19	63,63,63,63	0
56	MG	2a	3135	1/1	0.83	0.23	59,59,59,59	0
56	MG	2A	3395	1/1	0.83	0.14	66,66,66,66	0
56	MG	2a	3140	1/1	0.83	0.10	57,57,57,57	0
56	MG	1a	1646	1/1	0.83	0.15	56,56,56,56	0
56	MG	1A	3955	1/1	0.83	0.11	65,65,65,65	0
56	MG	1a	1781	1/1	0.83	0.13	75,75,75,75	0
56	MG	1A	3845	1/1	0.83	0.32	57,57,57,57	0
56	MG	1a	1659	1/1	0.83	0.38	55,55,55,55	0
56	MG	1A	3854	1/1	0.83	0.07	60,60,60,60	0
56	MG	1A	3747	1/1	0.83	0.17	54,54,54,54	0
56	MG	2a	3156	1/1	0.83	0.06	72,72,72,72	0
56	MG	1A	3018	1/1	0.83	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3713	1/1	0.83	0.13	48,48,48,48	0
56	MG	1a	1796	1/1	0.83	0.13	59,59,59,59	0
56	MG	2A	3251	1/1	0.83	0.15	62,62,62,62	0
56	MG	2A	3053	1/1	0.83	0.17	64,64,64,64	0
56	MG	2B	216	1/1	0.83	0.08	65,65,65,65	0
56	MG	2A	3059	1/1	0.83	0.30	58,58,58,58	0
56	MG	2F	302	1/1	0.83	0.15	64,64,64,64	0
56	MG	2a	3175	1/1	0.83	0.16	73,73,73,73	0
56	MG	1a	1797	1/1	0.83	0.07	65,65,65,65	0
56	MG	1A	4036	1/1	0.83	0.16	41,41,41,41	0
56	MG	2P	203	1/1	0.83	0.10	38,38,38,38	0
56	MG	1A	3510	1/1	0.83	0.15	41,41,41,41	0
56	MG	2A	3273	1/1	0.83	0.28	49,49,49,49	0
56	MG	2A	3480	1/1	0.83	0.37	46,46,46,46	0
56	MG	1A	3364	1/1	0.83	0.18	37,37,37,37	0
56	MG	2A	3282	1/1	0.83	0.16	63,63,63,63	0
56	MG	1A	3523	1/1	0.83	0.14	53,53,53,53	0
56	MG	2a	3005	1/1	0.83	0.17	66,66,66,66	0
56	MG	1A	3533	1/1	0.83	0.25	55,55,55,55	0
56	MG	2A	3796	1/1	0.83	0.28	77,77,77,77	0
56	MG	2a	3009	1/1	0.83	0.12	72,72,72,72	0
56	MG	1D	310	1/1	0.83	0.17	24,24,24,24	0
56	MG	1A	3693	1/1	0.83	0.23	42,42,42,42	0
56	MG	2a	3025	1/1	0.83	0.27	59,59,59,59	0
56	MG	1A	3270	1/1	0.83	0.12	55,55,55,55	0
56	MG	1A	3799	1/1	0.83	0.10	38,38,38,38	0
56	MG	1A	3136	1/1	0.83	0.14	41,41,41,41	0
56	MG	2a	3001	1/1	0.84	0.26	57,57,57,57	0
56	MG	2a	3002	1/1	0.84	0.13	63,63,63,63	0
56	MG	2A	3186	1/1	0.84	0.15	53,53,53,53	0
56	MG	1A	3635	1/1	0.84	0.19	33,33,33,33	0
56	MG	2A	3726	1/1	0.84	0.19	50,50,50,50	0
56	MG	2A	3202	1/1	0.84	0.15	47,47,47,47	0
56	MG	1a	1826	1/1	0.84	0.22	58,58,58,58	0
56	MG	2A	3400	1/1	0.84	0.45	59,59,59,59	0
56	MG	2A	3737	1/1	0.84	0.14	70,70,70,70	0
56	MG	1A	3339	1/1	0.84	0.25	42,42,42,42	0
56	MG	1A	3766	1/1	0.84	0.13	26,26,26,26	0
56	MG	2a	3037	1/1	0.84	0.15	48,48,48,48	0
56	MG	2A	3753	1/1	0.84	0.13	42,42,42,42	0
56	MG	1a	1715	1/1	0.84	0.11	53,53,53,53	0
56	MG	1t	201	1/1	0.84	0.17	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3767	1/1	0.84	0.18	51,51,51,51	0
56	MG	1A	3643	1/1	0.84	0.18	56,56,56,56	0
56	MG	2A	3418	1/1	0.84	0.16	66,66,66,66	0
56	MG	2A	3236	1/1	0.84	0.19	45,45,45,45	0
56	MG	1a	1722	1/1	0.84	0.11	50,50,50,50	0
56	MG	1x	104	1/1	0.84	0.25	56,56,56,56	0
56	MG	1a	1730	1/1	0.84	0.25	65,65,65,65	0
56	MG	1A	3984	1/1	0.84	0.10	71,71,71,71	0
56	MG	1A	3207	1/1	0.84	0.16	47,47,47,47	0
56	MG	2a	3077	1/1	0.84	0.14	59,59,59,59	0
56	MG	1A	3096	1/1	0.84	0.23	57,57,57,57	0
56	MG	2A	3801	1/1	0.84	0.12	80,80,80,80	0
56	MG	2A	3014	1/1	0.84	0.64	55,55,55,55	0
56	MG	1A	3989	1/1	0.84	0.19	31,31,31,31	0
56	MG	1Q	206	1/1	0.84	0.16	51,51,51,51	0
56	MG	1A	4053	1/1	0.84	0.14	34,34,34,34	0
56	MG	1A	3143	1/1	0.84	0.20	37,37,37,37	0
56	MG	2A	3508	1/1	0.84	0.15	64,64,64,64	0
56	MG	2A	3051	1/1	0.84	0.13	72,72,72,72	0
56	MG	14	101	1/1	0.84	0.10	69,69,69,69	0
56	MG	2a	3138	1/1	0.84	0.12	67,67,67,67	0
56	MG	1A	3074	1/1	0.84	0.30	55,55,55,55	0
56	MG	1a	1606	1/1	0.84	0.25	71,71,71,71	0
56	MG	2A	3540	1/1	0.84	0.14	35,35,35,35	0
56	MG	1A	3358	1/1	0.84	0.15	45,45,45,45	0
56	MG	2A	3822	1/1	0.84	0.11	61,61,61,61	0
56	MG	1A	3251	1/1	0.84	0.11	69,69,69,69	0
56	MG	2A	3295	1/1	0.84	0.25	58,58,58,58	0
56	MG	2A	3552	1/1	0.84	0.10	43,43,43,43	0
56	MG	1A	3256	1/1	0.84	0.13	53,53,53,53	0
56	MG	2A	3297	1/1	0.84	0.14	72,72,72,72	0
56	MG	2A	3299	1/1	0.84	0.16	49,49,49,49	0
56	MG	1a	1638	1/1	0.84	0.21	61,61,61,61	0
56	MG	1a	1641	1/1	0.84	0.10	57,57,57,57	0
56	MG	2A	3850	1/1	0.84	0.15	55,55,55,55	0
56	MG	2A	3087	1/1	0.84	0.22	48,48,48,48	0
56	MG	1A	3367	1/1	0.84	0.26	57,57,57,57	0
56	MG	2A	3605	1/1	0.84	0.11	51,51,51,51	0
56	MG	2A	3608	1/1	0.84	0.14	34,34,34,34	0
56	MG	1A	3151	1/1	0.84	0.53	42,42,42,42	0
56	MG	2A	3098	1/1	0.84	0.17	61,61,61,61	0
56	MG	1A	3282	1/1	0.84	0.67	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3954	1/1	0.84	0.15	75,75,75,75	0
56	MG	1A	3732	1/1	0.84	0.11	61,61,61,61	0
56	MG	1a	1661	1/1	0.84	0.13	58,58,58,58	0
56	MG	1A	3958	1/1	0.84	0.11	50,50,50,50	0
56	MG	2B	213	1/1	0.84	0.22	56,56,56,56	0
56	MG	2A	3350	1/1	0.84	0.14	68,68,68,68	0
56	MG	1A	4092	1/1	0.84	0.23	54,54,54,54	0
56	MG	1a	1683	1/1	0.84	0.13	43,43,43,43	0
56	MG	1A	4095	1/1	0.84	0.12	38,38,38,38	0
56	MG	2a	3238	1/1	0.84	0.24	72,72,72,72	0
56	MG	1a	1696	1/1	0.84	0.25	44,44,44,44	0
56	MG	2A	3372	1/1	0.84	0.15	50,50,50,50	0
56	MG	1A	3039	1/1	0.84	0.21	54,54,54,54	0
56	MG	2w	101	1/1	0.84	0.15	69,69,69,69	0
56	MG	2A	3700	1/1	0.84	0.07	58,58,58,58	0
56	MG	1A	3607	1/1	0.84	0.20	27,27,27,27	0
56	MG	2A	3383	1/1	0.84	0.19	66,66,66,66	0
56	MG	1B	208	1/1	0.84	0.17	57,57,57,57	0
56	MG	2A	3004	1/1	0.85	0.11	58,58,58,58	0
56	MG	2A	3173	1/1	0.85	0.15	72,72,72,72	0
56	MG	2A	3005	1/1	0.85	0.15	55,55,55,55	0
56	MG	1a	1690	1/1	0.85	0.14	56,56,56,56	0
56	MG	1A	3378	1/1	0.85	0.19	42,42,42,42	0
56	MG	2A	3193	1/1	0.85	0.10	63,63,63,63	0
56	MG	2A	3339	1/1	0.85	0.23	64,64,64,64	0
56	MG	1A	4027	1/1	0.85	0.41	65,65,65,65	0
56	MG	1A	3927	1/1	0.85	0.16	55,55,55,55	0
56	MG	2A	3205	1/1	0.85	0.39	63,63,63,63	0
56	MG	1A	3405	1/1	0.85	0.20	52,52,52,52	0
56	MG	1A	4076	1/1	0.85	0.25	36,36,36,36	0
56	MG	1A	3131	1/1	0.85	0.19	63,63,63,63	0
56	MG	2A	3368	1/1	0.85	0.23	65,65,65,65	0
56	MG	2a	3098	1/1	0.85	0.11	62,62,62,62	0
56	MG	1A	3932	1/1	0.85	0.19	48,48,48,48	0
56	MG	2A	3831	1/1	0.85	0.20	56,56,56,56	0
56	MG	2a	3107	1/1	0.85	0.14	74,74,74,74	0
56	MG	2A	3373	1/1	0.85	0.17	67,67,67,67	0
56	MG	2A	3376	1/1	0.85	0.20	53,53,53,53	0
56	MG	2A	3377	1/1	0.85	0.24	65,65,65,65	0
56	MG	2A	3221	1/1	0.85	0.16	57,57,57,57	0
56	MG	2A	3225	1/1	0.85	0.10	62,62,62,62	0
56	MG	2A	3657	1/1	0.85	0.29	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3412	1/1	0.85	0.20	38,38,38,38	0
56	MG	2A	3234	1/1	0.85	0.52	60,60,60,60	0
56	MG	1a	1607	1/1	0.85	0.16	55,55,55,55	0
56	MG	1A	3526	1/1	0.85	0.43	42,42,42,42	0
56	MG	1A	3048	1/1	0.85	0.13	20,20,20,20	0
56	MG	2A	3074	1/1	0.85	0.45	41,41,41,41	0
56	MG	1A	3220	1/1	0.85	0.17	49,49,49,49	0
56	MG	1A	3947	1/1	0.85	0.17	27,27,27,27	0
56	MG	1A	3797	1/1	0.85	0.21	27,27,27,27	0
56	MG	2a	3163	1/1	0.85	0.29	68,68,68,68	0
56	MG	1B	214	1/1	0.85	0.13	46,46,46,46	0
56	MG	1A	3885	1/1	0.85	0.19	25,25,25,25	0
56	MG	1A	3202	1/1	0.85	0.14	40,40,40,40	0
56	MG	2A	3263	1/1	0.85	0.20	71,71,71,71	0
56	MG	2A	3419	1/1	0.85	0.16	62,62,62,62	0
56	MG	1a	1759	1/1	0.85	0.14	61,61,61,61	0
56	MG	2A	3439	1/1	0.85	0.22	55,55,55,55	0
56	MG	1a	1657	1/1	0.85	0.21	68,68,68,68	0
56	MG	1A	3733	1/1	0.85	0.15	45,45,45,45	0
56	MG	2Q	203	1/1	0.85	0.41	56,56,56,56	0
56	MG	2A	3114	1/1	0.85	0.14	64,64,64,64	0
56	MG	1A	3960	1/1	0.85	0.11	50,50,50,50	0
56	MG	1A	3468	1/1	0.85	0.41	57,57,57,57	0
56	MG	1E	301	1/1	0.85	0.39	28,28,28,28	0
56	MG	2A	3766	1/1	0.85	0.19	68,68,68,68	0
56	MG	2A	3129	1/1	0.85	0.43	54,54,54,54	0
56	MG	2A	3768	1/1	0.85	0.09	42,42,42,42	0
56	MG	2A	3292	1/1	0.85	0.11	57,57,57,57	0
56	MG	2A	3484	1/1	0.85	0.12	58,58,58,58	0
56	MG	1A	3685	1/1	0.85	0.21	31,31,31,31	0
56	MG	2a	3236	1/1	0.85	0.13	73,73,73,73	0
56	MG	1N	201	1/1	0.85	0.36	51,51,51,51	0
56	MG	1x	111	1/1	0.85	0.14	71,71,71,71	0
56	MG	2g	201	1/1	0.85	0.14	81,81,81,81	0
56	MG	2A	3159	1/1	0.85	0.21	66,66,66,66	0
56	MG	1a	1788	1/1	0.85	0.09	61,61,61,61	0
56	MG	2A	3309	1/1	0.85	0.19	55,55,55,55	0
56	MG	2A	3310	1/1	0.85	0.25	65,65,65,65	0
56	MG	2A	3163	1/1	0.85	0.12	57,57,57,57	0
56	MG	2y	103	1/1	0.85	0.17	76,76,76,76	0
56	MG	2A	3168	1/1	0.85	0.10	53,53,53,53	0
56	MG	1a	1685	1/1	0.85	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3416	1/1	0.86	0.20	64,64,64,64	0
56	MG	2A	3182	1/1	0.86	0.14	49,49,49,49	0
56	MG	1A	4014	1/1	0.86	0.15	46,46,46,46	0
56	MG	2A	3302	1/1	0.86	0.14	61,61,61,61	0
56	MG	2A	3679	1/1	0.86	0.10	52,52,52,52	0
56	MG	10	104	1/1	0.86	0.18	59,59,59,59	0
56	MG	2a	3084	1/1	0.86	0.15	58,58,58,58	0
56	MG	1a	1805	1/1	0.86	0.14	55,55,55,55	0
56	MG	2a	3089	1/1	0.86	0.26	69,69,69,69	0
56	MG	2A	3056	1/1	0.86	0.18	59,59,59,59	0
56	MG	2A	3314	1/1	0.86	0.26	60,60,60,60	0
56	MG	1A	3234	1/1	0.86	0.37	54,54,54,54	0
56	MG	1A	3237	1/1	0.86	0.25	30,30,30,30	0
56	MG	2A	3457	1/1	0.86	0.14	50,50,50,50	0
56	MG	2a	3106	1/1	0.86	0.12	65,65,65,65	0
56	MG	1A	3675	1/1	0.86	0.10	24,24,24,24	0
56	MG	2a	3117	1/1	0.86	0.13	65,65,65,65	0
56	MG	1A	4031	1/1	0.86	0.10	60,60,60,60	0
56	MG	1A	3907	1/1	0.86	0.09	48,48,48,48	0
56	MG	2A	3479	1/1	0.86	0.24	52,52,52,52	0
56	MG	1A	3682	1/1	0.86	0.17	61,61,61,61	0
56	MG	2a	3137	1/1	0.86	0.13	75,75,75,75	0
56	MG	1a	1817	1/1	0.86	0.25	58,58,58,58	0
56	MG	1A	3400	1/1	0.86	0.54	42,42,42,42	0
56	MG	2A	3490	1/1	0.86	0.15	53,53,53,53	0
56	MG	1A	3528	1/1	0.86	0.34	47,47,47,47	0
56	MG	2B	217	1/1	0.86	0.21	84,84,84,84	0
56	MG	2D	307	1/1	0.86	0.53	47,47,47,47	0
56	MG	1A	3686	1/1	0.86	0.17	54,54,54,54	0
56	MG	2A	3495	1/1	0.86	0.16	57,57,57,57	0
56	MG	2A	3497	1/1	0.86	0.17	51,51,51,51	0
56	MG	1A	3349	1/1	0.86	0.25	56,56,56,56	0
56	MG	1A	3333	1/1	0.86	0.30	56,56,56,56	0
56	MG	1A	3041	1/1	0.86	0.55	34,34,34,34	0
56	MG	2A	3104	1/1	0.86	0.15	51,51,51,51	0
56	MG	2A	3356	1/1	0.86	0.35	62,62,62,62	0
56	MG	1A	3114	1/1	0.86	0.25	32,32,32,32	0
56	MG	1A	3990	1/1	0.86	0.14	33,33,33,33	0
56	MG	2A	3367	1/1	0.86	0.13	54,54,54,54	0
56	MG	2X	101	1/1	0.86	0.12	56,56,56,56	0
56	MG	25	104	1/1	0.86	0.25	54,54,54,54	0
56	MG	25	105	1/1	0.86	0.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1658	1/1	0.86	0.08	63,63,63,63	0
56	MG	1A	3062	1/1	0.86	0.27	51,51,51,51	0
56	MG	2A	3121	1/1	0.86	0.17	48,48,48,48	0
56	MG	1A	3261	1/1	0.86	0.16	52,52,52,52	0
56	MG	1A	3713	1/1	0.86	0.26	63,63,63,63	0
56	MG	1F	308	1/1	0.86	0.20	49,49,49,49	0
56	MG	2A	3265	1/1	0.86	0.12	57,57,57,57	0
56	MG	1x	112	1/1	0.86	0.15	58,58,58,58	0
56	MG	1A	3147	1/1	0.86	0.26	39,39,39,39	0
56	MG	2A	3391	1/1	0.86	0.12	68,68,68,68	0
56	MG	2a	3027	1/1	0.86	0.43	70,70,70,70	0
56	MG	2a	3216	1/1	0.86	0.17	72,72,72,72	0
56	MG	1a	1679	1/1	0.86	0.11	66,66,66,66	0
56	MG	2a	3227	1/1	0.86	0.21	78,78,78,78	0
56	MG	2a	3034	1/1	0.86	0.22	72,72,72,72	0
56	MG	1A	3626	1/1	0.86	0.12	47,47,47,47	0
56	MG	2A	3613	1/1	0.86	0.12	46,46,46,46	0
56	MG	2A	3283	1/1	0.86	0.09	57,57,57,57	0
56	MG	2a	3045	1/1	0.86	0.22	72,72,72,72	0
56	MG	2q	201	1/1	0.86	0.24	68,68,68,68	0
56	MG	1N	203	1/1	0.86	0.16	46,46,46,46	0
56	MG	2a	3050	1/1	0.86	0.18	47,47,47,47	0
56	MG	1A	3434	1/1	0.86	0.16	40,40,40,40	0
56	MG	1a	1692	1/1	0.86	0.17	70,70,70,70	0
56	MG	1A	3504	1/1	0.86	0.32	54,54,54,54	0
56	MG	1P	209	1/1	0.86	0.14	40,40,40,40	0
56	MG	1A	3440	1/1	0.86	0.13	36,36,36,36	0
56	MG	2A	3715	1/1	0.87	0.17	68,68,68,68	0
56	MG	2A	3716	1/1	0.87	0.08	51,51,51,51	0
56	MG	1a	1779	1/1	0.87	0.19	88,88,88,88	0
56	MG	1A	3334	1/1	0.87	0.16	43,43,43,43	0
56	MG	1A	3017	1/1	0.87	0.39	50,50,50,50	0
56	MG	2A	3069	1/1	0.87	0.09	54,54,54,54	0
56	MG	1A	3776	1/1	0.87	0.12	31,31,31,31	0
56	MG	2A	3432	1/1	0.87	0.22	40,40,40,40	0
56	MG	1a	1627	1/1	0.87	0.12	55,55,55,55	0
56	MG	2A	3267	1/1	0.87	0.82	67,67,67,67	0
56	MG	2A	3268	1/1	0.87	0.17	57,57,57,57	0
56	MG	2a	3047	1/1	0.87	0.13	55,55,55,55	0
56	MG	1A	3475	1/1	0.87	0.26	48,48,48,48	0
56	MG	1A	3157	1/1	0.87	0.20	40,40,40,40	0
56	MG	2a	3051	1/1	0.87	0.15	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	3116	1/1	0.87	0.22	36,36,36,36	0
56	MG	2A	3461	1/1	0.87	0.15	44,44,44,44	0
56	MG	2A	3463	1/1	0.87	0.12	55,55,55,55	0
56	MG	1A	3534	1/1	0.87	0.20	63,63,63,63	0
56	MG	1A	4100	1/1	0.87	0.42	85,85,85,85	0
56	MG	1A	3170	1/1	0.87	0.18	47,47,47,47	0
56	MG	2a	3064	1/1	0.87	0.23	64,64,64,64	0
56	MG	1A	3488	1/1	0.87	0.17	33,33,33,33	0
56	MG	1A	3279	1/1	0.87	0.31	39,39,39,39	0
56	MG	2A	3483	1/1	0.87	0.19	68,68,68,68	0
56	MG	1B	212	1/1	0.87	0.14	40,40,40,40	0
56	MG	2a	3080	1/1	0.87	0.28	62,62,62,62	0
56	MG	1A	4028	1/1	0.87	0.07	61,61,61,61	0
56	MG	1a	1668	1/1	0.87	0.11	66,66,66,66	0
56	MG	1a	1669	1/1	0.87	0.28	75,75,75,75	0
56	MG	1A	3493	1/1	0.87	0.17	48,48,48,48	0
56	MG	1A	3816	1/1	0.87	0.23	54,54,54,54	0
56	MG	1a	1810	1/1	0.87	0.10	59,59,59,59	0
56	MG	2A	3506	1/1	0.87	0.11	36,36,36,36	0
56	MG	1A	3823	1/1	0.87	0.60	50,50,50,50	0
56	MG	2A	3515	1/1	0.87	0.15	36,36,36,36	0
56	MG	1A	3836	1/1	0.87	0.20	50,50,50,50	0
56	MG	2A	3136	1/1	0.87	0.16	38,38,38,38	0
56	MG	2A	3525	1/1	0.87	0.14	60,60,60,60	0
56	MG	2a	3118	1/1	0.87	0.13	62,62,62,62	0
56	MG	2A	3531	1/1	0.87	0.17	55,55,55,55	0
56	MG	2a	3122	1/1	0.87	0.09	73,73,73,73	0
56	MG	1B	237	1/1	0.87	0.12	68,68,68,68	0
56	MG	1a	1689	1/1	0.87	0.15	59,59,59,59	0
56	MG	1A	3578	1/1	0.87	0.19	43,43,43,43	0
56	MG	1A	3585	1/1	0.87	0.31	35,35,35,35	0
56	MG	2A	3826	1/1	0.87	0.14	55,55,55,55	0
56	MG	2A	3331	1/1	0.87	0.32	72,72,72,72	0
56	MG	1E	303	1/1	0.87	0.30	38,38,38,38	0
56	MG	2a	3143	1/1	0.87	0.12	75,75,75,75	0
56	MG	1E	313	1/1	0.87	0.27	54,54,54,54	0
56	MG	1A	4038	1/1	0.87	0.09	52,52,52,52	0
56	MG	2A	3562	1/1	0.87	0.16	35,35,35,35	0
56	MG	2A	3564	1/1	0.87	0.23	53,53,53,53	0
56	MG	1A	3391	1/1	0.87	0.10	42,42,42,42	0
56	MG	1f	202	1/1	0.87	0.13	70,70,70,70	0
56	MG	1A	3717	1/1	0.87	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3175	1/1	0.87	0.43	50,50,50,50	0
56	MG	2A	3858	1/1	0.87	0.28	64,64,64,64	0
56	MG	2A	3592	1/1	0.87	0.14	46,46,46,46	0
56	MG	1A	3431	1/1	0.87	0.21	54,54,54,54	0
56	MG	1N	205	1/1	0.87	0.23	57,57,57,57	0
56	MG	2A	3601	1/1	0.87	0.20	58,58,58,58	0
56	MG	2A	3602	1/1	0.87	0.14	55,55,55,55	0
56	MG	1A	3433	1/1	0.87	0.13	31,31,31,31	0
56	MG	1A	3627	1/1	0.87	0.22	18,18,18,18	0
56	MG	2A	3611	1/1	0.87	0.13	51,51,51,51	0
56	MG	2A	3358	1/1	0.87	0.13	56,56,56,56	0
56	MG	1P	207	1/1	0.87	0.08	51,51,51,51	0
56	MG	2A	3200	1/1	0.87	0.17	48,48,48,48	0
56	MG	1x	110	1/1	0.87	0.22	61,61,61,61	0
56	MG	2a	3183	1/1	0.87	0.14	60,60,60,60	0
56	MG	2a	3187	1/1	0.87	0.16	70,70,70,70	0
56	MG	2D	306	1/1	0.87	0.77	47,47,47,47	0
56	MG	1A	3101	1/1	0.87	0.17	56,56,56,56	0
56	MG	1a	1729	1/1	0.87	0.19	54,54,54,54	0
56	MG	1A	3888	1/1	0.87	0.32	44,44,44,44	0
56	MG	1A	3892	1/1	0.87	0.14	30,30,30,30	0
56	MG	2A	3003	1/1	0.87	0.23	44,44,44,44	0
56	MG	1Y	201	1/1	0.87	0.23	32,32,32,32	0
56	MG	2a	3213	1/1	0.87	0.08	75,75,75,75	0
56	MG	1A	3061	1/1	0.87	0.18	67,67,67,67	0
56	MG	1A	3505	1/1	0.87	0.16	39,39,39,39	0
56	MG	1a	1752	1/1	0.87	0.19	74,74,74,74	0
56	MG	2A	3022	1/1	0.87	0.29	56,56,56,56	0
56	MG	12	101	1/1	0.87	0.15	54,54,54,54	0
56	MG	1a	1754	1/1	0.87	0.16	57,57,57,57	0
56	MG	2A	3692	1/1	0.87	0.07	66,66,66,66	0
56	MG	20	101	1/1	0.87	0.11	67,67,67,67	0
56	MG	1A	3917	1/1	0.87	0.16	34,34,34,34	0
56	MG	2t	201	1/1	0.87	0.14	47,47,47,47	0
56	MG	2A	3043	1/1	0.87	0.19	57,57,57,57	0
56	MG	2A	3702	1/1	0.87	0.10	31,31,31,31	0
56	MG	1A	3296	1/1	0.87	0.12	32,32,32,32	0
56	MG	2A	3248	1/1	0.87	0.57	65,65,65,65	0
56	MG	1A	3664	1/1	0.87	0.08	40,40,40,40	0
56	MG	1A	3997	1/1	0.87	0.20	45,45,45,45	0
56	MG	2A	3252	1/1	0.87	0.11	48,48,48,48	0
56	MG	2W	201	1/1	0.88	0.26	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	2W	202	1/1	0.88	0.28	45,45,45,45	0
56	MG	1A	3575	1/1	0.88	0.22	55,55,55,55	0
56	MG	1a	1623	1/1	0.88	0.23	55,55,55,55	0
56	MG	2A	3369	1/1	0.88	0.11	64,64,64,64	0
56	MG	25	103	1/1	0.88	0.22	45,45,45,45	0
56	MG	2A	3370	1/1	0.88	0.12	64,64,64,64	0
56	MG	2A	3664	1/1	0.88	0.13	57,57,57,57	0
56	MG	1A	3458	1/1	0.88	0.14	62,62,62,62	0
56	MG	1A	3109	1/1	0.88	0.41	31,31,31,31	0
56	MG	2A	3375	1/1	0.88	0.18	64,64,64,64	0
56	MG	1A	4070	1/1	0.88	0.07	52,52,52,52	0
56	MG	2A	3687	1/1	0.88	0.34	71,71,71,71	0
56	MG	2A	3688	1/1	0.88	0.16	57,57,57,57	0
56	MG	1a	1642	1/1	0.88	0.17	57,57,57,57	0
56	MG	2A	3379	1/1	0.88	0.15	56,56,56,56	0
56	MG	1A	4073	1/1	0.88	0.36	59,59,59,59	0
56	MG	2a	3020	1/1	0.88	0.14	71,71,71,71	0
56	MG	2a	3023	1/1	0.88	0.16	76,76,76,76	0
56	MG	2A	3181	1/1	0.88	0.11	44,44,44,44	0
56	MG	1A	3060	1/1	0.88	0.14	39,39,39,39	0
56	MG	1A	3470	1/1	0.88	0.24	49,49,49,49	0
56	MG	2A	3706	1/1	0.88	0.14	68,68,68,68	0
56	MG	1A	3709	1/1	0.88	0.19	41,41,41,41	0
56	MG	1A	4082	1/1	0.88	0.11	35,35,35,35	0
56	MG	2A	3712	1/1	0.88	0.18	70,70,70,70	0
56	MG	2A	3194	1/1	0.88	0.38	60,60,60,60	0
56	MG	2a	3046	1/1	0.88	0.11	66,66,66,66	0
56	MG	1A	3988	1/1	0.88	0.25	21,21,21,21	0
56	MG	1A	3606	1/1	0.88	0.20	36,36,36,36	0
56	MG	1A	3870	1/1	0.88	0.20	30,30,30,30	0
56	MG	2A	3721	1/1	0.88	0.11	62,62,62,62	0
56	MG	1a	1666	1/1	0.88	0.14	63,63,63,63	0
56	MG	1a	1667	1/1	0.88	0.21	58,58,58,58	0
56	MG	1A	4094	1/1	0.88	0.22	47,47,47,47	0
56	MG	2A	3409	1/1	0.88	0.15	66,66,66,66	0
56	MG	1A	3991	1/1	0.88	0.19	22,22,22,22	0
56	MG	1A	3506	1/1	0.88	0.27	47,47,47,47	0
56	MG	2A	3743	1/1	0.88	0.09	59,59,59,59	0
56	MG	2A	3746	1/1	0.88	0.11	57,57,57,57	0
56	MG	1A	3722	1/1	0.88	0.16	59,59,59,59	0
56	MG	1w	102	1/1	0.88	0.20	75,75,75,75	0
56	MG	2A	3228	1/1	0.88	0.40	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1677	1/1	0.88	0.29	57,57,57,57	0
56	MG	2A	3428	1/1	0.88	0.20	50,50,50,50	0
56	MG	1A	3725	1/1	0.88	0.08	66,66,66,66	0
56	MG	1A	3617	1/1	0.88	0.13	36,36,36,36	0
56	MG	2A	3770	1/1	0.88	0.31	54,54,54,54	0
56	MG	1B	211	1/1	0.88	0.32	51,51,51,51	0
56	MG	1A	3889	1/1	0.88	0.18	44,44,44,44	0
56	MG	1A	3625	1/1	0.88	0.12	53,53,53,53	0
56	MG	1a	1691	1/1	0.88	0.14	64,64,64,64	0
56	MG	2A	3792	1/1	0.88	0.41	63,63,63,63	0
56	MG	1A	3238	1/1	0.88	0.23	56,56,56,56	0
56	MG	2A	3459	1/1	0.88	0.11	41,41,41,41	0
56	MG	1A	3734	1/1	0.88	0.11	49,49,49,49	0
56	MG	2A	3462	1/1	0.88	0.20	60,60,60,60	0
56	MG	1A	3739	1/1	0.88	0.11	51,51,51,51	0
56	MG	1B	233	1/1	0.88	0.09	63,63,63,63	0
56	MG	2A	3470	1/1	0.88	0.62	62,62,62,62	0
56	MG	2a	3131	1/1	0.88	0.19	60,60,60,60	0
56	MG	1A	3276	1/1	0.88	0.12	45,45,45,45	0
56	MG	1A	3519	1/1	0.88	0.11	45,45,45,45	0
56	MG	2A	3011	1/1	0.88	0.09	53,53,53,53	0
56	MG	1A	4018	1/1	0.88	0.17	35,35,35,35	0
56	MG	1a	1709	1/1	0.88	0.18	50,50,50,50	0
56	MG	1a	1710	1/1	0.88	0.15	53,53,53,53	0
56	MG	2A	3030	1/1	0.88	0.12	46,46,46,46	0
56	MG	1A	3750	1/1	0.88	0.14	34,34,34,34	0
56	MG	2A	3270	1/1	0.88	0.20	57,57,57,57	0
56	MG	2a	3148	1/1	0.88	0.14	63,63,63,63	0
56	MG	1a	1712	1/1	0.88	0.27	53,53,53,53	0
56	MG	1A	3388	1/1	0.88	0.18	44,44,44,44	0
56	MG	1A	3303	1/1	0.88	0.39	55,55,55,55	0
56	MG	2A	3503	1/1	0.88	0.19	39,39,39,39	0
56	MG	1F	304	1/1	0.88	0.13	34,34,34,34	0
56	MG	1A	3644	1/1	0.88	0.17	58,58,58,58	0
56	MG	2A	3509	1/1	0.88	0.15	41,41,41,41	0
56	MG	1a	1726	1/1	0.88	0.14	61,61,61,61	0
56	MG	1A	3335	1/1	0.88	0.17	36,36,36,36	0
56	MG	1G	204	1/1	0.88	0.12	52,52,52,52	0
56	MG	1A	3770	1/1	0.88	0.15	32,32,32,32	0
56	MG	1A	3123	1/1	0.88	0.27	41,41,41,41	0
56	MG	2A	3847	1/1	0.88	0.11	47,47,47,47	0
56	MG	1A	3155	1/1	0.88	0.21	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	3667	1/1	0.88	0.18	28,28,28,28	0
56	MG	2A	3853	1/1	0.88	0.13	49,49,49,49	0
56	MG	1A	4037	1/1	0.88	0.10	68,68,68,68	0
56	MG	2a	3179	1/1	0.88	0.08	69,69,69,69	0
56	MG	1A	3438	1/1	0.88	0.16	50,50,50,50	0
56	MG	1A	3787	1/1	0.88	0.08	44,44,44,44	0
56	MG	1Q	205	1/1	0.88	0.21	55,55,55,55	0
56	MG	1A	3681	1/1	0.88	0.08	47,47,47,47	0
56	MG	1a	1762	1/1	0.88	0.19	61,61,61,61	0
56	MG	2A	3862	1/1	0.88	0.09	57,57,57,57	0
56	MG	1A	3949	1/1	0.88	0.07	54,54,54,54	0
56	MG	1A	4046	1/1	0.88	0.15	44,44,44,44	0
56	MG	1O	102	1/1	0.88	0.16	41,41,41,41	0
56	MG	1A	3547	1/1	0.88	0.18	42,42,42,42	0
56	MG	2a	3202	1/1	0.88	0.27	75,75,75,75	0
56	MG	1A	3361	1/1	0.88	0.17	56,56,56,56	0
56	MG	1A	4051	1/1	0.88	0.32	58,58,58,58	0
56	MG	2B	212	1/1	0.88	0.18	57,57,57,57	0
56	MG	1Z	102	1/1	0.88	0.21	39,39,39,39	0
56	MG	1A	3563	1/1	0.88	0.16	53,53,53,53	0
56	MG	2a	3231	1/1	0.88	0.15	58,58,58,58	0
56	MG	2a	3233	1/1	0.88	0.15	67,67,67,67	0
56	MG	1S	103	1/1	0.88	0.24	51,51,51,51	0
56	MG	1U	107	1/1	0.88	0.30	56,56,56,56	0
56	MG	2A	3130	1/1	0.88	0.21	54,54,54,54	0
56	MG	2A	3343	1/1	0.88	0.08	57,57,57,57	0
56	MG	1a	1791	1/1	0.88	0.10	64,64,64,64	0
56	MG	2A	3348	1/1	0.88	0.14	65,65,65,65	0
56	MG	1A	3456	1/1	0.88	0.12	49,49,49,49	0
56	MG	1A	3802	1/1	0.88	0.24	60,60,60,60	0
56	MG	2A	3150	1/1	0.88	0.35	53,53,53,53	0
56	MG	1A	3963	1/1	0.88	0.11	33,33,33,33	0
56	MG	2Q	204	1/1	0.88	0.42	62,62,62,62	0
56	MG	1A	3566	1/1	0.88	0.15	52,52,52,52	0
56	MG	2A	3160	1/1	0.88	0.53	57,57,57,57	0
56	MG	1A	3690	1/1	0.88	0.20	19,19,19,19	0
56	MG	1a	1732	1/1	0.89	0.20	64,64,64,64	0
56	MG	2A	3041	1/1	0.89	0.12	70,70,70,70	0
56	MG	1A	3451	1/1	0.89	0.31	42,42,42,42	0
56	MG	1A	3314	1/1	0.89	0.23	48,48,48,48	0
56	MG	2A	3254	1/1	0.89	0.17	63,63,63,63	0
56	MG	2a	3008	1/1	0.89	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3315	1/1	0.89	0.14	51,51,51,51	0
56	MG	2A	3442	1/1	0.89	0.21	57,57,57,57	0
56	MG	2A	3257	1/1	0.89	0.16	62,62,62,62	0
56	MG	1A	3964	1/1	0.89	0.07	33,33,33,33	0
56	MG	1A	3263	1/1	0.89	0.11	64,64,64,64	0
56	MG	2a	3024	1/1	0.89	0.16	59,59,59,59	0
56	MG	15	102	1/1	0.89	0.32	42,42,42,42	0
56	MG	2A	3456	1/1	0.89	0.11	61,61,61,61	0
56	MG	1A	3970	1/1	0.89	0.16	20,20,20,20	0
56	MG	1A	3974	1/1	0.89	0.08	54,54,54,54	0
56	MG	2a	3036	1/1	0.89	0.15	72,72,72,72	0
56	MG	1A	3976	1/1	0.89	0.14	47,47,47,47	0
56	MG	1A	3398	1/1	0.89	0.20	23,23,23,23	0
56	MG	1A	3822	1/1	0.89	0.09	25,25,25,25	0
56	MG	2A	3465	1/1	0.89	0.11	48,48,48,48	0
56	MG	1A	3981	1/1	0.89	0.18	60,60,60,60	0
56	MG	1A	3538	1/1	0.89	0.18	50,50,50,50	0
56	MG	2A	3473	1/1	0.89	0.14	60,60,60,60	0
56	MG	1A	3344	1/1	0.89	0.19	53,53,53,53	0
56	MG	1A	3552	1/1	0.89	0.18	27,27,27,27	0
56	MG	1a	1786	1/1	0.89	0.10	73,73,73,73	0
56	MG	2A	3771	1/1	0.89	0.10	62,62,62,62	0
56	MG	2A	3089	1/1	0.89	0.14	61,61,61,61	0
56	MG	2a	3056	1/1	0.89	0.11	57,57,57,57	0
56	MG	1A	3696	1/1	0.89	0.14	20,20,20,20	0
56	MG	2A	3781	1/1	0.89	0.09	57,57,57,57	0
56	MG	1A	3555	1/1	0.89	0.21	23,23,23,23	0
56	MG	2A	3788	1/1	0.89	0.19	51,51,51,51	0
56	MG	1A	3401	1/1	0.89	0.28	35,35,35,35	0
56	MG	1A	3473	1/1	0.89	0.42	65,65,65,65	0
56	MG	2A	3491	1/1	0.89	0.14	50,50,50,50	0
56	MG	1A	3226	1/1	0.89	0.23	43,43,43,43	0
56	MG	1a	1654	1/1	0.89	0.16	71,71,71,71	0
56	MG	2A	3115	1/1	0.89	0.09	41,41,41,41	0
56	MG	1A	3565	1/1	0.89	0.11	58,58,58,58	0
56	MG	1A	4099	1/1	0.89	0.21	40,40,40,40	0
56	MG	1A	3712	1/1	0.89	0.07	54,54,54,54	0
56	MG	2A	3312	1/1	0.89	0.16	50,50,50,50	0
56	MG	1A	3129	1/1	0.89	0.27	47,47,47,47	0
56	MG	1A	3572	1/1	0.89	0.30	39,39,39,39	0
56	MG	1A	3006	1/1	0.89	0.21	47,47,47,47	0
56	MG	1A	3891	1/1	0.89	0.21	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3105	1/1	0.89	0.12	45,45,45,45	0
56	MG	1a	1665	1/1	0.89	0.21	51,51,51,51	0
56	MG	2A	3326	1/1	0.89	0.24	61,61,61,61	0
56	MG	1A	3479	1/1	0.89	0.14	53,53,53,53	0
56	MG	2A	3149	1/1	0.89	0.13	63,63,63,63	0
56	MG	1A	4002	1/1	0.89	0.12	31,31,31,31	0
56	MG	2A	3152	1/1	0.89	0.28	71,71,71,71	0
56	MG	1A	3029	1/1	0.89	0.14	23,23,23,23	0
56	MG	1B	227	1/1	0.89	0.14	60,60,60,60	0
56	MG	2A	3338	1/1	0.89	0.18	62,62,62,62	0
56	MG	1a	1671	1/1	0.89	0.12	49,49,49,49	0
56	MG	2A	3341	1/1	0.89	0.31	66,66,66,66	0
56	MG	1A	3484	1/1	0.89	0.25	59,59,59,59	0
56	MG	2a	3139	1/1	0.89	0.09	70,70,70,70	0
56	MG	1A	3486	1/1	0.89	0.18	44,44,44,44	0
56	MG	1A	3246	1/1	0.89	0.27	50,50,50,50	0
56	MG	2A	3834	1/1	0.89	0.15	48,48,48,48	0
56	MG	1A	3416	1/1	0.89	0.22	36,36,36,36	0
56	MG	2A	3839	1/1	0.89	0.10	35,35,35,35	0
56	MG	2A	3575	1/1	0.89	0.20	65,65,65,65	0
56	MG	2A	3845	1/1	0.89	0.09	44,44,44,44	0
56	MG	2A	3581	1/1	0.89	0.11	46,46,46,46	0
56	MG	2A	3583	1/1	0.89	0.08	61,61,61,61	0
56	MG	1a	1680	1/1	0.89	0.15	63,63,63,63	0
56	MG	1B	236	1/1	0.89	0.14	49,49,49,49	0
56	MG	1a	1827	1/1	0.89	0.15	52,52,52,52	0
56	MG	1A	3613	1/1	0.89	0.15	42,42,42,42	0
56	MG	1A	4019	1/1	0.89	0.14	22,22,22,22	0
56	MG	1A	3490	1/1	0.89	0.23	35,35,35,35	0
56	MG	2A	3603	1/1	0.89	0.09	60,60,60,60	0
56	MG	2A	3183	1/1	0.89	0.20	52,52,52,52	0
56	MG	1A	4026	1/1	0.89	0.12	35,35,35,35	0
56	MG	2A	3189	1/1	0.89	0.20	60,60,60,60	0
56	MG	1A	3063	1/1	0.89	0.16	43,43,43,43	0
56	MG	2A	3873	1/1	0.89	0.40	75,75,75,75	0
56	MG	1A	3419	1/1	0.89	0.11	32,32,32,32	0
56	MG	1a	1695	1/1	0.89	0.27	52,52,52,52	0
56	MG	2A	3885	1/1	0.89	0.24	59,59,59,59	0
56	MG	2A	3198	1/1	0.89	0.15	68,68,68,68	0
56	MG	2A	3619	1/1	0.89	0.12	36,36,36,36	0
56	MG	2B	209	1/1	0.89	0.17	59,59,59,59	0
56	MG	1A	3420	1/1	0.89	0.15	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	1x	103	1/1	0.89	0.15	48,48,48,48	0
56	MG	2A	3627	1/1	0.89	0.13	44,44,44,44	0
56	MG	1A	3209	1/1	0.89	0.17	38,38,38,38	0
56	MG	1A	3159	1/1	0.89	0.30	30,30,30,30	0
56	MG	2A	3643	1/1	0.89	0.11	62,62,62,62	0
56	MG	2A	3206	1/1	0.89	0.32	53,53,53,53	0
56	MG	2D	309	1/1	0.89	0.20	35,35,35,35	0
56	MG	2F	301	1/1	0.89	0.35	46,46,46,46	0
56	MG	1A	3379	1/1	0.89	0.15	48,48,48,48	0
56	MG	2a	3214	1/1	0.89	0.08	74,74,74,74	0
56	MG	2F	303	1/1	0.89	0.40	48,48,48,48	0
56	MG	2a	3220	1/1	0.89	0.06	63,63,63,63	0
56	MG	1A	3091	1/1	0.89	0.13	50,50,50,50	0
56	MG	1A	3940	1/1	0.89	0.14	28,28,28,28	0
56	MG	2A	3670	1/1	0.89	0.34	47,47,47,47	0
56	MG	1A	3646	1/1	0.89	0.16	30,30,30,30	0
56	MG	1A	3650	1/1	0.89	0.20	49,49,49,49	0
56	MG	1A	3306	1/1	0.89	0.21	41,41,41,41	0
56	MG	1A	3390	1/1	0.89	0.23	36,36,36,36	0
56	MG	2A	3686	1/1	0.89	0.18	53,53,53,53	0
56	MG	1A	3446	1/1	0.89	0.17	52,52,52,52	0
56	MG	1a	1720	1/1	0.89	0.28	51,51,51,51	0
56	MG	2A	3689	1/1	0.89	0.09	59,59,59,59	0
56	MG	1A	3447	1/1	0.89	0.19	51,51,51,51	0
56	MG	1A	3956	1/1	0.89	0.23	45,45,45,45	0
56	MG	2A	3408	1/1	0.89	0.40	52,52,52,52	0
56	MG	2w	103	1/1	0.89	0.07	64,64,64,64	0
56	MG	2x	102	1/1	0.89	0.10	70,70,70,70	0
56	MG	1W	201	1/1	0.89	0.29	49,49,49,49	0
56	MG	1A	3957	1/1	0.89	0.08	50,50,50,50	0
56	MG	1Z	302	1/1	0.89	0.08	60,60,60,60	0
56	MG	1A	3450	1/1	0.89	0.43	50,50,50,50	0
56	MG	2A	3727	1/1	0.90	0.15	61,61,61,61	0
56	MG	1A	3055	1/1	0.90	0.15	23,23,23,23	0
56	MG	2A	3732	1/1	0.90	0.10	72,72,72,72	0
56	MG	1A	3168	1/1	0.90	0.48	40,40,40,40	0
56	MG	2A	3472	1/1	0.90	0.15	64,64,64,64	0
56	MG	1A	3025	1/1	0.90	0.15	30,30,30,30	0
56	MG	2a	3011	1/1	0.90	0.12	66,66,66,66	0
56	MG	1A	4065	1/1	0.90	0.13	36,36,36,36	0
56	MG	1a	1815	1/1	0.90	0.19	66,66,66,66	0
56	MG	2a	3017	1/1	0.90	0.10	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3132	1/1	0.90	0.15	36,36,36,36	0
56	MG	2A	3748	1/1	0.90	0.42	68,68,68,68	0
56	MG	2A	3301	1/1	0.90	0.17	57,57,57,57	0
56	MG	1A	3586	1/1	0.90	0.36	31,31,31,31	0
56	MG	1A	3601	1/1	0.90	0.42	43,43,43,43	0
56	MG	2a	3028	1/1	0.90	0.09	62,62,62,62	0
56	MG	2A	3761	1/1	0.90	0.18	62,62,62,62	0
56	MG	1a	1819	1/1	0.90	0.21	68,68,68,68	0
56	MG	1T	203	1/1	0.90	0.13	53,53,53,53	0
56	MG	1T	204	1/1	0.90	0.10	59,59,59,59	0
56	MG	1A	3604	1/1	0.90	0.17	27,27,27,27	0
56	MG	1A	4071	1/1	0.90	0.14	51,51,51,51	0
56	MG	2A	3317	1/1	0.90	0.45	49,49,49,49	0
56	MG	2A	3777	1/1	0.90	0.23	47,47,47,47	0
56	MG	1a	1699	1/1	0.90	0.30	47,47,47,47	0
56	MG	1A	3051	1/1	0.90	0.28	31,31,31,31	0
56	MG	1A	3791	1/1	0.90	0.24	63,63,63,63	0
56	MG	2A	3782	1/1	0.90	0.08	55,55,55,55	0
56	MG	2A	3783	1/1	0.90	0.15	58,58,58,58	0
56	MG	2A	3786	1/1	0.90	0.12	51,51,51,51	0
56	MG	1A	3308	1/1	0.90	0.17	32,32,32,32	0
56	MG	2A	3329	1/1	0.90	0.14	60,60,60,60	0
56	MG	2a	3059	1/1	0.90	0.08	80,80,80,80	0
56	MG	1A	3253	1/1	0.90	0.13	54,54,54,54	0
56	MG	1A	3609	1/1	0.90	0.20	25,25,25,25	0
56	MG	1A	3290	1/1	0.90	0.18	40,40,40,40	0
56	MG	1A	4085	1/1	0.90	0.17	17,17,17,17	0
56	MG	1A	3424	1/1	0.90	0.17	48,48,48,48	0
56	MG	1A	3942	1/1	0.90	0.13	51,51,51,51	0
56	MG	1x	107	1/1	0.90	0.23	49,49,49,49	0
56	MG	15	104	1/1	0.90	0.24	42,42,42,42	0
56	MG	2A	3541	1/1	0.90	0.09	49,49,49,49	0
56	MG	2a	3081	1/1	0.90	0.14	60,60,60,60	0
56	MG	16	102	1/1	0.90	0.43	40,40,40,40	0
56	MG	1A	4013	1/1	0.90	0.07	62,62,62,62	0
56	MG	2a	3085	1/1	0.90	0.16	73,73,73,73	0
56	MG	18	105	1/1	0.90	0.14	45,45,45,45	0
56	MG	1x	115	1/1	0.90	0.17	64,64,64,64	0
56	MG	2a	3093	1/1	0.90	0.20	53,53,53,53	0
56	MG	2A	3553	1/1	0.90	0.12	49,49,49,49	0
56	MG	2A	3811	1/1	0.90	0.16	54,54,54,54	0
56	MG	1A	3428	1/1	0.90	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3815	1/1	0.90	0.07	73,73,73,73	0
56	MG	2A	3561	1/1	0.90	0.15	36,36,36,36	0
56	MG	2a	3102	1/1	0.90	0.11	54,54,54,54	0
56	MG	1A	3393	1/1	0.90	0.21	43,43,43,43	0
56	MG	1A	4017	1/1	0.90	0.07	39,39,39,39	0
56	MG	1A	3316	1/1	0.90	0.21	40,40,40,40	0
56	MG	2a	3114	1/1	0.90	0.11	65,65,65,65	0
56	MG	1A	3363	1/1	0.90	0.20	51,51,51,51	0
56	MG	2A	3569	1/1	0.90	0.09	46,46,46,46	0
56	MG	2A	3359	1/1	0.90	0.39	51,51,51,51	0
56	MG	2A	3572	1/1	0.90	0.15	51,51,51,51	0
56	MG	1A	3010	1/1	0.90	0.20	36,36,36,36	0
56	MG	2A	3578	1/1	0.90	0.15	54,54,54,54	0
56	MG	2a	3132	1/1	0.90	0.14	54,54,54,54	0
56	MG	1A	3718	1/1	0.90	0.19	31,31,31,31	0
56	MG	1a	1622	1/1	0.90	0.10	40,40,40,40	0
56	MG	1A	3641	1/1	0.90	0.14	22,22,22,22	0
56	MG	2A	3586	1/1	0.90	0.09	60,60,60,60	0
56	MG	2A	3837	1/1	0.90	0.07	66,66,66,66	0
56	MG	2A	3212	1/1	0.90	0.25	66,66,66,66	0
56	MG	2A	3594	1/1	0.90	0.18	66,66,66,66	0
56	MG	2A	3027	1/1	0.90	0.18	71,71,71,71	0
56	MG	2A	3215	1/1	0.90	0.14	56,56,56,56	0
56	MG	1a	1626	1/1	0.90	0.20	52,52,52,52	0
56	MG	1a	1758	1/1	0.90	0.12	32,32,32,32	0
56	MG	2A	3219	1/1	0.90	0.09	52,52,52,52	0
56	MG	1A	3724	1/1	0.90	0.09	53,53,53,53	0
56	MG	2A	3222	1/1	0.90	0.35	61,61,61,61	0
56	MG	2A	3380	1/1	0.90	0.13	75,75,75,75	0
56	MG	1a	1636	1/1	0.90	0.12	49,49,49,49	0
56	MG	1A	3365	1/1	0.90	0.09	55,55,55,55	0
56	MG	2a	3162	1/1	0.90	0.07	82,82,82,82	0
56	MG	1A	3443	1/1	0.90	0.20	49,49,49,49	0
56	MG	2A	3384	1/1	0.90	0.27	62,62,62,62	0
56	MG	2A	3046	1/1	0.90	0.13	48,48,48,48	0
56	MG	2A	3387	1/1	0.90	0.25	62,62,62,62	0
56	MG	1A	3866	1/1	0.90	0.14	22,22,22,22	0
56	MG	2A	3624	1/1	0.90	0.14	40,40,40,40	0
56	MG	2A	3238	1/1	0.90	0.22	45,45,45,45	0
56	MG	2A	3879	1/1	0.90	0.11	47,47,47,47	0
56	MG	2A	3881	1/1	0.90	0.15	62,62,62,62	0
56	MG	2A	3630	1/1	0.90	0.21	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3635	1/1	0.90	0.29	61,61,61,61	0
56	MG	1a	1775	1/1	0.90	0.12	65,65,65,65	0
56	MG	1A	3491	1/1	0.90	0.13	38,38,38,38	0
56	MG	1A	3366	1/1	0.90	0.26	40,40,40,40	0
56	MG	1A	3967	1/1	0.90	0.12	46,46,46,46	0
56	MG	1A	3654	1/1	0.90	0.14	37,37,37,37	0
56	MG	2A	3249	1/1	0.90	0.30	55,55,55,55	0
56	MG	2A	3065	1/1	0.90	0.16	68,68,68,68	0
56	MG	2a	3194	1/1	0.90	0.14	55,55,55,55	0
56	MG	2D	302	1/1	0.90	0.16	55,55,55,55	0
56	MG	2D	303	1/1	0.90	0.33	42,42,42,42	0
56	MG	1A	3403	1/1	0.90	0.27	53,53,53,53	0
56	MG	2A	3070	1/1	0.90	0.28	56,56,56,56	0
56	MG	1D	306	1/1	0.90	0.30	33,33,33,33	0
56	MG	2a	3207	1/1	0.90	0.08	62,62,62,62	0
56	MG	1A	3971	1/1	0.90	0.31	32,32,32,32	0
56	MG	2E	301	1/1	0.90	0.15	49,49,49,49	0
56	MG	2A	3680	1/1	0.90	0.24	54,54,54,54	0
56	MG	1A	3878	1/1	0.90	0.41	30,30,30,30	0
56	MG	2A	3256	1/1	0.90	0.11	68,68,68,68	0
56	MG	2A	3075	1/1	0.90	0.23	48,48,48,48	0
56	MG	1A	3662	1/1	0.90	0.15	19,19,19,19	0
56	MG	1A	3663	1/1	0.90	0.17	21,21,21,21	0
56	MG	1A	3748	1/1	0.90	0.16	47,47,47,47	0
56	MG	1a	1795	1/1	0.90	0.20	64,64,64,64	0
56	MG	1A	3081	1/1	0.90	0.15	27,27,27,27	0
56	MG	1F	309	1/1	0.90	0.16	53,53,53,53	0
56	MG	2A	3445	1/1	0.90	0.28	60,60,60,60	0
56	MG	2A	3446	1/1	0.90	0.14	63,63,63,63	0
56	MG	2l	201	1/1	0.90	0.25	55,55,55,55	0
56	MG	2l	204	1/1	0.90	0.12	72,72,72,72	0
56	MG	1G	201	1/1	0.90	0.20	43,43,43,43	0
56	MG	1A	3376	1/1	0.90	0.37	44,44,44,44	0
56	MG	1A	3898	1/1	0.90	0.19	32,32,32,32	0
56	MG	2A	3274	1/1	0.90	0.17	59,59,59,59	0
56	MG	1A	3406	1/1	0.90	0.33	43,43,43,43	0
56	MG	2O	102	1/1	0.90	0.18	65,65,65,65	0
56	MG	1a	1676	1/1	0.90	0.10	72,72,72,72	0
56	MG	1A	3409	1/1	0.90	0.26	41,41,41,41	0
56	MG	2A	3284	1/1	0.90	0.29	59,59,59,59	0
56	MG	1A	3916	1/1	0.90	0.17	22,22,22,22	0
56	MG	1O	201	1/1	0.90	0.16	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	1V	202	1/1	0.91	0.30	39,39,39,39	0
56	MG	2A	3671	1/1	0.91	0.08	59,59,59,59	0
56	MG	2A	3398	1/1	0.91	0.17	58,58,58,58	0
56	MG	1V	207	1/1	0.91	0.12	52,52,52,52	0
56	MG	2A	3226	1/1	0.91	0.52	57,57,57,57	0
56	MG	2A	3401	1/1	0.91	0.22	54,54,54,54	0
56	MG	1A	3328	1/1	0.91	0.19	48,48,48,48	0
56	MG	2A	3685	1/1	0.91	0.13	60,60,60,60	0
56	MG	1W	204	1/1	0.91	0.12	34,34,34,34	0
56	MG	2A	3231	1/1	0.91	0.23	50,50,50,50	0
56	MG	1A	3213	1/1	0.91	0.21	44,44,44,44	0
56	MG	23	102	1/1	0.91	0.18	45,45,45,45	0
56	MG	1Z	301	1/1	0.91	0.23	48,48,48,48	0
56	MG	2A	3690	1/1	0.91	0.08	40,40,40,40	0
56	MG	1A	3350	1/1	0.91	0.33	51,51,51,51	0
56	MG	10	101	1/1	0.91	0.13	38,38,38,38	0
56	MG	2A	3694	1/1	0.91	0.12	50,50,50,50	0
56	MG	1a	1718	1/1	0.91	0.14	53,53,53,53	0
56	MG	1a	1719	1/1	0.91	0.11	41,41,41,41	0
56	MG	2A	3701	1/1	0.91	0.13	58,58,58,58	0
56	MG	1A	3906	1/1	0.91	0.08	49,49,49,49	0
56	MG	1A	3758	1/1	0.91	0.16	40,40,40,40	0
56	MG	2A	3427	1/1	0.91	0.23	42,42,42,42	0
56	MG	1A	3271	1/1	0.91	0.24	44,44,44,44	0
56	MG	11	105	1/1	0.91	0.19	53,53,53,53	0
56	MG	1a	1728	1/1	0.91	0.21	51,51,51,51	0
56	MG	1A	3671	1/1	0.91	0.11	29,29,29,29	0
56	MG	1A	3994	1/1	0.91	0.07	70,70,70,70	0
56	MG	1A	3459	1/1	0.91	0.12	49,49,49,49	0
56	MG	1A	3768	1/1	0.91	0.15	38,38,38,38	0
56	MG	1A	3680	1/1	0.91	0.27	38,38,38,38	0
56	MG	2A	3723	1/1	0.91	0.11	51,51,51,51	0
56	MG	1A	3273	1/1	0.91	0.28	35,35,35,35	0
56	MG	2A	3449	1/1	0.91	0.21	56,56,56,56	0
56	MG	2a	3032	1/1	0.91	0.18	65,65,65,65	0
56	MG	1A	3775	1/1	0.91	0.18	21,21,21,21	0
56	MG	2A	3454	1/1	0.91	0.17	50,50,50,50	0
56	MG	18	103	1/1	0.91	0.13	22,22,22,22	0
56	MG	1A	3499	1/1	0.91	0.16	44,44,44,44	0
56	MG	2A	3736	1/1	0.91	0.24	57,57,57,57	0
56	MG	2A	3458	1/1	0.91	0.14	53,53,53,53	0
56	MG	2A	3066	1/1	0.91	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	3500	1/1	0.91	0.18	37,37,37,37	0
56	MG	1a	1602	1/1	0.91	0.17	61,61,61,61	0
56	MG	2A	3269	1/1	0.91	0.13	53,53,53,53	0
56	MG	1a	1603	1/1	0.91	0.27	61,61,61,61	0
56	MG	2A	3466	1/1	0.91	0.19	47,47,47,47	0
56	MG	2A	3754	1/1	0.91	0.43	67,67,67,67	0
56	MG	1A	3467	1/1	0.91	0.13	46,46,46,46	0
56	MG	1A	3582	1/1	0.91	0.18	30,30,30,30	0
56	MG	1a	1763	1/1	0.91	0.14	62,62,62,62	0
56	MG	2A	3765	1/1	0.91	0.11	53,53,53,53	0
56	MG	2A	3275	1/1	0.91	0.12	59,59,59,59	0
56	MG	1a	1765	1/1	0.91	0.16	51,51,51,51	0
56	MG	2A	3475	1/1	0.91	0.32	56,56,56,56	0
56	MG	2A	3280	1/1	0.91	0.15	57,57,57,57	0
56	MG	2A	3281	1/1	0.91	0.07	70,70,70,70	0
56	MG	2A	3773	1/1	0.91	0.23	73,73,73,73	0
56	MG	2a	3072	1/1	0.91	0.14	51,51,51,51	0
56	MG	2a	3076	1/1	0.91	0.08	53,53,53,53	0
56	MG	2A	3081	1/1	0.91	0.41	52,52,52,52	0
56	MG	2a	3078	1/1	0.91	0.22	50,50,50,50	0
56	MG	1B	206	1/1	0.91	0.14	40,40,40,40	0
56	MG	1A	3191	1/1	0.91	0.09	43,43,43,43	0
56	MG	1A	3796	1/1	0.91	0.18	20,20,20,20	0
56	MG	2A	3488	1/1	0.91	0.15	56,56,56,56	0
56	MG	2A	3286	1/1	0.91	0.16	56,56,56,56	0
56	MG	2A	3784	1/1	0.91	0.32	64,64,64,64	0
56	MG	1a	1617	1/1	0.91	0.15	53,53,53,53	0
56	MG	1A	3195	1/1	0.91	0.15	55,55,55,55	0
56	MG	2A	3090	1/1	0.91	0.30	45,45,45,45	0
56	MG	2A	3091	1/1	0.91	0.29	48,48,48,48	0
56	MG	2A	3496	1/1	0.91	0.08	55,55,55,55	0
56	MG	2A	3093	1/1	0.91	0.23	37,37,37,37	0
56	MG	1A	3309	1/1	0.91	0.18	38,38,38,38	0
56	MG	2A	3504	1/1	0.91	0.16	49,49,49,49	0
56	MG	2A	3298	1/1	0.91	0.12	57,57,57,57	0
56	MG	1A	3427	1/1	0.91	0.18	43,43,43,43	0
56	MG	1A	3399	1/1	0.91	0.19	48,48,48,48	0
56	MG	2a	3110	1/1	0.91	0.10	62,62,62,62	0
56	MG	2A	3511	1/1	0.91	0.12	58,58,58,58	0
56	MG	2A	3514	1/1	0.91	0.13	67,67,67,67	0
56	MG	1A	3056	1/1	0.91	0.16	45,45,45,45	0
56	MG	1a	1630	1/1	0.91	0.17	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	3521	1/1	0.91	0.11	38,38,38,38	0
56	MG	2a	3126	1/1	0.91	0.12	66,66,66,66	0
56	MG	1a	1631	1/1	0.91	0.12	33,33,33,33	0
56	MG	2A	3810	1/1	0.91	0.32	78,78,78,78	0
56	MG	1A	3521	1/1	0.91	0.10	47,47,47,47	0
56	MG	2A	3526	1/1	0.91	0.09	30,30,30,30	0
56	MG	2A	3527	1/1	0.91	0.16	44,44,44,44	0
56	MG	2A	3816	1/1	0.91	0.29	68,68,68,68	0
56	MG	1A	3951	1/1	0.91	0.10	42,42,42,42	0
56	MG	1A	3285	1/1	0.91	0.32	26,26,26,26	0
56	MG	1A	4029	1/1	0.91	0.12	50,50,50,50	0
56	MG	1a	1643	1/1	0.91	0.15	51,51,51,51	0
56	MG	2A	3319	1/1	0.91	0.15	53,53,53,53	0
56	MG	2A	3542	1/1	0.91	0.10	46,46,46,46	0
56	MG	1a	1645	1/1	0.91	0.14	52,52,52,52	0
56	MG	1A	4030	1/1	0.91	0.08	61,61,61,61	0
56	MG	1A	3812	1/1	0.91	0.11	54,54,54,54	0
56	MG	1A	3524	1/1	0.91	0.20	51,51,51,51	0
56	MG	2a	3152	1/1	0.91	0.20	70,70,70,70	0
56	MG	1A	3140	1/1	0.91	0.26	40,40,40,40	0
56	MG	2A	3144	1/1	0.91	0.21	54,54,54,54	0
56	MG	2A	3832	1/1	0.91	0.15	38,38,38,38	0
56	MG	1A	3369	1/1	0.91	0.12	44,44,44,44	0
56	MG	2a	3158	1/1	0.91	0.14	54,54,54,54	0
56	MG	2a	3159	1/1	0.91	0.07	56,56,56,56	0
56	MG	1A	3715	1/1	0.91	0.17	48,48,48,48	0
56	MG	1E	308	1/1	0.91	0.12	31,31,31,31	0
56	MG	1E	310	1/1	0.91	0.16	61,61,61,61	0
56	MG	1a	1809	1/1	0.91	0.13	72,72,72,72	0
56	MG	2A	3841	1/1	0.91	0.09	47,47,47,47	0
56	MG	2a	3169	1/1	0.91	0.10	77,77,77,77	0
56	MG	1A	3961	1/1	0.91	0.11	56,56,56,56	0
56	MG	1A	3532	1/1	0.91	0.21	52,52,52,52	0
56	MG	1A	3483	1/1	0.91	0.11	59,59,59,59	0
56	MG	2A	3574	1/1	0.91	0.14	46,46,46,46	0
56	MG	2A	3342	1/1	0.91	0.10	55,55,55,55	0
56	MG	1A	3370	1/1	0.91	0.14	40,40,40,40	0
56	MG	2A	3164	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	3965	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3536	1/1	0.91	0.12	69,69,69,69	0
56	MG	1A	3861	1/1	0.91	0.27	61,61,61,61	0
56	MG	1I	201	1/1	0.91	0.14	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	3485	1/1	0.91	0.24	42,42,42,42	0
56	MG	2A	3595	1/1	0.91	0.23	65,65,65,65	0
56	MG	2a	3190	1/1	0.91	0.09	77,77,77,77	0
56	MG	2A	3357	1/1	0.91	0.13	50,50,50,50	0
56	MG	1a	1674	1/1	0.91	0.17	53,53,53,53	0
56	MG	2A	3178	1/1	0.91	0.09	48,48,48,48	0
56	MG	1a	1675	1/1	0.91	0.20	64,64,64,64	0
56	MG	2A	3878	1/1	0.91	0.23	38,38,38,38	0
56	MG	1A	3291	1/1	0.91	0.12	32,32,32,32	0
56	MG	1a	1833	1/1	0.91	0.23	43,43,43,43	0
56	MG	2a	3203	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3606	1/1	0.91	0.18	62,62,62,62	0
56	MG	2a	3208	1/1	0.91	0.08	69,69,69,69	0
56	MG	1A	4050	1/1	0.91	0.09	46,46,46,46	0
56	MG	1A	3972	1/1	0.91	0.15	43,43,43,43	0
56	MG	1A	3539	1/1	0.91	0.32	45,45,45,45	0
56	MG	2B	204	1/1	0.91	0.18	61,61,61,61	0
56	MG	1A	3541	1/1	0.91	0.17	43,43,43,43	0
56	MG	2a	3223	1/1	0.91	0.18	64,64,64,64	0
56	MG	2a	3224	1/1	0.91	0.12	61,61,61,61	0
56	MG	2B	211	1/1	0.91	0.17	75,75,75,75	0
56	MG	1A	3977	1/1	0.91	0.21	59,59,59,59	0
56	MG	1v	101	1/1	0.91	0.14	65,65,65,65	0
56	MG	2B	214	1/1	0.91	0.19	62,62,62,62	0
56	MG	1a	1686	1/1	0.91	0.14	62,62,62,62	0
56	MG	1w	104	1/1	0.91	0.17	72,72,72,72	0
56	MG	2a	3240	1/1	0.91	0.14	67,67,67,67	0
56	MG	1A	3545	1/1	0.91	0.15	46,46,46,46	0
56	MG	1A	3737	1/1	0.91	0.11	41,41,41,41	0
56	MG	2D	304	1/1	0.91	0.54	57,57,57,57	0
56	MG	1w	112	1/1	0.91	0.12	53,53,53,53	0
56	MG	1A	3487	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3632	1/1	0.91	0.12	39,39,39,39	0
56	MG	1Q	207	1/1	0.91	0.09	44,44,44,44	0
56	MG	2A	3636	1/1	0.91	0.47	55,55,55,55	0
56	MG	1Q	208	1/1	0.91	0.41	47,47,47,47	0
56	MG	1S	203	1/1	0.91	0.14	66,66,66,66	0
56	MG	1T	202	1/1	0.91	0.16	45,45,45,45	0
56	MG	2F	304	1/1	0.91	0.18	54,54,54,54	0
56	MG	2A	3390	1/1	0.91	0.24	54,54,54,54	0
56	MG	2x	104	1/1	0.91	0.10	62,62,62,62	0
56	MG	2y	101	1/1	0.91	0.19	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	3740	1/1	0.91	0.13	49,49,49,49	0
56	MG	1A	3124	1/1	0.91	0.18	46,46,46,46	0
56	MG	1A	3189	1/1	0.91	0.65	47,47,47,47	0
56	MG	2A	3645	1/1	0.92	0.14	37,37,37,37	0
56	MG	1A	3574	1/1	0.92	0.24	40,40,40,40	0
56	MG	2A	3656	1/1	0.92	0.15	59,59,59,59	0
56	MG	1a	1635	1/1	0.92	0.09	55,55,55,55	0
56	MG	2R	202	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	3437	1/1	0.92	0.10	53,53,53,53	0
56	MG	1a	1637	1/1	0.92	0.29	54,54,54,54	0
56	MG	1A	3289	1/1	0.92	0.11	49,49,49,49	0
56	MG	1A	3026	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	3700	1/1	0.92	0.18	25,25,25,25	0
56	MG	1B	213	1/1	0.92	0.13	56,56,56,56	0
56	MG	2Z	301	1/1	0.92	0.10	72,72,72,72	0
56	MG	1A	3986	1/1	0.92	0.24	70,70,70,70	0
56	MG	1A	3848	1/1	0.92	0.13	54,54,54,54	0
56	MG	20	103	1/1	0.92	0.25	66,66,66,66	0
56	MG	2A	3681	1/1	0.92	0.15	54,54,54,54	0
56	MG	25	101	1/1	0.92	0.16	58,58,58,58	0
56	MG	1B	224	1/1	0.92	0.21	52,52,52,52	0
56	MG	1A	3849	1/1	0.92	0.11	52,52,52,52	0
56	MG	1a	1821	1/1	0.92	0.05	53,53,53,53	0
56	MG	1A	3851	1/1	0.92	0.17	11,11,11,11	0
56	MG	2A	3201	1/1	0.92	0.27	70,70,70,70	0
56	MG	1a	1823	1/1	0.92	0.06	59,59,59,59	0
56	MG	1A	3580	1/1	0.92	0.35	29,29,29,29	0
56	MG	1B	230	1/1	0.92	0.07	61,61,61,61	0
56	MG	1A	3860	1/1	0.92	0.19	36,36,36,36	0
56	MG	1a	1829	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3410	1/1	0.92	0.27	70,70,70,70	0
56	MG	1A	3705	1/1	0.92	0.23	28,28,28,28	0
56	MG	2A	3213	1/1	0.92	0.15	61,61,61,61	0
56	MG	1A	3084	1/1	0.92	0.15	33,33,33,33	0
56	MG	1a	1662	1/1	0.92	0.17	60,60,60,60	0
56	MG	1A	3867	1/1	0.92	0.11	55,55,55,55	0
56	MG	2a	3021	1/1	0.92	0.07	69,69,69,69	0
56	MG	1A	3707	1/1	0.92	0.17	25,25,25,25	0
56	MG	2A	3422	1/1	0.92	0.10	42,42,42,42	0
56	MG	1A	3243	1/1	0.92	0.42	33,33,33,33	0
56	MG	2a	3026	1/1	0.92	0.36	60,60,60,60	0
56	MG	1D	312	1/1	0.92	0.21	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	3043	1/1	0.92	0.23	33,33,33,33	0
56	MG	2A	3433	1/1	0.92	0.22	49,49,49,49	0
56	MG	2A	3438	1/1	0.92	0.25	56,56,56,56	0
56	MG	2A	3718	1/1	0.92	0.16	41,41,41,41	0
56	MG	2A	3719	1/1	0.92	0.08	60,60,60,60	0
56	MG	1a	1670	1/1	0.92	0.09	60,60,60,60	0
56	MG	2A	3440	1/1	0.92	0.18	61,61,61,61	0
56	MG	1w	106	1/1	0.92	0.06	61,61,61,61	0
56	MG	1E	302	1/1	0.92	0.21	47,47,47,47	0
56	MG	1A	3589	1/1	0.92	0.17	35,35,35,35	0
56	MG	1w	111	1/1	0.92	0.07	69,69,69,69	0
56	MG	1A	3590	1/1	0.92	0.14	26,26,26,26	0
56	MG	1A	3882	1/1	0.92	0.18	44,44,44,44	0
56	MG	1A	3597	1/1	0.92	0.19	49,49,49,49	0
56	MG	1A	3005	1/1	0.92	0.15	37,37,37,37	0
56	MG	2A	3240	1/1	0.92	0.14	51,51,51,51	0
56	MG	1A	3602	1/1	0.92	0.10	47,47,47,47	0
56	MG	1a	1678	1/1	0.92	0.30	59,59,59,59	0
56	MG	2a	3058	1/1	0.92	0.10	74,74,74,74	0
56	MG	1A	3206	1/1	0.92	0.18	42,42,42,42	0
56	MG	1A	3454	1/1	0.92	0.59	39,39,39,39	0
56	MG	1x	113	1/1	0.92	0.10	65,65,65,65	0
56	MG	1a	1681	1/1	0.92	0.21	56,56,56,56	0
56	MG	2a	3063	1/1	0.92	0.11	63,63,63,63	0
56	MG	1A	3896	1/1	0.92	0.24	60,60,60,60	0
56	MG	2A	3464	1/1	0.92	0.15	63,63,63,63	0
56	MG	1A	3897	1/1	0.92	0.11	56,56,56,56	0
56	MG	2A	3763	1/1	0.92	0.09	60,60,60,60	0
56	MG	2A	3764	1/1	0.92	0.08	44,44,44,44	0
56	MG	1A	3050	1/1	0.92	0.21	21,21,21,21	0
56	MG	1A	4022	1/1	0.92	0.08	31,31,31,31	0
56	MG	2A	3469	1/1	0.92	0.19	64,64,64,64	0
56	MG	1A	3727	1/1	0.92	0.16	39,39,39,39	0
56	MG	1A	3059	1/1	0.92	0.24	47,47,47,47	0
56	MG	2A	3010	1/1	0.92	0.17	46,46,46,46	0
56	MG	2a	3083	1/1	0.92	0.45	65,65,65,65	0
56	MG	1A	3513	1/1	0.92	0.16	63,63,63,63	0
56	MG	1A	3515	1/1	0.92	0.18	47,47,47,47	0
56	MG	2A	3015	1/1	0.92	0.13	39,39,39,39	0
56	MG	2A	3016	1/1	0.92	0.17	57,57,57,57	0
56	MG	2a	3092	1/1	0.92	0.09	77,77,77,77	0
56	MG	1A	3257	1/1	0.92	0.17	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	3025	1/1	0.92	0.11	44,44,44,44	0
56	MG	1A	3258	1/1	0.92	0.35	25,25,25,25	0
56	MG	1A	3463	1/1	0.92	0.45	47,47,47,47	0
56	MG	2A	3785	1/1	0.92	0.08	53,53,53,53	0
56	MG	1A	3465	1/1	0.92	0.68	48,48,48,48	0
56	MG	1A	3744	1/1	0.92	0.13	50,50,50,50	0
56	MG	2a	3104	1/1	0.92	0.21	54,54,54,54	0
56	MG	2A	3034	1/1	0.92	0.17	56,56,56,56	0
56	MG	1A	3926	1/1	0.92	0.12	28,28,28,28	0
56	MG	2A	3278	1/1	0.92	0.09	65,65,65,65	0
56	MG	2a	3108	1/1	0.92	0.07	65,65,65,65	0
56	MG	1A	3632	1/1	0.92	0.16	34,34,34,34	0
56	MG	2a	3112	1/1	0.92	0.32	62,62,62,62	0
56	MG	2A	3795	1/1	0.92	0.17	55,55,55,55	0
56	MG	1S	201	1/1	0.92	0.66	40,40,40,40	0
56	MG	1A	3352	1/1	0.92	0.42	41,41,41,41	0
56	MG	2A	3499	1/1	0.92	0.16	47,47,47,47	0
56	MG	1A	3929	1/1	0.92	0.17	39,39,39,39	0
56	MG	2a	3123	1/1	0.92	0.23	68,68,68,68	0
56	MG	1A	3357	1/1	0.92	0.17	48,48,48,48	0
56	MG	2A	3052	1/1	0.92	0.09	63,63,63,63	0
56	MG	1A	3640	1/1	0.92	0.28	49,49,49,49	0
56	MG	1A	4041	1/1	0.92	0.11	42,42,42,42	0
56	MG	1U	205	1/1	0.92	0.65	38,38,38,38	0
56	MG	2A	3289	1/1	0.92	0.52	61,61,61,61	0
56	MG	2A	3061	1/1	0.92	0.27	63,63,63,63	0
56	MG	1U	209	1/1	0.92	0.79	44,44,44,44	0
56	MG	2A	3519	1/1	0.92	0.13	33,33,33,33	0
56	MG	1A	3531	1/1	0.92	0.45	47,47,47,47	0
56	MG	2A	3814	1/1	0.92	0.25	60,60,60,60	0
56	MG	1A	3761	1/1	0.92	0.18	36,36,36,36	0
56	MG	2A	3524	1/1	0.92	0.38	69,69,69,69	0
56	MG	1A	3936	1/1	0.92	0.09	14,14,14,14	0
56	MG	1A	3764	1/1	0.92	0.17	14,14,14,14	0
56	MG	1W	205	1/1	0.92	0.13	39,39,39,39	0
56	MG	2A	3529	1/1	0.92	0.16	52,52,52,52	0
56	MG	2A	3300	1/1	0.92	0.10	52,52,52,52	0
56	MG	1A	3312	1/1	0.92	0.10	34,34,34,34	0
56	MG	2A	3533	1/1	0.92	0.14	60,60,60,60	0
56	MG	2A	3535	1/1	0.92	0.14	51,51,51,51	0
56	MG	2A	3537	1/1	0.92	0.11	56,56,56,56	0
56	MG	1A	3163	1/1	0.92	0.24	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3408	1/1	0.92	0.40	32,32,32,32	0
56	MG	1A	3080	1/1	0.92	0.17	47,47,47,47	0
56	MG	1a	1736	1/1	0.92	0.18	46,46,46,46	0
56	MG	1A	3265	1/1	0.92	0.20	43,43,43,43	0
56	MG	1A	4055	1/1	0.92	0.07	41,41,41,41	0
56	MG	1A	3214	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	3773	1/1	0.92	0.11	46,46,46,46	0
56	MG	1A	3167	1/1	0.92	0.14	38,38,38,38	0
56	MG	1A	3417	1/1	0.92	0.18	48,48,48,48	0
56	MG	2A	3556	1/1	0.92	0.18	50,50,50,50	0
56	MG	1A	3542	1/1	0.92	0.23	37,37,37,37	0
56	MG	1A	3781	1/1	0.92	0.17	41,41,41,41	0
56	MG	2A	3324	1/1	0.92	0.36	49,49,49,49	0
56	MG	2A	3849	1/1	0.92	0.08	63,63,63,63	0
56	MG	2A	3565	1/1	0.92	0.18	68,68,68,68	0
56	MG	1A	3112	1/1	0.92	0.24	35,35,35,35	0
56	MG	2A	3095	1/1	0.92	0.07	59,59,59,59	0
56	MG	15	105	1/1	0.92	0.18	49,49,49,49	0
56	MG	2A	3857	1/1	0.92	0.22	66,66,66,66	0
56	MG	1A	3325	1/1	0.92	0.23	26,26,26,26	0
56	MG	1A	3789	1/1	0.92	0.09	43,43,43,43	0
56	MG	17	104	1/1	0.92	0.15	37,37,37,37	0
56	MG	2A	3108	1/1	0.92	0.12	65,65,65,65	0
56	MG	2a	3195	1/1	0.92	0.18	52,52,52,52	0
56	MG	2A	3111	1/1	0.92	0.18	59,59,59,59	0
56	MG	2A	3579	1/1	0.92	0.19	45,45,45,45	0
56	MG	2a	3198	1/1	0.92	0.11	62,62,62,62	0
56	MG	17	105	1/1	0.92	0.21	37,37,37,37	0
56	MG	17	106	1/1	0.92	0.21	25,25,25,25	0
56	MG	2A	3340	1/1	0.92	0.16	53,53,53,53	0
56	MG	1a	1777	1/1	0.92	0.18	59,59,59,59	0
56	MG	1a	1778	1/1	0.92	0.14	55,55,55,55	0
56	MG	1A	3548	1/1	0.92	0.37	46,46,46,46	0
56	MG	1A	3368	1/1	0.92	0.16	37,37,37,37	0
56	MG	1A	3678	1/1	0.92	0.16	23,23,23,23	0
56	MG	1A	3327	1/1	0.92	0.24	36,36,36,36	0
56	MG	2B	201	1/1	0.92	0.16	66,66,66,66	0
56	MG	2a	3219	1/1	0.92	0.12	68,68,68,68	0
56	MG	2A	3600	1/1	0.92	0.16	56,56,56,56	0
56	MG	2B	203	1/1	0.92	0.18	60,60,60,60	0
56	MG	2A	3351	1/1	0.92	0.33	59,59,59,59	0
56	MG	2B	208	1/1	0.92	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	4079	1/1	0.92	0.23	53,53,53,53	0
56	MG	2a	3230	1/1	0.92	0.29	65,65,65,65	0
56	MG	1A	3016	1/1	0.92	0.20	45,45,45,45	0
56	MG	1A	3562	1/1	0.92	0.27	43,43,43,43	0
56	MG	1A	3683	1/1	0.92	0.21	20,20,20,20	0
56	MG	1A	3230	1/1	0.92	0.14	36,36,36,36	0
56	MG	1A	3188	1/1	0.92	0.08	37,37,37,37	0
56	MG	2d	301	1/1	0.92	0.09	65,65,65,65	0
56	MG	1a	1792	1/1	0.92	0.08	60,60,60,60	0
56	MG	2A	3362	1/1	0.92	0.18	43,43,43,43	0
56	MG	2i	201	1/1	0.92	0.08	62,62,62,62	0
56	MG	1A	4090	1/1	0.92	0.23	53,53,53,53	0
56	MG	2A	3365	1/1	0.92	0.27	54,54,54,54	0
56	MG	1a	1618	1/1	0.92	0.21	49,49,49,49	0
56	MG	2A	3156	1/1	0.92	0.13	54,54,54,54	0
56	MG	1A	3973	1/1	0.92	0.20	50,50,50,50	0
56	MG	1A	3809	1/1	0.92	0.17	39,39,39,39	0
56	MG	1A	3284	1/1	0.92	0.58	35,35,35,35	0
56	MG	2E	304	1/1	0.92	0.08	43,43,43,43	0
56	MG	1a	1625	1/1	0.92	0.15	55,55,55,55	0
56	MG	2A	3374	1/1	0.92	0.08	57,57,57,57	0
56	MG	1A	3815	1/1	0.92	0.15	28,28,28,28	0
56	MG	2A	3166	1/1	0.92	0.14	50,50,50,50	0
56	MG	1a	1802	1/1	0.92	0.13	63,63,63,63	0
56	MG	1A	3380	1/1	0.92	0.18	48,48,48,48	0
56	MG	2y	104	1/1	0.92	0.13	50,50,50,50	0
56	MG	2P	202	1/1	0.92	0.16	47,47,47,47	0
56	MG	1A	3235	1/1	0.92	0.14	59,59,59,59	0
56	MG	2A	3244	1/1	0.93	0.23	43,43,43,43	0
56	MG	2A	3245	1/1	0.93	0.26	47,47,47,47	0
56	MG	2A	3437	1/1	0.93	0.23	56,56,56,56	0
56	MG	1A	3881	1/1	0.93	0.19	36,36,36,36	0
56	MG	1a	1740	1/1	0.93	0.18	43,43,43,43	0
56	MG	1A	3264	1/1	0.93	0.17	36,36,36,36	0
56	MG	2A	3039	1/1	0.93	0.14	65,65,65,65	0
56	MG	2A	3693	1/1	0.93	0.13	62,62,62,62	0
56	MG	1A	4098	1/1	0.93	0.11	50,50,50,50	0
56	MG	25	102	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3444	1/1	0.93	0.13	57,57,57,57	0
56	MG	1A	3883	1/1	0.93	0.09	66,66,66,66	0
56	MG	1a	1750	1/1	0.93	0.07	39,39,39,39	0
56	MG	28	101	1/1	0.93	0.28	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	17	108	1/1	0.93	0.15	45,45,45,45	0
56	MG	18	102	1/1	0.93	0.44	41,41,41,41	0
56	MG	2A	3050	1/1	0.93	0.20	57,57,57,57	0
56	MG	2A	3709	1/1	0.93	0.23	48,48,48,48	0
56	MG	1A	3651	1/1	0.93	0.12	37,37,37,37	0
56	MG	2A	3453	1/1	0.93	0.15	52,52,52,52	0
56	MG	2A	3259	1/1	0.93	0.14	60,60,60,60	0
56	MG	2A	3261	1/1	0.93	0.15	59,59,59,59	0
56	MG	1a	1755	1/1	0.93	0.08	88,88,88,88	0
56	MG	2a	3012	1/1	0.93	0.11	70,70,70,70	0
56	MG	1A	3242	1/1	0.93	0.23	22,22,22,22	0
56	MG	2A	3054	1/1	0.93	0.10	63,63,63,63	0
56	MG	2A	3460	1/1	0.93	0.14	57,57,57,57	0
56	MG	2a	3019	1/1	0.93	0.13	54,54,54,54	0
56	MG	2A	3055	1/1	0.93	0.26	53,53,53,53	0
56	MG	1A	3657	1/1	0.93	0.10	44,44,44,44	0
56	MG	1A	3658	1/1	0.93	0.11	42,42,42,42	0
56	MG	1A	3993	1/1	0.93	0.14	27,27,27,27	0
56	MG	1A	3267	1/1	0.93	0.27	40,40,40,40	0
56	MG	1A	3995	1/1	0.93	0.06	61,61,61,61	0
56	MG	1A	3301	1/1	0.93	0.26	24,24,24,24	0
56	MG	1a	1767	1/1	0.93	0.10	67,67,67,67	0
56	MG	1a	1770	1/1	0.93	0.10	49,49,49,49	0
56	MG	1a	1771	1/1	0.93	0.12	40,40,40,40	0
56	MG	1A	3462	1/1	0.93	0.58	54,54,54,54	0
56	MG	1A	3371	1/1	0.93	0.21	46,46,46,46	0
56	MG	2A	3742	1/1	0.93	0.09	72,72,72,72	0
56	MG	2a	3039	1/1	0.93	0.16	55,55,55,55	0
56	MG	1B	221	1/1	0.93	0.20	56,56,56,56	0
56	MG	2A	3076	1/1	0.93	0.21	31,31,31,31	0
56	MG	2A	3747	1/1	0.93	0.19	66,66,66,66	0
56	MG	2A	3478	1/1	0.93	0.10	43,43,43,43	0
56	MG	2A	3749	1/1	0.93	0.23	58,58,58,58	0
56	MG	1B	223	1/1	0.93	0.21	51,51,51,51	0
56	MG	2A	3078	1/1	0.93	0.14	59,59,59,59	0
56	MG	2A	3482	1/1	0.93	0.49	42,42,42,42	0
56	MG	2A	3757	1/1	0.93	0.08	66,66,66,66	0
56	MG	1A	3302	1/1	0.93	0.31	52,52,52,52	0
56	MG	1a	1621	1/1	0.93	0.09	51,51,51,51	0
56	MG	1B	225	1/1	0.93	0.14	53,53,53,53	0
56	MG	2A	3487	1/1	0.93	0.17	48,48,48,48	0
56	MG	1A	3377	1/1	0.93	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3489	1/1	0.93	0.31	62,62,62,62	0
56	MG	1a	1785	1/1	0.93	0.08	65,65,65,65	0
56	MG	1A	3668	1/1	0.93	0.14	21,21,21,21	0
56	MG	2A	3293	1/1	0.93	0.07	52,52,52,52	0
56	MG	1A	3911	1/1	0.93	0.08	55,55,55,55	0
56	MG	1A	3915	1/1	0.93	0.15	26,26,26,26	0
56	MG	2A	3772	1/1	0.93	0.07	66,66,66,66	0
56	MG	1A	4009	1/1	0.93	0.21	23,23,23,23	0
56	MG	1A	4011	1/1	0.93	0.27	65,65,65,65	0
56	MG	2A	3498	1/1	0.93	0.18	58,58,58,58	0
56	MG	1A	3268	1/1	0.93	0.17	35,35,35,35	0
56	MG	2A	3096	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3218	1/1	0.93	0.14	34,34,34,34	0
56	MG	1D	304	1/1	0.93	0.20	35,35,35,35	0
56	MG	2A	3306	1/1	0.93	0.12	50,50,50,50	0
56	MG	2A	3102	1/1	0.93	0.15	59,59,59,59	0
56	MG	2A	3103	1/1	0.93	0.16	58,58,58,58	0
56	MG	1a	1794	1/1	0.93	0.08	60,60,60,60	0
56	MG	1A	3772	1/1	0.93	0.17	28,28,28,28	0
56	MG	1D	308	1/1	0.93	0.19	36,36,36,36	0
56	MG	2a	3091	1/1	0.93	0.19	62,62,62,62	0
56	MG	2A	3790	1/1	0.93	0.08	61,61,61,61	0
56	MG	1A	3676	1/1	0.93	0.16	16,16,16,16	0
56	MG	2A	3113	1/1	0.93	0.24	59,59,59,59	0
56	MG	2A	3794	1/1	0.93	0.09	65,65,65,65	0
56	MG	2A	3318	1/1	0.93	0.72	50,50,50,50	0
56	MG	1A	3581	1/1	0.93	0.18	15,15,15,15	0
56	MG	1A	3205	1/1	0.93	0.11	46,46,46,46	0
56	MG	1A	3272	1/1	0.93	0.17	22,22,22,22	0
56	MG	1a	1650	1/1	0.93	0.12	56,56,56,56	0
56	MG	1A	3387	1/1	0.93	0.18	48,48,48,48	0
56	MG	1E	306	1/1	0.93	0.15	26,26,26,26	0
56	MG	1A	3587	1/1	0.93	0.35	35,35,35,35	0
56	MG	1A	3425	1/1	0.93	0.20	60,60,60,60	0
56	MG	2a	3109	1/1	0.93	0.23	72,72,72,72	0
56	MG	1A	3133	1/1	0.93	0.32	35,35,35,35	0
56	MG	2a	3111	1/1	0.93	0.10	63,63,63,63	0
56	MG	2A	3807	1/1	0.93	0.11	65,65,65,65	0
56	MG	2A	3134	1/1	0.93	0.20	39,39,39,39	0
56	MG	1A	3592	1/1	0.93	0.20	22,22,22,22	0
56	MG	1A	3594	1/1	0.93	0.18	55,55,55,55	0
56	MG	2A	3336	1/1	0.93	0.60	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	3141	1/1	0.93	0.17	39,39,39,39	0
56	MG	1A	3596	1/1	0.93	0.16	29,29,29,29	0
56	MG	1A	3529	1/1	0.93	0.37	28,28,28,28	0
56	MG	1A	3600	1/1	0.93	0.41	39,39,39,39	0
56	MG	1A	3938	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3939	1/1	0.93	0.17	21,21,21,21	0
56	MG	1A	3024	1/1	0.93	0.11	43,43,43,43	0
56	MG	2A	3555	1/1	0.93	0.18	27,27,27,27	0
56	MG	2A	3345	1/1	0.93	0.12	39,39,39,39	0
56	MG	2A	3559	1/1	0.93	0.12	53,53,53,53	0
56	MG	1N	202	1/1	0.93	0.12	42,42,42,42	0
56	MG	1A	3044	1/1	0.93	0.13	29,29,29,29	0
56	MG	2A	3563	1/1	0.93	0.13	36,36,36,36	0
56	MG	1A	3603	1/1	0.93	0.18	39,39,39,39	0
56	MG	2a	3144	1/1	0.93	0.15	65,65,65,65	0
56	MG	1A	3806	1/1	0.93	0.10	26,26,26,26	0
56	MG	1A	3807	1/1	0.93	0.39	27,27,27,27	0
56	MG	1P	202	1/1	0.93	0.36	23,23,23,23	0
56	MG	2A	3354	1/1	0.93	0.10	62,62,62,62	0
56	MG	2a	3150	1/1	0.93	0.12	76,76,76,76	0
56	MG	2A	3165	1/1	0.93	0.22	65,65,65,65	0
56	MG	2A	3836	1/1	0.93	0.14	62,62,62,62	0
56	MG	1A	3481	1/1	0.93	0.22	40,40,40,40	0
56	MG	2A	3573	1/1	0.93	0.19	62,62,62,62	0
56	MG	1A	3232	1/1	0.93	0.09	56,56,56,56	0
56	MG	2A	3840	1/1	0.93	0.08	51,51,51,51	0
56	MG	1a	1832	1/1	0.93	0.14	55,55,55,55	0
56	MG	2A	3842	1/1	0.93	0.16	42,42,42,42	0
56	MG	2a	3161	1/1	0.93	0.06	67,67,67,67	0
56	MG	2A	3576	1/1	0.93	0.10	26,26,26,26	0
56	MG	1A	3953	1/1	0.93	0.05	50,50,50,50	0
56	MG	2a	3164	1/1	0.93	0.17	58,58,58,58	0
56	MG	1A	3130	1/1	0.93	0.18	29,29,29,29	0
56	MG	2A	3363	1/1	0.93	0.28	51,51,51,51	0
56	MG	1A	3436	1/1	0.93	0.22	49,49,49,49	0
56	MG	1f	201	1/1	0.93	0.20	44,44,44,44	0
56	MG	2A	3852	1/1	0.93	0.11	53,53,53,53	0
56	MG	1A	3608	1/1	0.93	0.18	39,39,39,39	0
56	MG	2A	3588	1/1	0.93	0.15	37,37,37,37	0
56	MG	2A	3589	1/1	0.93	0.07	44,44,44,44	0
56	MG	2A	3180	1/1	0.93	0.27	47,47,47,47	0
56	MG	1A	3320	1/1	0.93	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3321	1/1	0.93	0.11	48,48,48,48	0
56	MG	2A	3371	1/1	0.93	0.06	64,64,64,64	0
56	MG	1a	1684	1/1	0.93	0.20	63,63,63,63	0
56	MG	1A	3829	1/1	0.93	0.26	32,32,32,32	0
56	MG	1A	3832	1/1	0.93	0.13	59,59,59,59	0
56	MG	2A	3866	1/1	0.93	0.16	38,38,38,38	0
56	MG	2A	3868	1/1	0.93	0.14	70,70,70,70	0
56	MG	2A	3190	1/1	0.93	0.12	67,67,67,67	0
56	MG	2a	3192	1/1	0.93	0.12	56,56,56,56	0
56	MG	1A	4054	1/1	0.93	0.48	53,53,53,53	0
56	MG	1A	3616	1/1	0.93	0.15	19,19,19,19	0
56	MG	2A	3378	1/1	0.93	0.66	55,55,55,55	0
56	MG	2A	3607	1/1	0.93	0.12	57,57,57,57	0
56	MG	1A	3212	1/1	0.93	0.11	35,35,35,35	0
56	MG	2A	3609	1/1	0.93	0.16	29,29,29,29	0
56	MG	2A	3610	1/1	0.93	0.06	41,41,41,41	0
56	MG	2a	3200	1/1	0.93	0.13	77,77,77,77	0
56	MG	1A	3441	1/1	0.93	0.14	41,41,41,41	0
56	MG	2A	3887	1/1	0.93	0.15	56,56,56,56	0
56	MG	1A	3288	1/1	0.93	0.21	34,34,34,34	0
56	MG	1U	212	1/1	0.93	0.12	37,37,37,37	0
56	MG	1A	3966	1/1	0.93	0.14	36,36,36,36	0
56	MG	1x	105	1/1	0.93	0.13	49,49,49,49	0
56	MG	1V	203	1/1	0.93	0.32	26,26,26,26	0
56	MG	2A	3620	1/1	0.93	0.14	64,64,64,64	0
56	MG	2A	3621	1/1	0.93	0.12	63,63,63,63	0
56	MG	1A	3260	1/1	0.93	0.15	47,47,47,47	0
56	MG	1A	4064	1/1	0.93	0.16	34,34,34,34	0
56	MG	1A	3629	1/1	0.93	0.08	29,29,29,29	0
56	MG	1A	3197	1/1	0.93	0.22	38,38,38,38	0
56	MG	2A	3628	1/1	0.93	0.11	55,55,55,55	0
56	MG	2B	218	1/1	0.93	0.20	67,67,67,67	0
56	MG	2a	3229	1/1	0.93	0.23	61,61,61,61	0
56	MG	2B	220	1/1	0.93	0.12	65,65,65,65	0
56	MG	1A	3633	1/1	0.93	0.12	28,28,28,28	0
56	MG	2a	3232	1/1	0.93	0.14	63,63,63,63	0
56	MG	1A	3858	1/1	0.93	0.23	43,43,43,43	0
56	MG	1A	3551	1/1	0.93	0.15	50,50,50,50	0
56	MG	1A	3262	1/1	0.93	0.19	59,59,59,59	0
56	MG	1A	3864	1/1	0.93	0.14	52,52,52,52	0
56	MG	2a	3241	1/1	0.93	0.12	63,63,63,63	0
56	MG	10	103	1/1	0.93	0.15	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	3107	1/1	0.93	0.10	27,27,27,27	0
56	MG	1A	3978	1/1	0.93	0.15	36,36,36,36	0
56	MG	2E	302	1/1	0.93	0.13	61,61,61,61	0
56	MG	1A	3735	1/1	0.93	0.13	45,45,45,45	0
56	MG	2A	3652	1/1	0.93	0.10	50,50,50,50	0
56	MG	2l	202	1/1	0.93	0.08	64,64,64,64	0
56	MG	1A	3736	1/1	0.93	0.08	38,38,38,38	0
56	MG	2A	3013	1/1	0.93	0.30	50,50,50,50	0
56	MG	2A	3658	1/1	0.93	0.11	69,69,69,69	0
56	MG	1A	3558	1/1	0.93	0.25	54,54,54,54	0
56	MG	1A	3560	1/1	0.93	0.14	51,51,51,51	0
56	MG	2A	3415	1/1	0.93	0.12	62,62,62,62	0
56	MG	2A	3235	1/1	0.93	0.27	44,44,44,44	0
56	MG	1A	4087	1/1	0.93	0.11	53,53,53,53	0
56	MG	2A	3237	1/1	0.93	0.46	44,44,44,44	0
56	MG	2A	3677	1/1	0.93	0.10	51,51,51,51	0
56	MG	2x	105	1/1	0.93	0.09	67,67,67,67	0
56	MG	15	103	1/1	0.93	0.30	33,33,33,33	0
56	MG	2A	3023	1/1	0.93	0.59	51,51,51,51	0
56	MG	1A	3453	1/1	0.93	0.43	31,31,31,31	0
56	MG	2y	105	1/1	0.93	0.07	76,76,76,76	0
56	MG	1A	3877	1/1	0.93	0.25	30,30,30,30	0
56	MG	1A	3331	1/1	0.93	0.30	43,43,43,43	0
59	ZN	2n	501	1/1	0.93	0.08	107,107,107,107	0
56	MG	1A	3920	1/1	0.94	0.20	65,65,65,65	0
56	MG	1A	4044	1/1	0.94	0.08	43,43,43,43	0
56	MG	1A	3762	1/1	0.94	0.20	21,21,21,21	0
56	MG	2D	310	1/1	0.94	0.18	56,56,56,56	0
56	MG	1A	3414	1/1	0.94	0.10	43,43,43,43	0
56	MG	1a	1756	1/1	0.94	0.17	54,54,54,54	0
56	MG	1A	4048	1/1	0.94	0.09	34,34,34,34	0
56	MG	1A	3015	1/1	0.94	0.15	39,39,39,39	0
56	MG	2A	3349	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3319	1/1	0.94	0.24	51,51,51,51	0
56	MG	1A	3649	1/1	0.94	0.14	29,29,29,29	0
56	MG	1l	101	1/1	0.94	0.59	33,33,33,33	0
56	MG	1l	103	1/1	0.94	0.21	36,36,36,36	0
56	MG	1A	3557	1/1	0.94	0.16	47,47,47,47	0
56	MG	1A	3769	1/1	0.94	0.19	25,25,25,25	0
56	MG	1a	1768	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	3022	1/1	0.94	0.18	34,34,34,34	0
56	MG	1A	3482	1/1	0.94	0.23	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	3360	1/1	0.94	0.09	56,56,56,56	0
56	MG	1A	3192	1/1	0.94	0.22	25,25,25,25	0
56	MG	1A	4058	1/1	0.94	0.27	28,28,28,28	0
56	MG	1A	3194	1/1	0.94	0.35	33,33,33,33	0
56	MG	2U	202	1/1	0.94	0.79	58,58,58,58	0
56	MG	2A	3119	1/1	0.94	0.22	36,36,36,36	0
56	MG	1A	3111	1/1	0.94	0.16	37,37,37,37	0
56	MG	1A	3423	1/1	0.94	0.14	42,42,42,42	0
56	MG	1A	3324	1/1	0.94	0.22	39,39,39,39	0
56	MG	2A	3638	1/1	0.94	0.29	55,55,55,55	0
56	MG	1A	3780	1/1	0.94	0.14	34,34,34,34	0
56	MG	1a	1782	1/1	0.94	0.08	79,79,79,79	0
56	MG	2A	3644	1/1	0.94	0.41	43,43,43,43	0
56	MG	21	101	1/1	0.94	0.57	55,55,55,55	0
56	MG	17	102	1/1	0.94	0.11	32,32,32,32	0
56	MG	23	103	1/1	0.94	0.24	55,55,55,55	0
56	MG	2A	3649	1/1	0.94	0.08	68,68,68,68	0
56	MG	2A	3133	1/1	0.94	0.46	55,55,55,55	0
56	MG	1A	3086	1/1	0.94	0.47	28,28,28,28	0
56	MG	2A	3135	1/1	0.94	0.16	51,51,51,51	0
56	MG	1A	3567	1/1	0.94	0.18	29,29,29,29	0
56	MG	27	101	1/1	0.94	0.21	46,46,46,46	0
56	MG	1A	3568	1/1	0.94	0.20	30,30,30,30	0
56	MG	28	103	1/1	0.94	0.17	42,42,42,42	0
56	MG	2A	3140	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3662	1/1	0.94	0.09	59,59,59,59	0
56	MG	17	107	1/1	0.94	0.10	49,49,49,49	0
56	MG	2A	3143	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3944	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3090	1/1	0.94	0.23	30,30,30,30	0
56	MG	2A	3148	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3573	1/1	0.94	0.16	34,34,34,34	0
56	MG	2A	3678	1/1	0.94	0.13	76,76,76,76	0
56	MG	1A	3793	1/1	0.94	0.21	56,56,56,56	0
56	MG	2a	3013	1/1	0.94	0.15	58,58,58,58	0
56	MG	2A	3385	1/1	0.94	0.10	53,53,53,53	0
56	MG	18	106	1/1	0.94	0.14	26,26,26,26	0
56	MG	1A	3374	1/1	0.94	0.14	30,30,30,30	0
56	MG	1A	4077	1/1	0.94	0.16	27,27,27,27	0
56	MG	2A	3157	1/1	0.94	0.87	44,44,44,44	0
56	MG	2A	3392	1/1	0.94	0.13	58,58,58,58	0
56	MG	2A	3393	1/1	0.94	0.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3158	1/1	0.94	0.45	56,56,56,56	0
56	MG	1A	3429	1/1	0.94	0.13	44,44,44,44	0
56	MG	1A	3576	1/1	0.94	0.23	43,43,43,43	0
56	MG	1A	3430	1/1	0.94	0.10	47,47,47,47	0
56	MG	1a	1799	1/1	0.94	0.20	46,46,46,46	0
56	MG	2a	3030	1/1	0.94	0.19	63,63,63,63	0
56	MG	1A	3245	1/1	0.94	0.13	43,43,43,43	0
56	MG	2A	3696	1/1	0.94	0.10	55,55,55,55	0
56	MG	2a	3033	1/1	0.94	0.12	81,81,81,81	0
56	MG	1A	3496	1/1	0.94	0.18	25,25,25,25	0
56	MG	2a	3035	1/1	0.94	0.32	76,76,76,76	0
56	MG	1A	3203	1/1	0.94	0.15	24,24,24,24	0
56	MG	2A	3403	1/1	0.94	0.31	57,57,57,57	0
56	MG	1a	1614	1/1	0.94	0.14	58,58,58,58	0
56	MG	2a	3040	1/1	0.94	0.10	77,77,77,77	0
56	MG	1a	1804	1/1	0.94	0.07	53,53,53,53	0
56	MG	2A	3407	1/1	0.94	0.06	57,57,57,57	0
56	MG	1A	3803	1/1	0.94	0.09	26,26,26,26	0
56	MG	1A	3008	1/1	0.94	0.21	26,26,26,26	0
56	MG	1a	1619	1/1	0.94	0.22	52,52,52,52	0
56	MG	2A	3412	1/1	0.94	0.19	53,53,53,53	0
56	MG	1A	3435	1/1	0.94	0.25	42,42,42,42	0
56	MG	1A	3117	1/1	0.94	0.26	35,35,35,35	0
56	MG	1A	3092	1/1	0.94	0.11	45,45,45,45	0
56	MG	1A	3588	1/1	0.94	0.38	36,36,36,36	0
56	MG	1A	3813	1/1	0.94	0.17	40,40,40,40	0
56	MG	1A	3814	1/1	0.94	0.18	63,63,63,63	0
56	MG	2a	3057	1/1	0.94	0.11	65,65,65,65	0
56	MG	2A	3420	1/1	0.94	0.10	60,60,60,60	0
56	MG	2A	3722	1/1	0.94	0.13	40,40,40,40	0
56	MG	2A	3185	1/1	0.94	0.08	47,47,47,47	0
56	MG	1A	3381	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	3694	1/1	0.94	0.18	41,41,41,41	0
56	MG	2A	3728	1/1	0.94	0.11	64,64,64,64	0
56	MG	1A	3817	1/1	0.94	0.59	39,39,39,39	0
56	MG	2a	3065	1/1	0.94	0.05	77,77,77,77	0
56	MG	1a	1632	1/1	0.94	0.14	58,58,58,58	0
56	MG	2A	3733	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3192	1/1	0.94	0.14	60,60,60,60	0
56	MG	1A	3093	1/1	0.94	0.16	51,51,51,51	0
56	MG	1A	3052	1/1	0.94	0.13	40,40,40,40	0
56	MG	2A	3196	1/1	0.94	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	3739	1/1	0.94	0.14	59,59,59,59	0
56	MG	1A	3826	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3741	1/1	0.94	0.09	42,42,42,42	0
56	MG	2A	3199	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	3299	1/1	0.94	0.07	30,30,30,30	0
56	MG	1a	1640	1/1	0.94	0.14	69,69,69,69	0
56	MG	1A	3337	1/1	0.94	0.15	37,37,37,37	0
56	MG	1A	3835	1/1	0.94	0.14	33,33,33,33	0
56	MG	1a	1830	1/1	0.94	0.15	42,42,42,42	0
56	MG	1B	217	1/1	0.94	0.24	47,47,47,47	0
56	MG	2A	3751	1/1	0.94	0.11	67,67,67,67	0
56	MG	1B	220	1/1	0.94	0.14	32,32,32,32	0
56	MG	2A	3208	1/1	0.94	0.13	53,53,53,53	0
56	MG	2A	3209	1/1	0.94	0.16	43,43,43,43	0
56	MG	2A	3210	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3211	1/1	0.94	0.19	45,45,45,45	0
56	MG	1b	301	1/1	0.94	0.18	74,74,74,74	0
56	MG	1b	302	1/1	0.94	0.17	71,71,71,71	0
56	MG	1A	3098	1/1	0.94	0.12	44,44,44,44	0
56	MG	1a	1649	1/1	0.94	0.18	44,44,44,44	0
56	MG	1B	222	1/1	0.94	0.18	55,55,55,55	0
56	MG	1a	1652	1/1	0.94	0.10	48,48,48,48	0
56	MG	1l	201	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3220	1/1	0.94	0.12	52,52,52,52	0
56	MG	1n	101	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	3598	1/1	0.94	0.33	35,35,35,35	0
56	MG	1A	3449	1/1	0.94	0.35	32,32,32,32	0
56	MG	2a	3113	1/1	0.94	0.11	56,56,56,56	0
56	MG	2A	3775	1/1	0.94	0.09	66,66,66,66	0
56	MG	2A	3468	1/1	0.94	0.26	51,51,51,51	0
56	MG	1A	3518	1/1	0.94	0.29	54,54,54,54	0
56	MG	2a	3119	1/1	0.94	0.08	69,69,69,69	0
56	MG	2A	3227	1/1	0.94	0.08	56,56,56,56	0
56	MG	1w	101	1/1	0.94	0.19	65,65,65,65	0
56	MG	1A	3708	1/1	0.94	0.07	45,45,45,45	0
56	MG	1A	3035	1/1	0.94	0.14	39,39,39,39	0
56	MG	1A	3850	1/1	0.94	0.19	47,47,47,47	0
56	MG	1w	107	1/1	0.94	0.16	69,69,69,69	0
56	MG	1A	3711	1/1	0.94	0.16	48,48,48,48	0
56	MG	2a	3133	1/1	0.94	0.20	66,66,66,66	0
56	MG	1A	3852	1/1	0.94	0.20	39,39,39,39	0
56	MG	1A	3853	1/1	0.94	0.15	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	2A	3481	1/1	0.94	0.78	60,60,60,60	0
56	MG	1a	1663	1/1	0.94	0.23	52,52,52,52	0
56	MG	1B	235	1/1	0.94	0.22	47,47,47,47	0
56	MG	1A	3102	1/1	0.94	0.15	46,46,46,46	0
56	MG	2a	3141	1/1	0.94	0.08	68,68,68,68	0
56	MG	2A	3485	1/1	0.94	0.63	44,44,44,44	0
56	MG	1A	3855	1/1	0.94	0.14	20,20,20,20	0
56	MG	1A	3857	1/1	0.94	0.22	36,36,36,36	0
56	MG	1A	3522	1/1	0.94	0.31	53,53,53,53	0
56	MG	2A	3246	1/1	0.94	0.26	49,49,49,49	0
56	MG	1A	3215	1/1	0.94	0.15	39,39,39,39	0
56	MG	1A	3396	1/1	0.94	0.28	26,26,26,26	0
56	MG	2A	3492	1/1	0.94	0.38	58,58,58,58	0
56	MG	1D	311	1/1	0.94	0.20	50,50,50,50	0
56	MG	1A	3304	1/1	0.94	0.32	21,21,21,21	0
56	MG	1A	3865	1/1	0.94	0.10	65,65,65,65	0
56	MG	1A	3343	1/1	0.94	0.25	47,47,47,47	0
56	MG	2A	3001	1/1	0.94	0.14	55,55,55,55	0
56	MG	1A	3217	1/1	0.94	0.12	39,39,39,39	0
56	MG	1E	304	1/1	0.94	0.19	34,34,34,34	0
56	MG	1A	3611	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3999	1/1	0.94	0.17	39,39,39,39	0
56	MG	2A	3006	1/1	0.94	0.17	54,54,54,54	0
56	MG	1A	3612	1/1	0.94	0.20	51,51,51,51	0
56	MG	1A	3054	1/1	0.94	0.19	42,42,42,42	0
56	MG	1E	314	1/1	0.94	0.20	30,30,30,30	0
56	MG	2A	3512	1/1	0.94	0.08	58,58,58,58	0
56	MG	2A	3513	1/1	0.94	0.13	50,50,50,50	0
56	MG	1A	3728	1/1	0.94	0.19	44,44,44,44	0
56	MG	1A	3729	1/1	0.94	0.07	32,32,32,32	0
56	MG	1A	4005	1/1	0.94	0.08	26,26,26,26	0
56	MG	1a	1687	1/1	0.94	0.13	50,50,50,50	0
56	MG	1A	3615	1/1	0.94	0.12	33,33,33,33	0
56	MG	1A	3347	1/1	0.94	0.51	41,41,41,41	0
56	MG	1A	3175	1/1	0.94	0.28	30,30,30,30	0
56	MG	2a	3177	1/1	0.94	0.25	65,65,65,65	0
56	MG	1A	3623	1/1	0.94	0.17	26,26,26,26	0
56	MG	1A	3624	1/1	0.94	0.14	46,46,46,46	0
56	MG	1A	3887	1/1	0.94	0.18	31,31,31,31	0
56	MG	2a	3181	1/1	0.94	0.15	64,64,64,64	0
56	MG	2A	3277	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	4015	1/1	0.94	0.13	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3464	1/1	0.94	0.10	46,46,46,46	0
56	MG	2A	3038	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	3738	1/1	0.94	0.13	45,45,45,45	0
56	MG	1A	3310	1/1	0.94	0.23	40,40,40,40	0
56	MG	1a	1701	1/1	0.94	0.24	53,53,53,53	0
56	MG	2A	3539	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3042	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3221	1/1	0.94	0.16	46,46,46,46	0
56	MG	2A	3044	1/1	0.94	0.11	59,59,59,59	0
56	MG	1P	203	1/1	0.94	0.21	25,25,25,25	0
56	MG	2A	3047	1/1	0.94	0.10	24,24,24,24	0
56	MG	2A	3547	1/1	0.94	0.17	34,34,34,34	0
56	MG	1a	1707	1/1	0.94	0.20	57,57,57,57	0
56	MG	1A	4021	1/1	0.94	0.19	32,32,32,32	0
56	MG	1A	3893	1/1	0.94	0.18	21,21,21,21	0
56	MG	2a	3206	1/1	0.94	0.17	62,62,62,62	0
56	MG	1A	3894	1/1	0.94	0.17	21,21,21,21	0
56	MG	1A	4025	1/1	0.94	0.18	40,40,40,40	0
56	MG	1A	3353	1/1	0.94	0.24	33,33,33,33	0
56	MG	2A	3557	1/1	0.94	0.13	59,59,59,59	0
56	MG	1A	3469	1/1	0.94	0.19	33,33,33,33	0
56	MG	2A	3560	1/1	0.94	0.12	38,38,38,38	0
56	MG	2a	3218	1/1	0.94	0.14	74,74,74,74	0
56	MG	1a	1716	1/1	0.94	0.15	49,49,49,49	0
56	MG	2A	3057	1/1	0.94	0.14	46,46,46,46	0
56	MG	2A	3058	1/1	0.94	0.11	52,52,52,52	0
56	MG	1A	3313	1/1	0.94	0.20	39,39,39,39	0
56	MG	2A	3867	1/1	0.94	0.12	35,35,35,35	0
56	MG	2A	3060	1/1	0.94	0.20	46,46,46,46	0
56	MG	2a	3228	1/1	0.94	0.25	62,62,62,62	0
56	MG	1R	203	1/1	0.94	0.24	46,46,46,46	0
56	MG	2A	3870	1/1	0.94	0.11	42,42,42,42	0
56	MG	2A	3062	1/1	0.94	0.18	66,66,66,66	0
56	MG	1A	3181	1/1	0.94	0.17	39,39,39,39	0
56	MG	1A	3902	1/1	0.94	0.19	43,43,43,43	0
56	MG	2A	3571	1/1	0.94	0.09	42,42,42,42	0
56	MG	1A	3903	1/1	0.94	0.15	45,45,45,45	0
56	MG	2A	3067	1/1	0.94	0.11	30,30,30,30	0
56	MG	2A	3884	1/1	0.94	0.10	61,61,61,61	0
56	MG	2A	3316	1/1	0.94	0.10	53,53,53,53	0
56	MG	1a	1724	1/1	0.94	0.28	49,49,49,49	0
56	MG	1A	3905	1/1	0.94	0.26	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	1A	3636	1/1	0.94	0.14	16,16,16,16	0
56	MG	1A	3185	1/1	0.94	0.14	37,37,37,37	0
56	MG	2k	201	1/1	0.94	0.16	55,55,55,55	0
56	MG	2A	3073	1/1	0.94	0.51	52,52,52,52	0
56	MG	1A	3909	1/1	0.94	0.17	49,49,49,49	0
56	MG	2l	203	1/1	0.94	0.12	61,61,61,61	0
56	MG	2B	205	1/1	0.94	0.15	66,66,66,66	0
56	MG	2B	206	1/1	0.94	0.21	60,60,60,60	0
56	MG	2B	207	1/1	0.94	0.17	61,61,61,61	0
56	MG	1A	3910	1/1	0.94	0.21	51,51,51,51	0
56	MG	1A	3757	1/1	0.94	0.17	50,50,50,50	0
56	MG	2B	210	1/1	0.94	0.15	67,67,67,67	0
56	MG	1A	3914	1/1	0.94	0.18	19,19,19,19	0
56	MG	2w	104	1/1	0.94	0.08	69,69,69,69	0
56	MG	2x	101	1/1	0.94	0.15	60,60,60,60	0
56	MG	1A	3134	1/1	0.94	0.36	41,41,41,41	0
56	MG	2A	3079	1/1	0.94	0.35	46,46,46,46	0
56	MG	2A	3593	1/1	0.94	0.18	46,46,46,46	0
56	MG	1a	1741	1/1	0.94	0.24	60,60,60,60	0
56	MG	2A	3082	1/1	0.94	0.17	43,43,43,43	0
56	MG	2A	3083	1/1	0.94	0.19	57,57,57,57	0
56	MG	2A	3597	1/1	0.94	0.23	58,58,58,58	0
56	MG	1V	205	1/1	0.94	0.20	29,29,29,29	0
56	MG	1A	4040	1/1	0.94	0.30	47,47,47,47	0
57	CLM	2A	3888	20/20	0.94	0.32	38,45,57,61	0
59	ZN	2Y	501	1/1	0.94	0.15	81,81,81,81	0
56	MG	1A	3759	1/1	0.94	0.16	15,15,15,15	0
56	MG	1A	3413	1/1	0.94	0.11	37,37,37,37	0
56	MG	1A	3421	1/1	0.95	0.18	32,32,32,32	0
56	MG	2A	3672	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3104	1/1	0.95	0.18	25,25,25,25	0
56	MG	1x	101	1/1	0.95	0.20	38,38,38,38	0
56	MG	1A	3106	1/1	0.95	0.17	26,26,26,26	0
56	MG	1A	3795	1/1	0.95	0.20	19,19,19,19	0
56	MG	1a	1682	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3216	1/1	0.95	0.33	32,32,32,32	0
56	MG	1A	3318	1/1	0.95	0.30	43,43,43,43	0
56	MG	1P	208	1/1	0.95	0.29	42,42,42,42	0
56	MG	1A	3492	1/1	0.95	0.15	33,33,33,33	0
56	MG	2A	3426	1/1	0.95	0.18	42,42,42,42	0
56	MG	1Q	204	1/1	0.95	0.12	44,44,44,44	0
56	MG	1a	1688	1/1	0.95	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3430	1/1	0.95	0.22	31,31,31,31	0
56	MG	1A	3426	1/1	0.95	0.15	44,44,44,44	0
56	MG	1x	116	1/1	0.95	0.14	65,65,65,65	0
56	MG	2A	3434	1/1	0.95	0.33	46,46,46,46	0
56	MG	1A	3088	1/1	0.95	0.17	37,37,37,37	0
56	MG	1A	3269	1/1	0.95	0.12	29,29,29,29	0
56	MG	2A	3218	1/1	0.95	0.54	35,35,35,35	0
56	MG	1A	3089	1/1	0.95	0.12	41,41,41,41	0
56	MG	2a	3004	1/1	0.95	0.21	51,51,51,51	0
56	MG	2A	3699	1/1	0.95	0.07	70,70,70,70	0
56	MG	2A	3441	1/1	0.95	0.14	60,60,60,60	0
56	MG	1A	3584	1/1	0.95	0.14	32,32,32,32	0
56	MG	1a	1694	1/1	0.95	0.06	56,56,56,56	0
56	MG	1A	3009	1/1	0.95	0.12	17,17,17,17	0
56	MG	2a	3010	1/1	0.95	0.19	60,60,60,60	0
56	MG	1A	3183	1/1	0.95	0.21	48,48,48,48	0
56	MG	2A	3707	1/1	0.95	0.15	36,36,36,36	0
56	MG	1A	3372	1/1	0.95	0.38	43,43,43,43	0
56	MG	1A	3502	1/1	0.95	0.15	47,47,47,47	0
56	MG	1A	3810	1/1	0.95	0.16	25,25,25,25	0
56	MG	1A	3222	1/1	0.95	0.26	29,29,29,29	0
56	MG	2A	3450	1/1	0.95	0.09	56,56,56,56	0
56	MG	1A	3274	1/1	0.95	0.15	38,38,38,38	0
56	MG	2A	3233	1/1	0.95	0.12	33,33,33,33	0
56	MG	1a	1705	1/1	0.95	0.13	56,56,56,56	0
56	MG	1U	208	1/1	0.95	0.29	30,30,30,30	0
56	MG	2A	3017	1/1	0.95	0.17	36,36,36,36	0
56	MG	2A	3020	1/1	0.95	0.39	39,39,39,39	0
56	MG	1A	3946	1/1	0.95	0.09	40,40,40,40	0
56	MG	1A	3184	1/1	0.95	0.10	64,64,64,64	0
56	MG	2A	3724	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3278	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3026	1/1	0.95	0.52	53,53,53,53	0
56	MG	1A	3595	1/1	0.95	0.14	34,34,34,34	0
56	MG	2A	3729	1/1	0.95	0.09	68,68,68,68	0
56	MG	2A	3028	1/1	0.95	0.16	48,48,48,48	0
56	MG	1A	3950	1/1	0.95	0.15	55,55,55,55	0
56	MG	1A	3509	1/1	0.95	0.18	31,31,31,31	0
56	MG	2A	3031	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	3819	1/1	0.95	0.14	44,44,44,44	0
56	MG	1A	3138	1/1	0.95	0.17	28,28,28,28	0
56	MG	1A	3511	1/1	0.95	0.21	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3044	1/1	0.95	0.24	56,56,56,56	0
56	MG	1X	104	1/1	0.95	0.36	61,61,61,61	0
56	MG	1X	105	1/1	0.95	0.17	29,29,29,29	0
56	MG	1A	3599	1/1	0.95	0.16	42,42,42,42	0
56	MG	1Y	203	1/1	0.95	0.19	47,47,47,47	0
56	MG	1A	3330	1/1	0.95	0.24	46,46,46,46	0
56	MG	1A	3830	1/1	0.95	0.18	48,48,48,48	0
56	MG	1A	3229	1/1	0.95	0.38	32,32,32,32	0
56	MG	1A	4072	1/1	0.95	0.13	48,48,48,48	0
56	MG	1A	3834	1/1	0.95	0.26	32,32,32,32	0
56	MG	2A	3049	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3186	1/1	0.95	0.22	37,37,37,37	0
56	MG	10	106	1/1	0.95	0.11	49,49,49,49	0
56	MG	1a	1734	1/1	0.95	0.14	53,53,53,53	0
56	MG	2A	3756	1/1	0.95	0.12	55,55,55,55	0
56	MG	1a	1735	1/1	0.95	0.16	53,53,53,53	0
56	MG	1A	3516	1/1	0.95	0.25	40,40,40,40	0
56	MG	2A	3760	1/1	0.95	0.13	54,54,54,54	0
56	MG	1a	1737	1/1	0.95	0.30	62,62,62,62	0
56	MG	1a	1738	1/1	0.95	0.09	57,57,57,57	0
56	MG	11	102	1/1	0.95	0.12	42,42,42,42	0
56	MG	2A	3272	1/1	0.95	0.15	56,56,56,56	0
56	MG	1A	3837	1/1	0.95	0.11	51,51,51,51	0
56	MG	1a	1743	1/1	0.95	0.12	61,61,61,61	0
56	MG	2a	3074	1/1	0.95	0.12	52,52,52,52	0
56	MG	1a	1745	1/1	0.95	0.12	54,54,54,54	0
56	MG	2A	3276	1/1	0.95	0.14	51,51,51,51	0
56	MG	1A	4078	1/1	0.95	0.10	24,24,24,24	0
56	MG	1A	3444	1/1	0.95	0.34	43,43,43,43	0
56	MG	1A	3840	1/1	0.95	0.12	22,22,22,22	0
56	MG	1a	1749	1/1	0.95	0.21	33,33,33,33	0
56	MG	2A	3774	1/1	0.95	0.14	64,64,64,64	0
56	MG	2A	3500	1/1	0.95	0.15	55,55,55,55	0
56	MG	2A	3776	1/1	0.95	0.10	56,56,56,56	0
56	MG	2A	3502	1/1	0.95	0.23	55,55,55,55	0
56	MG	2a	3088	1/1	0.95	0.15	55,55,55,55	0
56	MG	1A	3843	1/1	0.95	0.11	51,51,51,51	0
56	MG	1a	1751	1/1	0.95	0.11	52,52,52,52	0
56	MG	2A	3068	1/1	0.95	0.34	61,61,61,61	0
56	MG	2A	3507	1/1	0.95	0.18	44,44,44,44	0
56	MG	13	102	1/1	0.95	0.15	38,38,38,38	0
56	MG	13	103	1/1	0.95	0.18	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3097	1/1	0.95	0.19	49,49,49,49	0
56	MG	2A	3510	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	3139	1/1	0.95	0.22	36,36,36,36	0
56	MG	1A	3969	1/1	0.95	0.13	42,42,42,42	0
56	MG	1A	3721	1/1	0.95	0.17	27,27,27,27	0
56	MG	1A	4088	1/1	0.95	0.17	21,21,21,21	0
56	MG	1A	3846	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3847	1/1	0.95	0.07	51,51,51,51	0
56	MG	2A	3518	1/1	0.95	0.16	53,53,53,53	0
56	MG	1A	3520	1/1	0.95	0.24	56,56,56,56	0
56	MG	1A	4093	1/1	0.95	0.12	38,38,38,38	0
56	MG	1A	3075	1/1	0.95	0.18	21,21,21,21	0
56	MG	2A	3523	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3975	1/1	0.95	0.08	50,50,50,50	0
56	MG	1A	4096	1/1	0.95	0.17	46,46,46,46	0
56	MG	1A	4097	1/1	0.95	0.17	35,35,35,35	0
56	MG	2A	3084	1/1	0.95	0.13	46,46,46,46	0
56	MG	2A	3803	1/1	0.95	0.13	81,81,81,81	0
56	MG	1a	1769	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3303	1/1	0.95	0.48	71,71,71,71	0
56	MG	2A	3305	1/1	0.95	0.12	54,54,54,54	0
56	MG	1A	3389	1/1	0.95	0.33	23,23,23,23	0
56	MG	2a	3125	1/1	0.95	0.09	64,64,64,64	0
56	MG	1A	3113	1/1	0.95	0.41	37,37,37,37	0
56	MG	1A	3144	1/1	0.95	0.18	42,42,42,42	0
56	MG	1a	1773	1/1	0.95	0.12	54,54,54,54	0
56	MG	2A	3311	1/1	0.95	0.26	59,59,59,59	0
56	MG	1A	3525	1/1	0.95	0.27	31,31,31,31	0
56	MG	1B	203	1/1	0.95	0.16	33,33,33,33	0
56	MG	1B	204	1/1	0.95	0.29	42,42,42,42	0
56	MG	19	101	1/1	0.95	0.27	34,34,34,34	0
56	MG	2A	3544	1/1	0.95	0.12	35,35,35,35	0
56	MG	1a	1601	1/1	0.95	0.12	42,42,42,42	0
56	MG	1B	205	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3452	1/1	0.95	0.44	38,38,38,38	0
56	MG	1A	3527	1/1	0.95	0.28	32,32,32,32	0
56	MG	2A	3101	1/1	0.95	0.10	35,35,35,35	0
56	MG	1a	1605	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	3193	1/1	0.95	0.49	30,30,30,30	0
56	MG	2A	3825	1/1	0.95	0.07	43,43,43,43	0
56	MG	1B	209	1/1	0.95	0.17	47,47,47,47	0
56	MG	2A	3827	1/1	0.95	0.09	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	3327	1/1	0.95	0.17	51,51,51,51	0
56	MG	2A	3829	1/1	0.95	0.09	45,45,45,45	0
56	MG	2A	3105	1/1	0.95	0.34	57,57,57,57	0
56	MG	1a	1608	1/1	0.95	0.20	45,45,45,45	0
56	MG	1A	3240	1/1	0.95	0.19	34,34,34,34	0
56	MG	2a	3155	1/1	0.95	0.10	70,70,70,70	0
56	MG	2A	3110	1/1	0.95	0.15	61,61,61,61	0
56	MG	1A	3619	1/1	0.95	0.20	41,41,41,41	0
56	MG	1a	1612	1/1	0.95	0.09	62,62,62,62	0
56	MG	1a	1613	1/1	0.95	0.22	49,49,49,49	0
56	MG	2a	3160	1/1	0.95	0.28	84,84,84,84	0
56	MG	1A	3033	1/1	0.95	0.45	24,24,24,24	0
56	MG	1A	3067	1/1	0.95	0.16	32,32,32,32	0
56	MG	2A	3117	1/1	0.95	0.10	55,55,55,55	0
56	MG	2A	3118	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3397	1/1	0.95	0.30	30,30,30,30	0
56	MG	1A	3460	1/1	0.95	0.28	40,40,40,40	0
56	MG	1A	3535	1/1	0.95	0.11	57,57,57,57	0
56	MG	2a	3168	1/1	0.95	0.07	51,51,51,51	0
56	MG	2A	3846	1/1	0.95	0.16	62,62,62,62	0
56	MG	1A	3868	1/1	0.95	0.12	35,35,35,35	0
56	MG	2A	3124	1/1	0.95	0.05	66,66,66,66	0
56	MG	2A	3125	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3741	1/1	0.95	0.24	37,37,37,37	0
56	MG	1A	3298	1/1	0.95	0.14	36,36,36,36	0
56	MG	2A	3580	1/1	0.95	0.16	45,45,45,45	0
56	MG	1a	1624	1/1	0.95	0.11	62,62,62,62	0
56	MG	1A	3082	1/1	0.95	0.24	33,33,33,33	0
56	MG	2A	3584	1/1	0.95	0.12	59,59,59,59	0
56	MG	1A	3198	1/1	0.95	0.13	35,35,35,35	0
56	MG	1B	226	1/1	0.95	0.06	69,69,69,69	0
56	MG	1A	3152	1/1	0.95	0.14	29,29,29,29	0
56	MG	1A	3540	1/1	0.95	0.13	45,45,45,45	0
56	MG	2a	3185	1/1	0.95	0.16	52,52,52,52	0
56	MG	2a	3186	1/1	0.95	0.09	54,54,54,54	0
56	MG	2A	3591	1/1	0.95	0.18	46,46,46,46	0
56	MG	1A	3637	1/1	0.95	0.10	48,48,48,48	0
56	MG	1a	1634	1/1	0.95	0.25	66,66,66,66	0
56	MG	2A	3142	1/1	0.95	0.14	43,43,43,43	0
56	MG	1A	3755	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3345	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3249	1/1	0.95	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3871	1/1	0.95	0.14	39,39,39,39	0
56	MG	2A	3872	1/1	0.95	0.16	48,48,48,48	0
56	MG	2A	3146	1/1	0.95	0.20	38,38,38,38	0
56	MG	1A	3118	1/1	0.95	0.18	22,22,22,22	0
56	MG	2A	3876	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3760	1/1	0.95	0.19	45,45,45,45	0
56	MG	1A	3348	1/1	0.95	0.29	41,41,41,41	0
56	MG	1A	3156	1/1	0.95	0.38	39,39,39,39	0
56	MG	2a	3204	1/1	0.95	0.14	65,65,65,65	0
56	MG	2A	3882	1/1	0.95	0.15	42,42,42,42	0
56	MG	2A	3153	1/1	0.95	0.11	41,41,41,41	0
56	MG	2A	3154	1/1	0.95	0.12	52,52,52,52	0
56	MG	1A	3763	1/1	0.95	0.15	22,22,22,22	0
56	MG	1A	3069	1/1	0.95	0.24	28,28,28,28	0
56	MG	1a	1820	1/1	0.95	0.07	68,68,68,68	0
56	MG	2a	3215	1/1	0.95	0.09	59,59,59,59	0
56	MG	1D	309	1/1	0.95	0.34	20,20,20,20	0
56	MG	1A	3648	1/1	0.95	0.15	30,30,30,30	0
56	MG	1A	3895	1/1	0.95	0.15	18,18,18,18	0
56	MG	1a	1651	1/1	0.95	0.22	61,61,61,61	0
56	MG	2a	3222	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	3351	1/1	0.95	0.71	47,47,47,47	0
56	MG	1A	3554	1/1	0.95	0.27	41,41,41,41	0
56	MG	1A	3474	1/1	0.95	0.25	32,32,32,32	0
56	MG	2a	3226	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	3410	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3070	1/1	0.95	0.14	12,12,12,12	0
56	MG	1A	3072	1/1	0.95	0.39	31,31,31,31	0
56	MG	1A	3904	1/1	0.95	0.16	32,32,32,32	0
56	MG	1A	3356	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3164	1/1	0.95	0.14	52,52,52,52	0
56	MG	2A	3388	1/1	0.95	0.06	62,62,62,62	0
56	MG	2a	3234	1/1	0.95	0.16	60,60,60,60	0
56	MG	2A	3629	1/1	0.95	0.13	36,36,36,36	0
56	MG	2a	3237	1/1	0.95	0.21	61,61,61,61	0
56	MG	2A	3389	1/1	0.95	0.20	36,36,36,36	0
56	MG	1A	4023	1/1	0.95	0.18	30,30,30,30	0
56	MG	2A	3633	1/1	0.95	0.08	40,40,40,40	0
56	MG	2A	3634	1/1	0.95	0.51	56,56,56,56	0
56	MG	1E	315	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	3774	1/1	0.95	0.16	19,19,19,19	0
56	MG	1A	3415	1/1	0.95	0.18	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1m	3001	1/1	0.95	0.13	54,54,54,54	0
56	MG	2A	3639	1/1	0.95	0.15	42,42,42,42	0
56	MG	1A	3210	1/1	0.95	0.25	35,35,35,35	0
56	MG	2A	3641	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3359	1/1	0.95	0.23	58,58,58,58	0
56	MG	1G	202	1/1	0.95	0.21	51,51,51,51	0
56	MG	1A	3087	1/1	0.95	0.36	35,35,35,35	0
56	MG	2r	101	1/1	0.95	0.06	65,65,65,65	0
56	MG	2A	3646	1/1	0.95	0.30	59,59,59,59	0
56	MG	2A	3647	1/1	0.95	0.17	64,64,64,64	0
56	MG	1A	3166	1/1	0.95	0.27	34,34,34,34	0
56	MG	1A	3782	1/1	0.95	0.24	48,48,48,48	0
56	MG	1w	103	1/1	0.95	0.20	64,64,64,64	0
56	MG	2A	3654	1/1	0.95	0.18	57,57,57,57	0
56	MG	1A	3362	1/1	0.95	0.10	35,35,35,35	0
56	MG	1w	105	1/1	0.95	0.33	62,62,62,62	0
56	MG	2P	204	1/1	0.95	0.26	57,57,57,57	0
56	MG	2A	3195	1/1	0.95	0.12	44,44,44,44	0
56	MG	2A	3659	1/1	0.95	0.14	58,58,58,58	0
56	MG	1A	3918	1/1	0.95	0.30	28,28,28,28	0
56	MG	2y	102	1/1	0.95	0.40	74,74,74,74	0
56	MG	1A	3673	1/1	0.95	0.17	17,17,17,17	0
56	MG	2A	3663	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3788	1/1	0.95	0.07	35,35,35,35	0
56	MG	2A	3665	1/1	0.95	0.10	61,61,61,61	0
57	CLM	1A	4102	20/20	0.95	0.28	18,29,44,60	0
56	MG	2T	203	1/1	0.95	0.15	50,50,50,50	0
59	ZN	14	102	1/1	0.95	0.13	87,87,87,87	0
56	MG	1N	206	1/1	0.95	0.22	37,37,37,37	0
56	MG	2V	202	1/1	0.95	0.52	48,48,48,48	0
59	ZN	29	501	1/1	0.95	0.11	72,72,72,72	0
56	MG	2V	203	1/1	0.95	0.30	57,57,57,57	0
56	MG	2A	3517	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3020	1/1	0.96	0.18	33,33,33,33	0
56	MG	1A	3076	1/1	0.96	0.15	20,20,20,20	0
56	MG	1A	3169	1/1	0.96	0.14	49,49,49,49	0
56	MG	1A	3710	1/1	0.96	0.15	51,51,51,51	0
56	MG	1A	3078	1/1	0.96	0.17	31,31,31,31	0
56	MG	1A	3172	1/1	0.96	0.23	36,36,36,36	0
56	MG	2a	3029	1/1	0.96	0.38	40,40,40,40	0
56	MG	1P	201	1/1	0.96	0.26	25,25,25,25	0
56	MG	1A	3137	1/1	0.96	0.20	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3325	1/1	0.96	0.33	57,57,57,57	0
56	MG	2A	3528	1/1	0.96	0.18	59,59,59,59	0
56	MG	2A	3126	1/1	0.96	0.15	44,44,44,44	0
56	MG	2A	3530	1/1	0.96	0.17	49,49,49,49	0
56	MG	1A	3176	1/1	0.96	0.23	27,27,27,27	0
56	MG	2A	3769	1/1	0.96	0.12	39,39,39,39	0
56	MG	1P	205	1/1	0.96	0.16	16,16,16,16	0
56	MG	2A	3131	1/1	0.96	0.08	75,75,75,75	0
56	MG	2A	3534	1/1	0.96	0.10	41,41,41,41	0
56	MG	2a	3042	1/1	0.96	0.20	60,60,60,60	0
56	MG	1A	3544	1/1	0.96	0.23	37,37,37,37	0
56	MG	1A	3941	1/1	0.96	0.09	35,35,35,35	0
56	MG	1a	1831	1/1	0.96	0.22	43,43,43,43	0
56	MG	1A	3824	1/1	0.96	0.15	30,30,30,30	0
56	MG	1A	3943	1/1	0.96	0.14	38,38,38,38	0
56	MG	2a	3048	1/1	0.96	0.19	58,58,58,58	0
56	MG	1Q	203	1/1	0.96	0.24	24,24,24,24	0
56	MG	1A	3178	1/1	0.96	0.17	17,17,17,17	0
56	MG	1A	3828	1/1	0.96	0.17	45,45,45,45	0
56	MG	1A	3546	1/1	0.96	0.22	43,43,43,43	0
56	MG	1e	202	1/1	0.96	0.23	59,59,59,59	0
56	MG	1A	3179	1/1	0.96	0.13	29,29,29,29	0
56	MG	2A	3549	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3831	1/1	0.96	0.17	37,37,37,37	0
56	MG	2A	3344	1/1	0.96	0.51	48,48,48,48	0
56	MG	1A	3180	1/1	0.96	0.35	35,35,35,35	0
56	MG	1A	3549	1/1	0.96	0.28	30,30,30,30	0
56	MG	1m	3002	1/1	0.96	0.11	56,56,56,56	0
56	MG	1S	202	1/1	0.96	0.16	51,51,51,51	0
56	MG	1A	3550	1/1	0.96	0.16	40,40,40,40	0
56	MG	2A	3558	1/1	0.96	0.08	52,52,52,52	0
56	MG	1T	201	1/1	0.96	0.23	47,47,47,47	0
56	MG	1A	3110	1/1	0.96	0.16	26,26,26,26	0
56	MG	2a	3067	1/1	0.96	0.12	47,47,47,47	0
56	MG	2A	3797	1/1	0.96	0.08	40,40,40,40	0
56	MG	1A	3182	1/1	0.96	0.22	49,49,49,49	0
56	MG	2a	3071	1/1	0.96	0.18	62,62,62,62	0
56	MG	1A	4066	1/1	0.96	0.16	24,24,24,24	0
56	MG	2a	3073	1/1	0.96	0.13	50,50,50,50	0
56	MG	2A	3355	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3630	1/1	0.96	0.15	29,29,29,29	0
56	MG	1A	3553	1/1	0.96	0.35	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	3064	1/1	0.96	0.20	32,32,32,32	0
56	MG	1A	3634	1/1	0.96	0.17	52,52,52,52	0
56	MG	1U	210	1/1	0.96	0.23	25,25,25,25	0
56	MG	1w	108	1/1	0.96	0.11	74,74,74,74	0
56	MG	1A	3959	1/1	0.96	0.23	46,46,46,46	0
56	MG	1A	3030	1/1	0.96	0.27	32,32,32,32	0
56	MG	1A	3556	1/1	0.96	0.31	41,41,41,41	0
56	MG	1V	204	1/1	0.96	0.36	32,32,32,32	0
56	MG	1A	4075	1/1	0.96	0.30	48,48,48,48	0
56	MG	1A	3275	1/1	0.96	0.17	31,31,31,31	0
56	MG	2A	3813	1/1	0.96	0.15	53,53,53,53	0
56	MG	2A	3172	1/1	0.96	0.12	50,50,50,50	0
56	MG	1a	1697	1/1	0.96	0.28	49,49,49,49	0
56	MG	2A	3174	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	3432	1/1	0.96	0.29	36,36,36,36	0
56	MG	1A	3094	1/1	0.96	0.15	20,20,20,20	0
56	MG	1A	3277	1/1	0.96	0.33	44,44,44,44	0
56	MG	2A	3179	1/1	0.96	0.21	65,65,65,65	0
56	MG	1X	102	1/1	0.96	0.16	35,35,35,35	0
56	MG	2A	3587	1/1	0.96	0.20	56,56,56,56	0
56	MG	2a	3103	1/1	0.96	0.21	62,62,62,62	0
56	MG	1a	1702	1/1	0.96	0.29	53,53,53,53	0
56	MG	1A	3642	1/1	0.96	0.12	14,14,14,14	0
56	MG	2A	3590	1/1	0.96	0.15	64,64,64,64	0
56	MG	1A	3095	1/1	0.96	0.29	44,44,44,44	0
56	MG	1A	3383	1/1	0.96	0.33	31,31,31,31	0
56	MG	1A	3745	1/1	0.96	0.14	14,14,14,14	0
56	MG	1A	4086	1/1	0.96	0.16	28,28,28,28	0
56	MG	1x	118	1/1	0.96	0.14	58,58,58,58	0
56	MG	1A	3384	1/1	0.96	0.14	41,41,41,41	0
56	MG	1A	3231	1/1	0.96	0.11	33,33,33,33	0
56	MG	1A	3145	1/1	0.96	0.21	21,21,21,21	0
56	MG	2a	3115	1/1	0.96	0.14	61,61,61,61	0
56	MG	2a	3116	1/1	0.96	0.15	53,53,53,53	0
56	MG	1A	3751	1/1	0.96	0.18	42,42,42,42	0
56	MG	1A	3233	1/1	0.96	0.14	30,30,30,30	0
56	MG	1A	3863	1/1	0.96	0.17	34,34,34,34	0
56	MG	2A	3197	1/1	0.96	0.22	55,55,55,55	0
56	MG	2A	3007	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3754	1/1	0.96	0.15	18,18,18,18	0
56	MG	2a	3124	1/1	0.96	0.23	55,55,55,55	0
56	MG	2A	3009	1/1	0.96	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3394	1/1	0.96	0.18	51,51,51,51	0
56	MG	1A	3501	1/1	0.96	0.13	28,28,28,28	0
56	MG	2a	3130	1/1	0.96	0.08	68,68,68,68	0
56	MG	1A	3756	1/1	0.96	0.13	45,45,45,45	0
56	MG	2A	3012	1/1	0.96	0.12	40,40,40,40	0
56	MG	2A	3204	1/1	0.96	0.18	47,47,47,47	0
56	MG	2a	3134	1/1	0.96	0.10	58,58,58,58	0
56	MG	1A	3652	1/1	0.96	0.15	31,31,31,31	0
56	MG	1A	3653	1/1	0.96	0.09	35,35,35,35	0
56	MG	2A	3615	1/1	0.96	0.13	60,60,60,60	0
56	MG	2A	3616	1/1	0.96	0.10	63,63,63,63	0
56	MG	2A	3617	1/1	0.96	0.20	59,59,59,59	0
56	MG	2A	3854	1/1	0.96	0.11	35,35,35,35	0
56	MG	1a	1723	1/1	0.96	0.21	46,46,46,46	0
56	MG	1A	3570	1/1	0.96	0.21	29,29,29,29	0
56	MG	1A	3655	1/1	0.96	0.07	58,58,58,58	0
56	MG	2A	3404	1/1	0.96	0.21	45,45,45,45	0
56	MG	2A	3018	1/1	0.96	0.21	49,49,49,49	0
56	MG	2a	3146	1/1	0.96	0.08	68,68,68,68	0
56	MG	1a	1727	1/1	0.96	0.17	36,36,36,36	0
56	MG	2A	3021	1/1	0.96	0.17	55,55,55,55	0
56	MG	13	101	1/1	0.96	0.10	26,26,26,26	0
56	MG	1A	3571	1/1	0.96	0.53	29,29,29,29	0
56	MG	2A	3865	1/1	0.96	0.07	51,51,51,51	0
56	MG	2A	3024	1/1	0.96	0.42	48,48,48,48	0
56	MG	1B	202	1/1	0.96	0.33	47,47,47,47	0
56	MG	2A	3631	1/1	0.96	0.14	39,39,39,39	0
56	MG	1A	3872	1/1	0.96	0.25	33,33,33,33	0
56	MG	15	101	1/1	0.96	0.34	31,31,31,31	0
56	MG	1A	3875	1/1	0.96	0.39	35,35,35,35	0
56	MG	1A	3115	1/1	0.96	0.09	32,32,32,32	0
56	MG	1A	3659	1/1	0.96	0.19	24,24,24,24	0
56	MG	2A	3874	1/1	0.96	0.05	66,66,66,66	0
56	MG	1A	3287	1/1	0.96	0.12	43,43,43,43	0
56	MG	2A	3224	1/1	0.96	0.09	49,49,49,49	0
56	MG	16	101	1/1	0.96	0.19	41,41,41,41	0
56	MG	1a	1739	1/1	0.96	0.36	77,77,77,77	0
56	MG	2A	3424	1/1	0.96	0.22	49,49,49,49	0
56	MG	2A	3035	1/1	0.96	0.20	36,36,36,36	0
56	MG	2A	3036	1/1	0.96	0.08	28,28,28,28	0
56	MG	1A	3445	1/1	0.96	0.18	36,36,36,36	0
56	MG	1A	3011	1/1	0.96	0.21	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	17	101	1/1	0.96	0.19	31,31,31,31	0
56	MG	1a	1744	1/1	0.96	0.15	54,54,54,54	0
56	MG	1A	3149	1/1	0.96	0.25	29,29,29,29	0
56	MG	2A	3436	1/1	0.96	0.17	41,41,41,41	0
56	MG	17	103	1/1	0.96	0.11	22,22,22,22	0
56	MG	2A	3655	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3884	1/1	0.96	0.32	28,28,28,28	0
56	MG	2A	3045	1/1	0.96	0.20	53,53,53,53	0
56	MG	1A	3150	1/1	0.96	0.17	31,31,31,31	0
56	MG	1A	3886	1/1	0.96	0.14	23,23,23,23	0
56	MG	1A	3666	1/1	0.96	0.14	35,35,35,35	0
56	MG	1A	3395	1/1	0.96	0.23	40,40,40,40	0
56	MG	18	101	1/1	0.96	0.26	37,37,37,37	0
56	MG	1A	3068	1/1	0.96	0.18	48,48,48,48	0
56	MG	1A	3890	1/1	0.96	0.10	33,33,33,33	0
56	MG	2A	3666	1/1	0.96	0.16	44,44,44,44	0
56	MG	2A	3669	1/1	0.96	0.55	59,59,59,59	0
56	MG	18	104	1/1	0.96	0.08	49,49,49,49	0
56	MG	2a	3191	1/1	0.96	0.13	71,71,71,71	0
56	MG	1A	3670	1/1	0.96	0.19	28,28,28,28	0
56	MG	1A	3099	1/1	0.96	0.23	16,16,16,16	0
56	MG	2D	301	1/1	0.96	0.32	47,47,47,47	0
56	MG	2A	3673	1/1	0.96	0.15	57,57,57,57	0
56	MG	1A	3293	1/1	0.96	0.23	42,42,42,42	0
56	MG	2A	3451	1/1	0.96	0.26	37,37,37,37	0
56	MG	1A	3674	1/1	0.96	0.16	22,22,22,22	0
56	MG	1a	1761	1/1	0.96	0.14	51,51,51,51	0
56	MG	1A	4003	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3514	1/1	0.96	0.24	64,64,64,64	0
56	MG	1A	3295	1/1	0.96	0.18	22,22,22,22	0
56	MG	1A	3779	1/1	0.96	0.12	18,18,18,18	0
56	MG	1A	4008	1/1	0.96	0.39	33,33,33,33	0
56	MG	1A	3455	1/1	0.96	0.27	28,28,28,28	0
56	MG	1A	4010	1/1	0.96	0.17	28,28,28,28	0
56	MG	1A	3899	1/1	0.96	0.17	38,38,38,38	0
56	MG	1A	3900	1/1	0.96	0.16	20,20,20,20	0
56	MG	1A	3679	1/1	0.96	0.16	34,34,34,34	0
56	MG	2F	305	1/1	0.96	0.33	43,43,43,43	0
56	MG	1B	239	1/1	0.96	0.15	30,30,30,30	0
56	MG	1D	301	1/1	0.96	0.13	34,34,34,34	0
56	MG	2a	3217	1/1	0.96	0.12	72,72,72,72	0
56	MG	2P	201	1/1	0.96	0.34	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	1D	302	1/1	0.96	0.18	36,36,36,36	0
56	MG	1a	1616	1/1	0.96	0.09	55,55,55,55	0
56	MG	1D	303	1/1	0.96	0.13	17,17,17,17	0
56	MG	2A	3697	1/1	0.96	0.21	72,72,72,72	0
56	MG	1A	3120	1/1	0.96	0.17	36,36,36,36	0
56	MG	2A	3471	1/1	0.96	0.19	32,32,32,32	0
56	MG	1A	3100	1/1	0.96	0.11	41,41,41,41	0
56	MG	1D	307	1/1	0.96	0.26	44,44,44,44	0
56	MG	1a	1783	1/1	0.96	0.12	57,57,57,57	0
56	MG	1A	3200	1/1	0.96	0.13	33,33,33,33	0
56	MG	1A	3201	1/1	0.96	0.15	22,22,22,22	0
56	MG	2T	204	1/1	0.96	0.17	54,54,54,54	0
56	MG	1A	3248	1/1	0.96	0.18	51,51,51,51	0
56	MG	2U	203	1/1	0.96	0.41	54,54,54,54	0
56	MG	2V	201	1/1	0.96	0.56	69,69,69,69	0
56	MG	1A	3023	1/1	0.96	0.08	15,15,15,15	0
56	MG	1A	3908	1/1	0.96	0.14	32,32,32,32	0
56	MG	1D	313	1/1	0.96	0.35	34,34,34,34	0
56	MG	2a	3239	1/1	0.96	0.05	66,66,66,66	0
56	MG	1A	3250	1/1	0.96	0.23	36,36,36,36	0
56	MG	1a	1628	1/1	0.96	0.22	47,47,47,47	0
56	MG	1A	3794	1/1	0.96	0.19	48,48,48,48	0
56	MG	2e	201	1/1	0.96	0.14	64,64,64,64	0
56	MG	2f	201	1/1	0.96	0.11	48,48,48,48	0
56	MG	1A	3688	1/1	0.96	0.21	33,33,33,33	0
56	MG	1A	3912	1/1	0.96	0.37	31,31,31,31	0
56	MG	1a	1633	1/1	0.96	0.21	52,52,52,52	0
56	MG	1A	3013	1/1	0.96	0.35	26,26,26,26	0
56	MG	1A	3252	1/1	0.96	0.18	37,37,37,37	0
56	MG	2A	3290	1/1	0.96	0.13	36,36,36,36	0
56	MG	1E	309	1/1	0.96	0.37	47,47,47,47	0
56	MG	1A	3126	1/1	0.96	0.47	34,34,34,34	0
56	MG	2A	3097	1/1	0.96	0.15	45,45,45,45	0
56	MG	2A	3294	1/1	0.96	0.31	67,67,67,67	0
56	MG	1E	311	1/1	0.96	0.23	52,52,52,52	0
56	MG	1a	1639	1/1	0.96	0.19	56,56,56,56	0
56	MG	2A	3730	1/1	0.96	0.08	41,41,41,41	0
56	MG	2A	3100	1/1	0.96	0.09	53,53,53,53	0
56	MG	1A	3255	1/1	0.96	0.19	29,29,29,29	0
56	MG	1A	3695	1/1	0.96	0.11	25,25,25,25	0
56	MG	1A	3014	1/1	0.96	0.18	22,22,22,22	0
56	MG	1A	3530	1/1	0.96	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1F	307	1/1	0.96	0.25	30,30,30,30	0
56	MG	2A	3106	1/1	0.96	0.10	36,36,36,36	0
56	MG	2A	3738	1/1	0.96	0.10	48,48,48,48	0
56	MG	2A	3304	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3007	1/1	0.96	0.26	26,26,26,26	0
56	MG	1A	3805	1/1	0.96	0.09	35,35,35,35	0
56	MG	2A	3109	1/1	0.96	0.19	39,39,39,39	0
56	MG	1A	3311	1/1	0.96	0.19	40,40,40,40	0
56	MG	1A	3925	1/1	0.96	0.17	39,39,39,39	0
56	MG	1A	3701	1/1	0.96	0.18	23,23,23,23	0
56	MG	1A	3472	1/1	0.96	0.23	33,33,33,33	0
56	MG	2A	3313	1/1	0.96	0.07	57,57,57,57	0
56	MG	2a	3016	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3105	1/1	0.96	0.33	30,30,30,30	0
56	MG	2a	3018	1/1	0.96	0.12	61,61,61,61	0
56	MG	1A	3259	1/1	0.96	0.18	38,38,38,38	0
56	MG	2A	3752	1/1	0.96	0.22	54,54,54,54	0
56	MG	1A	3783	1/1	0.97	0.15	17,17,17,17	0
56	MG	1A	3294	1/1	0.97	0.13	41,41,41,41	0
56	MG	1A	3407	1/1	0.97	0.13	36,36,36,36	0
56	MG	2A	3683	1/1	0.97	0.10	64,64,64,64	0
56	MG	1A	4045	1/1	0.97	0.12	17,17,17,17	0
56	MG	2a	3087	1/1	0.97	0.10	59,59,59,59	0
56	MG	2A	3064	1/1	0.97	0.08	48,48,48,48	0
56	MG	1a	1811	1/1	0.97	0.10	38,38,38,38	0
56	MG	2a	3090	1/1	0.97	0.20	66,66,66,66	0
56	MG	1A	3583	1/1	0.97	0.11	44,44,44,44	0
56	MG	1A	3448	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3790	1/1	0.97	0.17	19,19,19,19	0
56	MG	1A	3122	1/1	0.97	0.30	37,37,37,37	0
56	MG	1A	3880	1/1	0.97	0.09	60,60,60,60	0
56	MG	1A	3714	1/1	0.97	0.14	14,14,14,14	0
56	MG	2A	3520	1/1	0.97	0.11	49,49,49,49	0
56	MG	2a	3099	1/1	0.97	0.16	52,52,52,52	0
56	MG	2A	3366	1/1	0.97	0.14	60,60,60,60	0
56	MG	2A	3695	1/1	0.97	0.08	60,60,60,60	0
56	MG	1A	3647	1/1	0.97	0.15	30,30,30,30	0
56	MG	1A	3038	1/1	0.97	0.21	30,30,30,30	0
56	MG	2A	3880	1/1	0.97	0.12	52,52,52,52	0
56	MG	1A	3146	1/1	0.97	0.35	25,25,25,25	0
56	MG	1A	3720	1/1	0.97	0.19	44,44,44,44	0
56	MG	1A	3027	1/1	0.97	0.13	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	3495	1/1	0.97	0.23	47,47,47,47	0
56	MG	1A	3040	1/1	0.97	0.15	30,30,30,30	0
56	MG	1E	307	1/1	0.97	0.22	57,57,57,57	0
56	MG	2A	3704	1/1	0.97	0.19	44,44,44,44	0
56	MG	2A	3705	1/1	0.97	0.16	51,51,51,51	0
56	MG	1A	3204	1/1	0.97	0.16	29,29,29,29	0
56	MG	1a	1704	1/1	0.97	0.29	60,60,60,60	0
56	MG	1A	3593	1/1	0.97	0.34	27,27,27,27	0
56	MG	1A	3543	1/1	0.97	0.38	34,34,34,34	0
56	MG	2A	3229	1/1	0.97	0.47	33,33,33,33	0
56	MG	1A	3656	1/1	0.97	0.18	34,34,34,34	0
56	MG	1A	3375	1/1	0.97	0.15	42,42,42,42	0
56	MG	1A	3731	1/1	0.97	0.14	24,24,24,24	0
56	MG	2a	3121	1/1	0.97	0.12	54,54,54,54	0
56	MG	1A	3031	1/1	0.97	0.28	31,31,31,31	0
56	MG	1A	3236	1/1	0.97	0.47	30,30,30,30	0
56	MG	1a	1713	1/1	0.97	0.14	50,50,50,50	0
56	MG	1F	305	1/1	0.97	0.10	45,45,45,45	0
56	MG	2A	3720	1/1	0.97	0.13	48,48,48,48	0
56	MG	1F	306	1/1	0.97	0.25	23,23,23,23	0
56	MG	1A	4069	1/1	0.97	0.14	20,20,20,20	0
56	MG	1a	1717	1/1	0.97	0.06	64,64,64,64	0
56	MG	2A	3241	1/1	0.97	0.24	62,62,62,62	0
56	MG	1A	3032	1/1	0.97	0.28	26,26,26,26	0
56	MG	2A	3550	1/1	0.97	0.17	57,57,57,57	0
56	MG	1A	3811	1/1	0.97	0.12	49,49,49,49	0
56	MG	1F	310	1/1	0.97	0.14	41,41,41,41	0
56	MG	1A	3085	1/1	0.97	0.18	23,23,23,23	0
56	MG	1A	3305	1/1	0.97	0.31	34,34,34,34	0
56	MG	1A	3239	1/1	0.97	0.18	25,25,25,25	0
56	MG	1A	3132	1/1	0.97	0.26	33,33,33,33	0
56	MG	1A	3154	1/1	0.97	0.43	39,39,39,39	0
56	MG	1A	3507	1/1	0.97	0.27	42,42,42,42	0
56	MG	1A	3508	1/1	0.97	0.18	23,23,23,23	0
56	MG	1A	3669	1/1	0.97	0.14	19,19,19,19	0
56	MG	1A	3028	1/1	0.97	0.17	21,21,21,21	0
56	MG	1A	3466	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3825	1/1	0.97	0.16	34,34,34,34	0
56	MG	1a	1733	1/1	0.97	0.31	53,53,53,53	0
56	MG	1O	202	1/1	0.97	0.42	47,47,47,47	0
56	MG	2F	306	1/1	0.97	0.60	51,51,51,51	0
56	MG	2A	3112	1/1	0.97	0.11	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2N	201	1/1	0.97	0.08	35,35,35,35	0
56	MG	2A	3745	1/1	0.97	0.09	50,50,50,50	0
56	MG	1O	203	1/1	0.97	0.14	40,40,40,40	0
56	MG	1O	204	1/1	0.97	0.14	46,46,46,46	0
56	MG	1x	102	1/1	0.97	0.16	46,46,46,46	0
56	MG	2A	3411	1/1	0.97	0.10	46,46,46,46	0
56	MG	1a	1615	1/1	0.97	0.07	43,43,43,43	0
56	MG	2A	3413	1/1	0.97	0.19	55,55,55,55	0
56	MG	1A	4084	1/1	0.97	0.24	14,14,14,14	0
56	MG	2A	3266	1/1	0.97	0.21	59,59,59,59	0
56	MG	1A	3746	1/1	0.97	0.25	46,46,46,46	0
56	MG	2A	3755	1/1	0.97	0.07	54,54,54,54	0
56	MG	1x	106	1/1	0.97	0.21	52,52,52,52	0
56	MG	1A	3672	1/1	0.97	0.10	35,35,35,35	0
56	MG	1x	108	1/1	0.97	0.20	62,62,62,62	0
56	MG	2U	201	1/1	0.97	0.26	54,54,54,54	0
56	MG	1A	3386	1/1	0.97	0.30	30,30,30,30	0
56	MG	2A	3582	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3913	1/1	0.97	0.50	34,34,34,34	0
56	MG	1A	3211	1/1	0.97	0.43	34,34,34,34	0
56	MG	2A	3423	1/1	0.97	0.17	35,35,35,35	0
56	MG	1A	3610	1/1	0.97	0.20	44,44,44,44	0
56	MG	2A	3425	1/1	0.97	0.14	43,43,43,43	0
56	MG	2A	3128	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	3752	1/1	0.97	0.14	37,37,37,37	0
56	MG	1x	114	1/1	0.97	0.21	51,51,51,51	0
56	MG	1A	3833	1/1	0.97	0.15	55,55,55,55	0
56	MG	2A	3431	1/1	0.97	0.20	49,49,49,49	0
56	MG	1Q	201	1/1	0.97	0.62	42,42,42,42	0
56	MG	1A	3559	1/1	0.97	0.21	54,54,54,54	0
56	MG	23	101	1/1	0.97	0.22	54,54,54,54	0
56	MG	2a	3184	1/1	0.97	0.11	57,57,57,57	0
56	MG	1A	3677	1/1	0.97	0.12	23,23,23,23	0
56	MG	2A	3435	1/1	0.97	0.12	28,28,28,28	0
56	MG	1A	3071	1/1	0.97	0.21	29,29,29,29	0
56	MG	2A	3598	1/1	0.97	0.15	42,42,42,42	0
56	MG	2a	3189	1/1	0.97	0.10	57,57,57,57	0
56	MG	2A	3778	1/1	0.97	0.11	58,58,58,58	0
56	MG	1A	3135	1/1	0.97	0.11	23,23,23,23	0
56	MG	2A	3137	1/1	0.97	0.34	40,40,40,40	0
56	MG	1A	3614	1/1	0.97	0.17	35,35,35,35	0
56	MG	1A	3839	1/1	0.97	0.16	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	1R	201	1/1	0.97	0.23	32,32,32,32	0
56	MG	2A	3604	1/1	0.97	0.14	44,44,44,44	0
56	MG	1R	202	1/1	0.97	0.42	36,36,36,36	0
56	MG	1a	1757	1/1	0.97	0.12	35,35,35,35	0
56	MG	1A	3158	1/1	0.97	0.31	60,60,60,60	0
56	MG	1A	3841	1/1	0.97	0.21	39,39,39,39	0
56	MG	1A	3842	1/1	0.97	0.18	31,31,31,31	0
56	MG	1A	3046	1/1	0.97	0.16	28,28,28,28	0
56	MG	2A	3791	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3280	1/1	0.97	0.15	21,21,21,21	0
56	MG	2a	3205	1/1	0.97	0.06	60,60,60,60	0
56	MG	1A	3281	1/1	0.97	0.26	31,31,31,31	0
56	MG	2A	3151	1/1	0.97	0.21	60,60,60,60	0
56	MG	1a	1764	1/1	0.97	0.11	58,58,58,58	0
56	MG	1A	3931	1/1	0.97	0.08	40,40,40,40	0
56	MG	2a	3210	1/1	0.97	0.09	57,57,57,57	0
56	MG	2a	3211	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3620	1/1	0.97	0.10	52,52,52,52	0
56	MG	1A	3161	1/1	0.97	0.18	22,22,22,22	0
56	MG	1U	202	1/1	0.97	0.20	27,27,27,27	0
56	MG	1U	203	1/1	0.97	0.32	28,28,28,28	0
56	MG	1a	1647	1/1	0.97	0.27	55,55,55,55	0
56	MG	1A	3476	1/1	0.97	0.13	40,40,40,40	0
56	MG	1U	206	1/1	0.97	0.16	33,33,33,33	0
56	MG	2A	3161	1/1	0.97	0.39	64,64,64,64	0
56	MG	2a	3221	1/1	0.97	0.08	55,55,55,55	0
56	MG	1A	3935	1/1	0.97	0.14	40,40,40,40	0
56	MG	2A	3626	1/1	0.97	0.17	33,33,33,33	0
56	MG	1a	1774	1/1	0.97	0.14	61,61,61,61	0
56	MG	1A	4020	1/1	0.97	0.10	33,33,33,33	0
56	MG	1a	1776	1/1	0.97	0.10	58,58,58,58	0
56	MG	1A	3283	1/1	0.97	0.44	33,33,33,33	0
56	MG	2A	3167	1/1	0.97	0.15	39,39,39,39	0
56	MG	1A	3569	1/1	0.97	0.22	42,42,42,42	0
56	MG	1V	201	1/1	0.97	0.45	30,30,30,30	0
56	MG	2A	3170	1/1	0.97	0.09	52,52,52,52	0
56	MG	1A	3691	1/1	0.97	0.16	24,24,24,24	0
56	MG	2A	3032	1/1	0.97	0.20	47,47,47,47	0
56	MG	1A	3190	1/1	0.97	0.25	25,25,25,25	0
56	MG	1B	218	1/1	0.97	0.15	39,39,39,39	0
56	MG	1B	219	1/1	0.97	0.28	34,34,34,34	0
56	MG	2a	3038	1/1	0.97	0.23	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	3628	1/1	0.97	0.12	51,51,51,51	0
56	MG	2A	3477	1/1	0.97	0.14	23,23,23,23	0
56	MG	2A	3177	1/1	0.97	0.17	35,35,35,35	0
56	MG	2A	3037	1/1	0.97	0.08	68,68,68,68	0
56	MG	1A	3034	1/1	0.97	0.30	23,23,23,23	0
56	MG	1W	202	1/1	0.97	0.15	50,50,50,50	0
56	MG	2A	3330	1/1	0.97	0.13	60,60,60,60	0
56	MG	2A	3648	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	3049	1/1	0.97	0.23	39,39,39,39	0
56	MG	1A	3254	1/1	0.97	0.17	36,36,36,36	0
56	MG	2A	3651	1/1	0.97	0.20	44,44,44,44	0
56	MG	1X	101	1/1	0.97	0.23	32,32,32,32	0
56	MG	2A	3653	1/1	0.97	0.21	61,61,61,61	0
56	MG	2A	3184	1/1	0.97	0.16	41,41,41,41	0
56	MG	1A	3698	1/1	0.97	0.21	28,28,28,28	0
56	MG	2m	201	1/1	0.97	0.12	73,73,73,73	0
56	MG	2A	3835	1/1	0.97	0.14	34,34,34,34	0
56	MG	2q	202	1/1	0.97	0.13	72,72,72,72	0
56	MG	1X	103	1/1	0.97	0.31	37,37,37,37	0
56	MG	2A	3187	1/1	0.97	0.21	56,56,56,56	0
56	MG	1A	3859	1/1	0.97	0.37	38,38,38,38	0
56	MG	1A	3119	1/1	0.97	0.26	23,23,23,23	0
56	MG	1A	3021	1/1	0.97	0.10	21,21,21,21	0
56	MG	1A	3862	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3326	1/1	0.97	0.18	48,48,48,48	0
56	MG	1A	3142	1/1	0.97	0.21	14,14,14,14	0
56	MG	1Z	303	1/1	0.97	0.20	42,42,42,42	0
56	MG	1B	231	1/1	0.97	0.21	39,39,39,39	0
56	MG	2A	3667	1/1	0.97	0.10	57,57,57,57	0
56	MG	2A	3668	1/1	0.97	0.19	54,54,54,54	0
56	MG	2A	3346	1/1	0.97	0.08	67,67,67,67	0
56	MG	2a	3069	1/1	0.97	0.23	62,62,62,62	0
56	MG	1A	3778	1/1	0.97	0.16	20,20,20,20	0
56	MG	2A	3851	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3952	1/1	0.97	0.18	39,39,39,39	0
56	MG	2A	3501	1/1	0.97	0.07	58,58,58,58	0
56	MG	1A	3037	1/1	0.97	0.16	32,32,32,32	0
56	MG	2a	3075	1/1	0.97	0.22	57,57,57,57	0
56	MG	10	105	1/1	0.97	0.13	53,53,53,53	0
59	ZN	1n	102	1/1	0.97	0.15	66,66,66,66	0
56	MG	2A	3675	1/1	0.97	0.06	57,57,57,57	0
56	MG	1A	3638	1/1	0.97	0.08	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3579	1/1	0.97	0.26	21,21,21,21	0
56	MG	1A	3227	1/1	0.97	0.26	37,37,37,37	0
60	SF4	1d	302	8/8	0.97	0.14	68,78,85,86	0
60	SF4	2d	302	8/8	0.97	0.15	59,73,81,82	0
56	MG	1A	3057	1/1	0.98	0.18	28,28,28,28	0
56	MG	2A	3877	1/1	0.98	0.24	49,49,49,49	0
56	MG	2A	3536	1/1	0.98	0.17	57,57,57,57	0
56	MG	1a	1825	1/1	0.98	0.23	43,43,43,43	0
56	MG	1a	1653	1/1	0.98	0.14	56,56,56,56	0
56	MG	1N	204	1/1	0.98	0.39	42,42,42,42	0
56	MG	1a	1828	1/1	0.98	0.25	42,42,42,42	0
56	MG	2A	3232	1/1	0.98	0.15	60,60,60,60	0
56	MG	1A	3012	1/1	0.98	0.20	28,28,28,28	0
56	MG	1A	3517	1/1	0.98	0.24	44,44,44,44	0
56	MG	1a	1742	1/1	0.98	0.12	55,55,55,55	0
56	MG	1A	3077	1/1	0.98	0.12	35,35,35,35	0
56	MG	2A	3139	1/1	0.98	0.13	34,34,34,34	0
56	MG	2A	3548	1/1	0.98	0.18	35,35,35,35	0
56	MG	2a	3171	1/1	0.98	0.12	64,64,64,64	0
56	MG	1B	216	1/1	0.98	0.16	47,47,47,47	0
56	MG	1A	3631	1/1	0.98	0.11	14,14,14,14	0
56	MG	1A	3873	1/1	0.98	0.16	35,35,35,35	0
56	MG	1A	3874	1/1	0.98	0.20	27,27,27,27	0
56	MG	1A	3716	1/1	0.98	0.19	31,31,31,31	0
56	MG	1A	3818	1/1	0.98	0.11	42,42,42,42	0
56	MG	1a	1664	1/1	0.98	0.08	60,60,60,60	0
56	MG	1A	3591	1/1	0.98	0.29	35,35,35,35	0
56	MG	1h	201	1/1	0.98	0.10	58,58,58,58	0
56	MG	1P	204	1/1	0.98	0.47	23,23,23,23	0
56	MG	1l	202	1/1	0.98	0.19	41,41,41,41	0
56	MG	1A	4057	1/1	0.98	0.21	23,23,23,23	0
56	MG	2B	215	1/1	0.98	0.15	69,69,69,69	0
56	MG	2A	3455	1/1	0.98	0.17	61,61,61,61	0
56	MG	1A	3820	1/1	0.98	0.09	18,18,18,18	0
56	MG	1A	3879	1/1	0.98	0.21	36,36,36,36	0
56	MG	2B	219	1/1	0.98	0.14	62,62,62,62	0
56	MG	1A	3821	1/1	0.98	0.13	26,26,26,26	0
56	MG	1A	3042	1/1	0.98	0.28	22,22,22,22	0
56	MG	1A	3187	1/1	0.98	0.17	31,31,31,31	0
56	MG	2A	3567	1/1	0.98	0.10	54,54,54,54	0
56	MG	1Q	202	1/1	0.98	0.36	34,34,34,34	0
56	MG	2D	305	1/1	0.98	0.14	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3125	1/1	0.98	0.47	34,34,34,34	0
56	MG	1A	3385	1/1	0.98	0.18	27,27,27,27	0
56	MG	2A	3258	1/1	0.98	0.08	67,67,67,67	0
56	MG	2A	3682	1/1	0.98	0.13	74,74,74,74	0
56	MG	1A	3723	1/1	0.98	0.17	40,40,40,40	0
56	MG	2A	3260	1/1	0.98	0.16	57,57,57,57	0
56	MG	1B	232	1/1	0.98	0.11	50,50,50,50	0
56	MG	2E	303	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	3827	1/1	0.98	0.15	39,39,39,39	0
56	MG	1A	3266	1/1	0.98	0.11	40,40,40,40	0
56	MG	2A	3577	1/1	0.98	0.16	57,57,57,57	0
56	MG	1A	4007	1/1	0.98	0.12	15,15,15,15	0
56	MG	2a	3079	1/1	0.98	0.09	56,56,56,56	0
56	MG	1A	3354	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3355	1/1	0.98	0.49	25,25,25,25	0
56	MG	1A	3047	1/1	0.98	0.20	23,23,23,23	0
56	MG	1A	3153	1/1	0.98	0.13	26,26,26,26	0
56	MG	2a	3212	1/1	0.98	0.13	59,59,59,59	0
56	MG	1A	3457	1/1	0.98	0.21	25,25,25,25	0
56	MG	1A	3730	1/1	0.98	0.16	19,19,19,19	0
56	MG	1A	3241	1/1	0.98	0.34	30,30,30,30	0
56	MG	1D	305	1/1	0.98	0.30	29,29,29,29	0
56	MG	1A	3128	1/1	0.98	0.18	36,36,36,36	0
56	MG	1A	3171	1/1	0.98	0.18	44,44,44,44	0
56	MG	2Q	201	1/1	0.98	0.13	49,49,49,49	0
56	MG	1A	3687	1/1	0.98	0.16	27,27,27,27	0
56	MG	1A	4080	1/1	0.98	0.09	39,39,39,39	0
56	MG	1U	204	1/1	0.98	0.17	22,22,22,22	0
56	MG	1A	3244	1/1	0.98	0.16	42,42,42,42	0
56	MG	1a	1610	1/1	0.98	0.11	23,23,23,23	0
56	MG	1A	3141	1/1	0.98	0.18	26,26,26,26	0
56	MG	1A	3786	1/1	0.98	0.09	24,24,24,24	0
56	MG	1A	3173	1/1	0.98	0.32	34,34,34,34	0
56	MG	2A	3708	1/1	0.98	0.09	31,31,31,31	0
56	MG	1A	3174	1/1	0.98	0.26	27,27,27,27	0
56	MG	1U	211	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	3692	1/1	0.98	0.14	55,55,55,55	0
56	MG	2A	3092	1/1	0.98	0.10	48,48,48,48	0
56	MG	2A	3188	1/1	0.98	0.11	43,43,43,43	0
56	MG	1A	3219	1/1	0.98	0.30	32,32,32,32	0
56	MG	2a	3235	1/1	0.98	0.06	66,66,66,66	0
56	MG	1A	3196	1/1	0.98	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3792	1/1	0.98	0.15	45,45,45,45	0
56	MG	2A	3717	1/1	0.98	0.04	51,51,51,51	0
56	MG	1A	3307	1/1	0.98	0.17	26,26,26,26	0
56	MG	1A	4091	1/1	0.98	0.20	31,31,31,31	0
56	MG	1V	206	1/1	0.98	0.10	29,29,29,29	0
56	MG	1a	1708	1/1	0.98	0.27	58,58,58,58	0
56	MG	1A	3743	1/1	0.98	0.12	22,22,22,22	0
56	MG	1A	3097	1/1	0.98	0.32	35,35,35,35	0
56	MG	1A	3066	1/1	0.98	0.13	29,29,29,29	0
56	MG	2A	3725	1/1	0.98	0.09	34,34,34,34	0
56	MG	1W	203	1/1	0.98	0.17	31,31,31,31	0
56	MG	2A	3505	1/1	0.98	0.17	57,57,57,57	0
56	MG	1E	312	1/1	0.98	0.13	39,39,39,39	0
56	MG	2A	3843	1/1	0.98	0.16	35,35,35,35	0
56	MG	1A	3223	1/1	0.98	0.08	46,46,46,46	0
56	MG	1a	1629	1/1	0.98	0.15	54,54,54,54	0
56	MG	1A	3199	1/1	0.98	0.21	20,20,20,20	0
56	MG	1A	3177	1/1	0.98	0.20	25,25,25,25	0
56	MG	28	102	1/1	0.98	0.10	48,48,48,48	0
56	MG	1F	301	1/1	0.98	0.16	27,27,27,27	0
56	MG	2a	3129	1/1	0.98	0.24	49,49,49,49	0
56	MG	1F	302	1/1	0.98	0.17	30,30,30,30	0
56	MG	1F	303	1/1	0.98	0.23	28,28,28,28	0
56	MG	1A	3749	1/1	0.98	0.11	30,30,30,30	0
56	MG	1Y	202	1/1	0.98	0.12	68,68,68,68	0
56	MG	1A	3856	1/1	0.98	0.14	16,16,16,16	0
56	MG	1A	3108	1/1	0.98	0.25	36,36,36,36	0
56	MG	1a	1725	1/1	0.98	0.16	42,42,42,42	0
56	MG	1A	3702	1/1	0.98	0.12	8,8,8,8	0
56	MG	1B	201	1/1	0.98	0.29	48,48,48,48	0
56	MG	1A	3439	1/1	0.98	0.19	44,44,44,44	0
56	MG	2A	3744	1/1	0.98	0.21	44,44,44,44	0
56	MG	1A	3804	1/1	0.98	0.17	22,22,22,22	0
56	MG	1A	3704	1/1	0.98	0.10	21,21,21,21	0
56	MG	2A	3122	1/1	0.98	0.24	53,53,53,53	0
56	MG	2A	3863	1/1	0.98	0.12	28,28,28,28	0
56	MG	1A	3073	1/1	0.98	0.16	14,14,14,14	0
56	MG	1A	3621	1/1	0.98	0.21	27,27,27,27	0
56	MG	2A	3322	1/1	0.98	0.10	48,48,48,48	0
56	MG	1A	3160	1/1	0.98	0.33	26,26,26,26	0
58	K	2A	3889	1/1	0.98	0.09	36,36,36,36	0
56	MG	1A	3442	1/1	0.98	0.40	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3223	1/1	0.98	0.10	45,45,45,45	0
56	MG	2A	3127	1/1	0.98	0.29	65,65,65,65	0
56	MG	1A	3003	1/1	0.98	0.16	19,19,19,19	0
59	ZN	25	106	1/1	0.98	0.20	57,57,57,57	0
56	MG	2A	3642	1/1	0.98	0.07	41,41,41,41	0
56	MG	2A	3328	1/1	0.98	0.09	41,41,41,41	0
56	MG	2A	3758	1/1	0.98	0.11	64,64,64,64	0
56	MG	1A	3162	1/1	0.98	0.81	31,31,31,31	0
56	MG	27	102	1/1	0.99	0.26	34,34,34,34	0
56	MG	1A	3001	1/1	0.99	0.13	39,39,39,39	0
56	MG	1U	207	1/1	0.99	0.13	29,29,29,29	0
56	MG	1A	3036	1/1	0.99	0.16	15,15,15,15	0
56	MG	1A	3622	1/1	0.99	0.14	22,22,22,22	0
56	MG	2A	3147	1/1	0.99	0.29	31,31,31,31	0
56	MG	1A	3919	1/1	0.99	0.16	30,30,30,30	0
56	MG	1A	3373	1/1	0.99	0.10	43,43,43,43	0
56	MG	2A	3625	1/1	0.99	0.14	57,57,57,57	0
56	MG	2A	3307	1/1	0.99	0.17	54,54,54,54	0
56	MG	1A	3228	1/1	0.99	0.21	32,32,32,32	0
56	MG	1B	238	1/1	0.99	0.12	37,37,37,37	0
56	MG	2A	3660	1/1	0.99	0.09	33,33,33,33	0
56	MG	1E	305	1/1	0.99	0.31	32,32,32,32	0
56	MG	1A	3645	1/1	0.99	0.21	20,20,20,20	0
56	MG	1a	1816	1/1	0.99	0.14	53,53,53,53	0
56	MG	1A	3045	1/1	0.99	0.12	28,28,28,28	0
56	MG	2A	3080	1/1	0.99	0.15	56,56,56,56	0
56	MG	1A	3079	1/1	0.99	0.23	26,26,26,26	0
56	MG	2A	3288	1/1	0.99	0.24	36,36,36,36	0
56	MG	2A	3545	1/1	0.99	0.13	35,35,35,35	0
56	MG	2A	3429	1/1	0.99	0.31	53,53,53,53	0
56	MG	1A	3719	1/1	0.99	0.13	47,47,47,47	0
56	MG	1A	3785	1/1	0.99	0.15	37,37,37,37	0
56	MG	2a	3055	1/1	0.99	0.12	60,60,60,60	0
56	MG	1a	1644	1/1	0.99	0.12	39,39,39,39	0
56	MG	2a	3128	1/1	0.99	0.06	44,44,44,44	0
58	K	1A	4103	1/1	0.99	0.10	21,21,21,21	0
56	MG	2a	3022	1/1	0.99	0.06	43,43,43,43	0
59	ZN	1Y	204	1/1	0.99	0.19	53,53,53,53	0
56	MG	1A	3225	1/1	0.99	0.19	39,39,39,39	0
59	ZN	15	106	1/1	0.99	0.20	38,38,38,38	0
59	ZN	16	104	1/1	0.99	0.21	37,37,37,37	0
59	ZN	19	102	1/1	0.99	0.22	40,40,40,40	0

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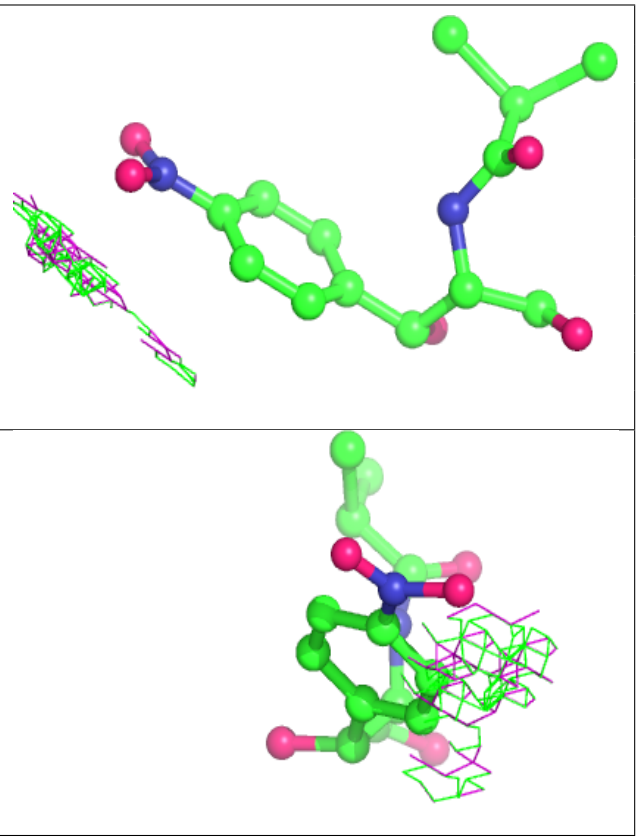
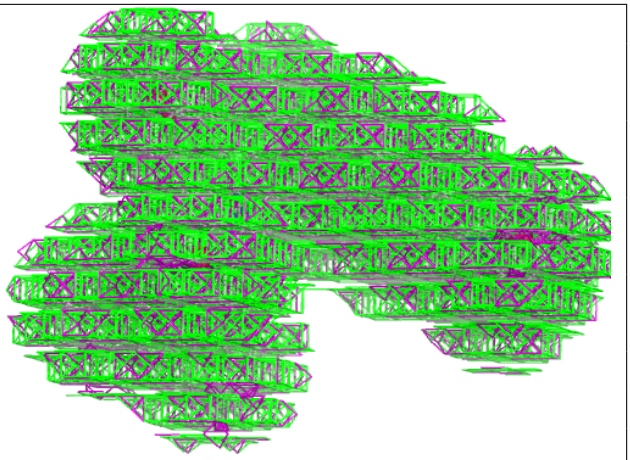
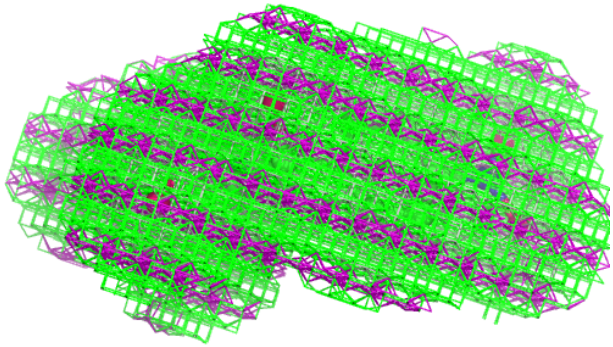
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3094	1/1	0.99	0.22	62,62,62,62	0
56	MG	1B	210	1/1	0.99	0.20	51,51,51,51	0
56	MG	1A	4063	1/1	0.99	0.12	46,46,46,46	0
56	MG	1a	1648	1/1	0.99	0.11	48,48,48,48	0
59	ZN	26	501	1/1	0.99	0.17	64,64,64,64	0
56	MG	1A	3660	1/1	0.99	0.20	31,31,31,31	0
56	MG	1A	3618	1/1	0.99	0.20	26,26,26,26	0
56	MG	1A	3286	1/1	0.99	0.37	42,42,42,42	0
56	MG	2A	3019	1/1	0.99	0.11	30,30,30,30	0
56	MG	1A	3127	1/1	1.00	0.14	42,42,42,42	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CLM 2A 3888:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLM 1A 4102: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.