



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:24 AM UTC

PDB ID : 4ZER / pdb_00004zer
Title : Crystal structure of the Onc112 antimicrobial peptide bound to the Thermus thermophilus 70S ribosome
Authors : Seefeldt, A.C.; Nguyen, F.; Antunes, S.; Perebaskine, N.; Graf, M.; Arenz, S.; Inampudi, K.K.; Douat, C.; Guichard, G.; Wilson, D.N.; Innis, C.A.
Deposited on : 2015-04-20
Resolution : 3.10 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

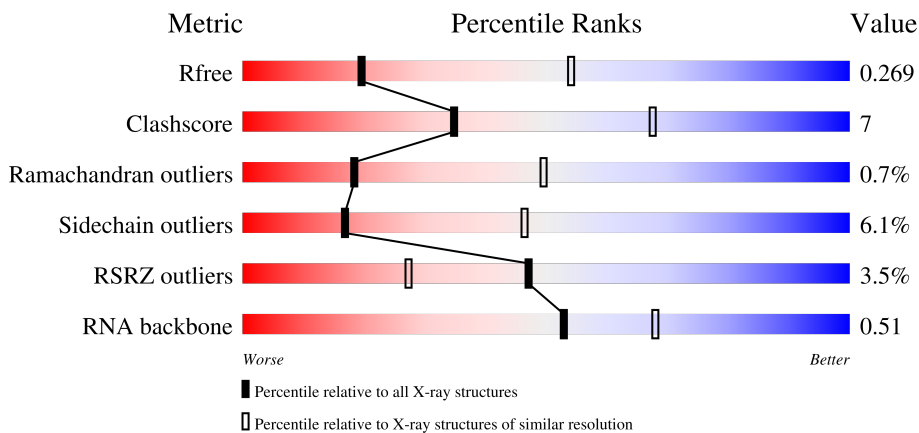
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

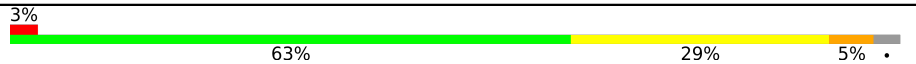
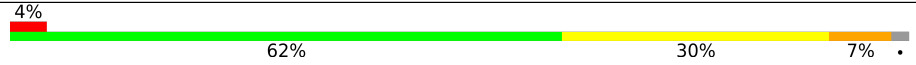


The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	 3% 63% 29% 5%
1	2A	2915	 4% 62% 30% 7%
2	1B	120	 63% 32%
2	2B	120	 70% 27%

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Mol	Chain	Length	Quality of chain
3	1D	275	 79% 19% .
3	2D	275	 79% 19% .
4	1E	204	 77% 19% .
4	2E	204	 76% 21% .
5	1F	203	 70% 26% .
5	2F	203	 72% 26% .
6	1G	181	 67% 30% .
6	2G	181	 68% 28% .
7	1H	174	 73% 24% .
7	2H	174	 68% 29% ..
8	1I	147	 76% 20% 5%
8	2I	147	 73% 24% ..
9	1N	140	 83% 16% .
9	2N	140	 79% 19% .
10	1O	122	 78% 20% .
10	2O	122	 75% 25% .
11	1P	149	 76% 22% .
11	2P	149	 80% 20%
12	1Q	141	 75% 22% .
12	2Q	141	 74% 23% .
13	1R	118	 74% 21% 5%
13	2R	118	 73% 22% 5%
14	1S	110	 73% 25% ..
14	2S	110	 75% 25% .
15	1T	131	 73% 26% .







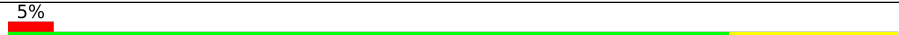
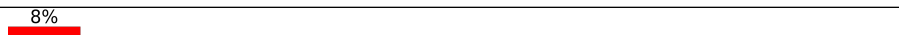
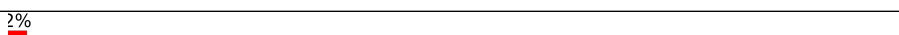
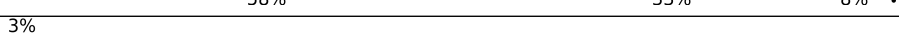
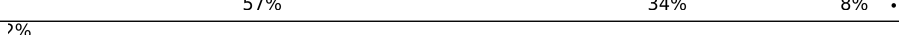
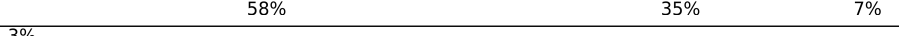













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Mol	Chain	Length	Quality of chain	
15	2T	131	%	76% 24%
16	1U	116	%	81% 18%
16	2U	116	%	80% 19%
17	1V	101		70% 28%
17	2V	101		72% 24%
18	1W	112		84% 16%
18	2W	112		75% 22%
19	1X	95	%	75% 25%
19	2X	95	3%	75% 24%
20	1Y	107	%	63% 35%
20	2Y	107	6%	69% 30%
21	1Z	203	7%	75% 23%
21	2Z	203	6%	75% 20%
22	10	77	3%	81% 16%
22	20	77	4%	78% 22%
23	11	97	2%	82% 18%
23	21	97	%	72% 28%
24	12	70	4%	81% 19%
24	22	70	4%	83% 17%
25	13	59		71% 22% 7%
25	23	59		80% 17%
26	14	69	%	54% 39% 6%
26	24	69	9%	59% 30% 10%
27	15	59	2%	86% 12%
27	25	59	2%	86% 14%

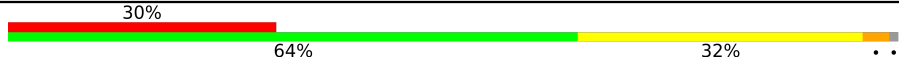
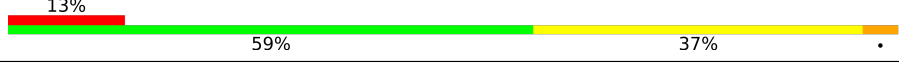
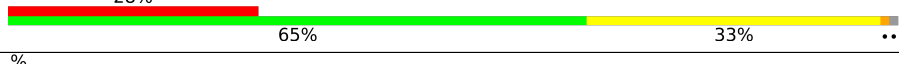


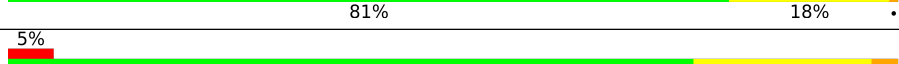
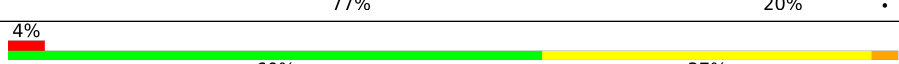
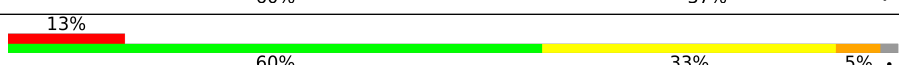
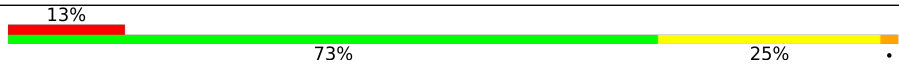


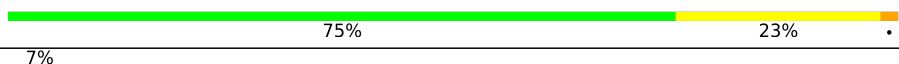
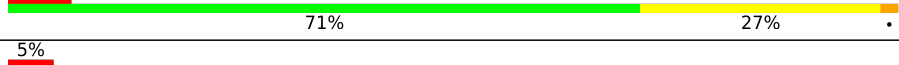

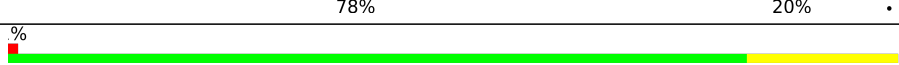










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Mol	Chain	Length	Quality of chain
28	16	53	
28	26	53	
29	17	48	
29	27	48	
30	18	64	
30	28	64	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	231	
33	2b	231	
34	1c	206	
34	2c	206	
35	1d	208	
35	2d	208	
36	1e	148	
36	2e	148	
37	1f	100	
37	2f	100	
38	1g	155	
38	2g	155	
39	1h	137	
39	2h	137	
40	1i	127	







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Mol	Chain	Length	Quality of chain
40	2i	127	
41	1j	97	
41	2j	97	
42	1k	114	
42	2k	114	
43	1l	122	
43	2l	122	
44	1m	116	
44	2m	116	
45	1n	60	
45	2n	60	
46	1o	88	
46	2o	88	
47	1p	82	
47	2p	82	
48	1q	99	
48	2q	99	
49	1r	68	
49	2r	68	
50	1s	83	
50	2s	83	
51	1t	98	
51	2t	98	
52	1u	23	
52	2u	23	

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Mol	Chain	Length	Quality of chain
53	1x	76	
53	2x	76	
54	1y	19	
54	2y	19	
55	A	27	
55	B	27	

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
56	MG	1a	1667	-	-	-	X
56	MG	1a	1713	-	-	-	X
56	MG	1a	1732	-	-	-	X
56	MG	2A	3081	-	-	-	X
56	MG	2D	302	-	-	-	X
56	MG	2a	1606	-	-	-	X
56	MG	2a	1608	-	-	-	X
56	MG	2a	1630	-	-	-	X
56	MG	2a	1639	-	-	-	X
56	MG	2a	1640	-	-	-	X
56	MG	2a	1675	-	-	-	X
56	MG	2p	101	-	-	-	X

2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 293672 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	2824	Total	C	N	O	P	0	0	0
			60842	27081	11388	19550	2823			
1	2A	2869	Total	C	N	O	P	0	0	0
			61801	27510	11560	19864	2867			

- 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	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- 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	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

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

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

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

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

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

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

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

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

- Molecule 32 is a RNA chain called 16s ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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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	116	914	564	189	159	2	0	0	0
44	2m	114	895	550	186	157	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
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

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

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

- Molecule 53 is a RNA chain called tRNA met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
53	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
53	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 54 is a protein called Onc112.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	1y	12	Total	C	N	O	0	0	0
			101	67	19	15			
54	2y	12	Total	C	N	O	0	0	0
			101	67	19	15			

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	A	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			
55	B	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	946	Total	Mg	0	0
			946	946		
56	1B	29	Total	Mg	0	0
			29	29		
56	1D	21	Total	Mg	0	0
			21	21		
56	1E	6	Total	Mg	0	0
			6	6		
56	1F	9	Total	Mg	0	0
			9	9		
56	1G	4	Total	Mg	0	0
			4	4		
56	1H	2	Total	Mg	0	0
			2	2		
56	1N	3	Total	Mg	0	0
			3	3		
56	1O	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1P	2	Total 2	Mg 2	0	0
56	1Q	4	Total 4	Mg 4	0	0
56	1R	4	Total 4	Mg 4	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	5	Total 5	Mg 5	0	0
56	1V	3	Total 3	Mg 3	0	0
56	1W	3	Total 3	Mg 3	0	0
56	1X	1	Total 1	Mg 1	0	0
56	1Y	1	Total 1	Mg 1	0	0
56	1Z	1	Total 1	Mg 1	0	0
56	10	7	Total 7	Mg 7	0	0
56	11	3	Total 3	Mg 3	0	0
56	13	3	Total 3	Mg 3	0	0
56	15	3	Total 3	Mg 3	0	0
56	17	2	Total 2	Mg 2	0	0
56	18	1	Total 1	Mg 1	0	0
56	19	2	Total 2	Mg 2	0	0
56	1a	261	Total 261	Mg 261	0	0
56	1b	1	Total 1	Mg 1	0	0
56	1d	4	Total 4	Mg 4	0	0
56	1e	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1f	1	Total Mg 1 1	0	0
56	1g	1	Total Mg 1 1	0	0
56	1i	1	Total Mg 1 1	0	0
56	1l	1	Total Mg 1 1	0	0
56	1n	1	Total Mg 1 1	0	0
56	1o	2	Total Mg 2 2	0	0
56	1r	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1x	12	Total Mg 12 12	0	0
56	2A	679	Total Mg 679 679	0	0
56	2B	17	Total Mg 17 17	0	0
56	2D	8	Total Mg 8 8	0	0
56	2E	7	Total Mg 7 7	0	0
56	2F	3	Total Mg 3 3	0	0
56	2G	2	Total Mg 2 2	0	0
56	2I	1	Total Mg 1 1	0	0
56	2N	1	Total Mg 1 1	0	0
56	2O	2	Total Mg 2 2	0	0
56	2P	1	Total Mg 1 1	0	0
56	2Q	2	Total Mg 2 2	0	0
56	2R	1	Total Mg 1 1	0	0

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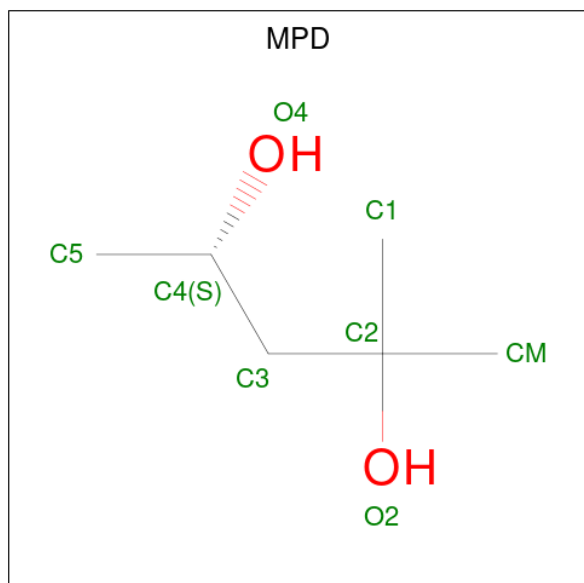
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2T	4	Total 4	Mg 4	0	0
56	2U	2	Total 2	Mg 2	0	0
56	2V	3	Total 3	Mg 3	0	0
56	2W	1	Total 1	Mg 1	0	0
56	2X	1	Total 1	Mg 1	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	20	1	Total 1	Mg 1	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0
56	28	2	Total 2	Mg 2	0	0
56	2a	183	Total 183	Mg 183	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2j	1	Total 1	Mg 1	0	0
56	2k	1	Total 1	Mg 1	0	0
56	2l	1	Total 1	Mg 1	0	0
56	2n	1	Total 1	Mg 1	0	0
56	2p	1	Total 1	Mg 1	0	0
56	2q	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2x	10	Total 10	Mg 10	0	0

- Molecule 57 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

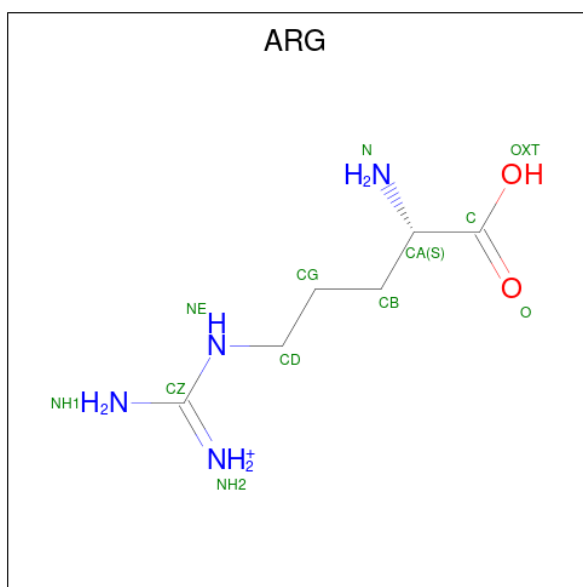
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total X 1 1	0	0
57	2A	1	Total X 1 1	0	0

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C O 8 6 2	0	0
58	1a	1	Total C O 8 6 2	0	0

- Molecule 59 is ARGinine (CCD ID: ARG) (formula: C₆H₁₅N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	1B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

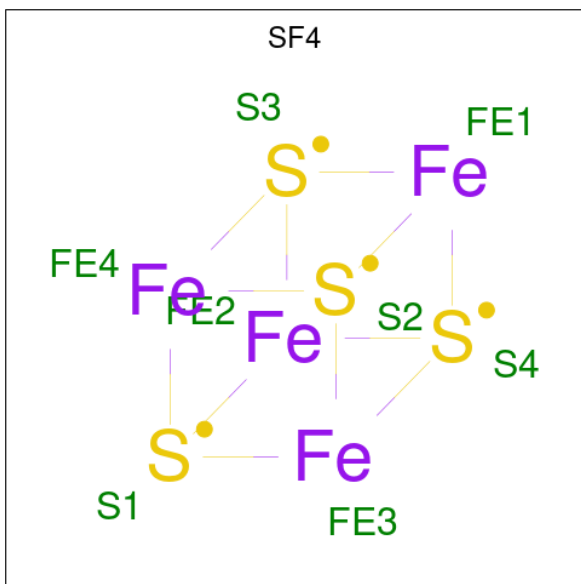
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		
60	29	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1d	1	Total Fe S 8 4 4	0	0
61	2d	1	Total Fe S 8 4 4	0	0

- Molecule 62 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2A	1	Total K 1 1	0	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1A	1632	Total O 1632 1632	0	0
63	1B	50	Total O 50 50	0	0
63	1D	20	Total O 20 20	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1E	17	Total O 17 17	0	0
63	1F	14	Total O 14 14	0	0
63	1G	5	Total O 5 5	0	0
63	1H	4	Total O 4 4	0	0
63	1N	7	Total O 7 7	0	0
63	1O	2	Total O 2 2	0	0
63	1P	18	Total O 18 18	0	0
63	1Q	5	Total O 5 5	0	0
63	1R	7	Total O 7 7	0	0
63	1T	4	Total O 4 4	0	0
63	1U	3	Total O 3 3	0	0
63	1V	3	Total O 3 3	0	0
63	1X	6	Total O 6 6	0	0
63	1Y	2	Total O 2 2	0	0
63	10	4	Total O 4 4	0	0
63	11	3	Total O 3 3	0	0
63	13	6	Total O 6 6	0	0
63	15	2	Total O 2 2	0	0
63	16	3	Total O 3 3	0	0
63	18	7	Total O 7 7	0	0
63	19	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1a	369	Total 369	O 369	0	0
63	1c	1	Total 1	O 1	0	0
63	1d	6	Total 6	O 6	0	0
63	1e	3	Total 3	O 3	0	0
63	1f	1	Total 1	O 1	0	0
63	1h	1	Total 1	O 1	0	0
63	1l	3	Total 3	O 3	0	0
63	1m	1	Total 1	O 1	0	0
63	1n	1	Total 1	O 1	0	0
63	1o	2	Total 2	O 2	0	0
63	1p	1	Total 1	O 1	0	0
63	1t	1	Total 1	O 1	0	0
63	1x	2	Total 2	O 2	0	0
63	2A	1221	Total 1221	O 1221	0	0
63	2B	33	Total 33	O 33	0	0
63	2D	13	Total 13	O 13	0	0
63	2E	12	Total 12	O 12	0	0
63	2F	4	Total 4	O 4	0	0
63	2N	2	Total 2	O 2	0	0
63	2O	4	Total 4	O 4	0	0
63	2P	7	Total 7	O 7	0	0

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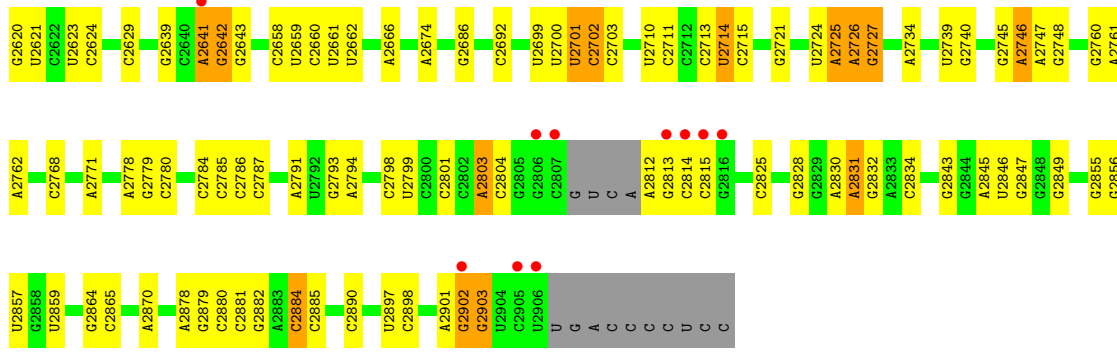
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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63	2R	2	Total 2	O 2	0	0
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63	2U	3	Total 3	O 3	0	0
63	2X	4	Total 4	O 4	0	0
63	2Y	1	Total 1	O 1	0	0
63	20	2	Total 2	O 2	0	0
63	21	2	Total 2	O 2	0	0
63	23	2	Total 2	O 2	0	0
63	25	1	Total 1	O 1	0	0
63	26	2	Total 2	O 2	0	0
63	28	5	Total 5	O 5	0	0
63	2a	305	Total 305	O 305	0	0
63	2d	3	Total 3	O 3	0	0
63	2e	1	Total 1	O 1	0	0
63	2j	2	Total 2	O 2	0	0
63	2l	1	Total 1	O 1	0	0
63	2n	1	Total 1	O 1	0	0
63	2p	1	Total 1	O 1	0	0
63	2r	1	Total 1	O 1	0	0
63	2t	1	Total 1	O 1	0	0

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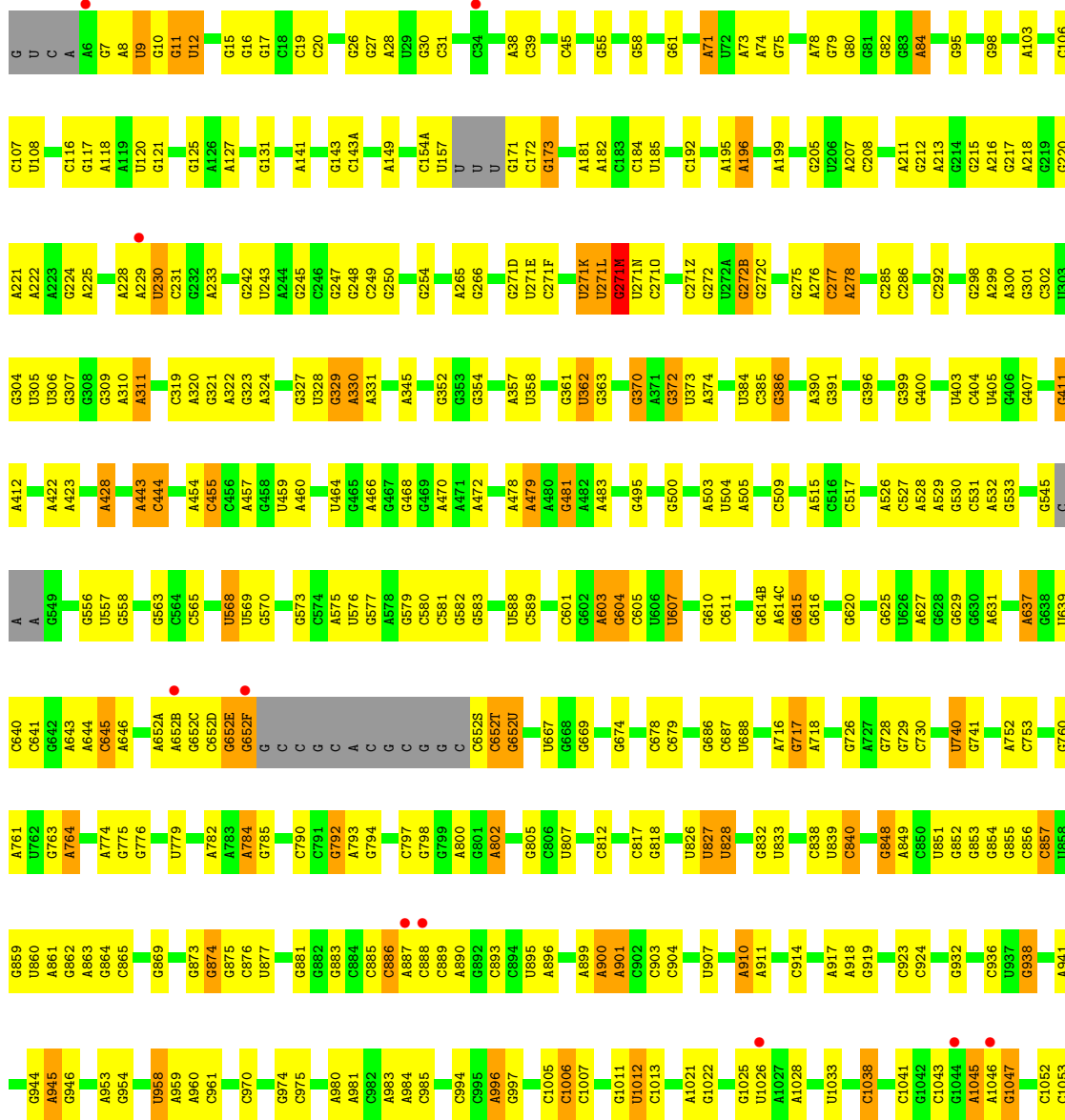
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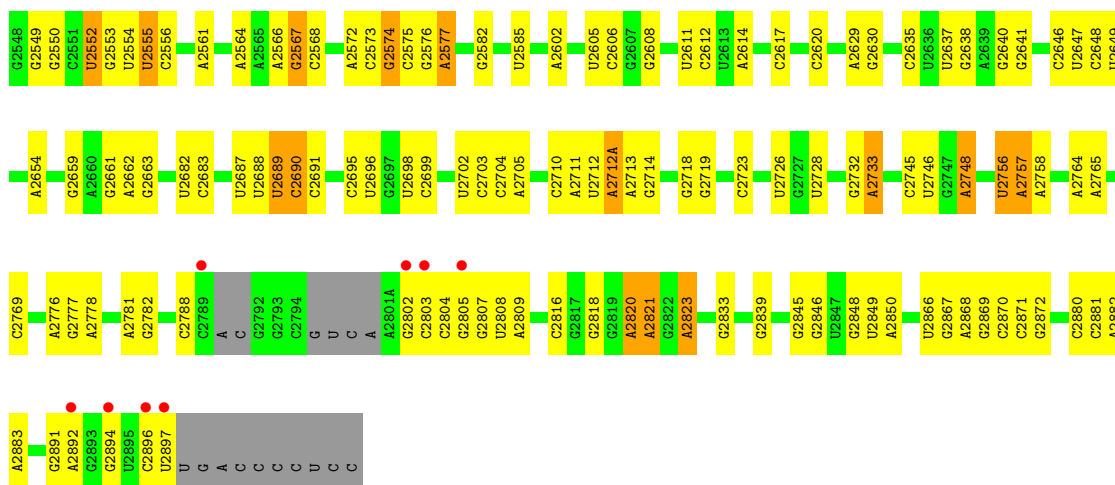
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	2x	2	Total O 2 2	0	0
63	A	1	Total O 1 1	0	0

A	A	A	U	G	C	U	C	A	C1150	C1151	C1152	C1153	C1154	C1155	C1156	C1157	C1158	C1159	C1160	C1161	C1162	C1170	C1171	C1174	C1175	C1176	C1180	C1181	C1184	C1185	C1186	C1187	C1188	C1195	C1199	C1200	C1201	C1202	C1211	C1212	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1231						
U1233	U1234	C1245	C1246	C1247	C1248	C1255	C1256	C1263	C1277	C1281	C1282	C1285	C1286	C1290	C1299	C1302	C1303	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1321	C1324	C1325	C1335	C1338	C1339	C1340	C1341	C1342	C1346	C1347	C1348	C1356	C1359	C1360															
C1361	C1362	C1363	C1367	C1378	C1386	C1387	C1388	C1389	C1390	C1391	C1398	C1399	C1400	C1401	C1404	C1405	C1406	C1411	C1414	C1415	C1416	C1417	C1418	C1425	C1426	C1430	C1431	C1432	C1433	C1438	C1441	C1442	C1451	C1452	C1458	C1459	C1462	C1463	C1464	C1465	C1466	C1467	C1471	C1472												
C1473	C1474	C1475	C1476	C1481	C1482	C1483	C1491	C1492	C1495	C1496	C1497	C1500	C1501	C1502	C1506	C1507	C1514	C1518	C1521	C1522	C1525	C1529	C1532	C1533	C1539	C1540	C1541	C1542	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1700										
A1575	C1579	G	U	A	C	G1584	G1585	G1586	G1587	G1588	A1589	C1594	C1595	C1596	C1597	C1604	A1605	A1613	A1616	U1625	U1626	C1629	A1630	A1632	G1639	G1640	C1653	A1654	A1655	A1656	A1662	G1668	G1682	C1683	U1686	C1687	A1688	G1689	G1690	C1691	C1695	A1699	G1700													
A1701	C1704	C1705	C1710	A1711	A1712	A1715	A1716	G1721	G1725	A1736	A1737	G1743	A1747	A1748	G1749	G1750	G1751	G1752	U1753	A1759	A1766	U1767	U1768	G1769	A1770	G1771	G1781	C1785	A1786	G1788	G1794	G1795	A1804	C1805	G1809	A1811	C1812	C1813	A1814	A1817																
A1821	G1822	G1823	U1829	G1830	G1831	A1833	A1834	C1835	U1836	A1841	G1842	A1846	G1847	G1854	G1857	C1858	G1859	G1870	G1873	G1874	G1875	G1876	G1877	G1878	G1889	A1890	G1893	G1894	U1895	G1896	C1897	A1898	A1899	G1900	C1901	G1904	G1905	A1911	G1921	C1922	A1925	G1926	C1927	G1928												
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C2207	C2208	C2209	C2210	U2211	C2212	C2213	C2214	A2220	A2221	C2222	C2226	G2227	C2228	A2229	U2230	C2231	C2232	C2235	C2236	A2237	C2238	A2239	G2240	U2244	U2245	C2246	C2250	C2251	C2252	A2253	C2254	U2255	U2256	U2257	C2258	A2259	C2263	A2280	A2281	A2285	A2286	G2289	A2290	C2291	C2295	C2296	C2297	A2298	A2299							
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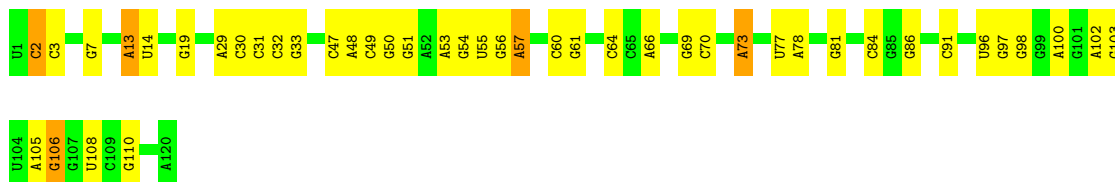


• Molecule 1: 23s ribosomal RNA





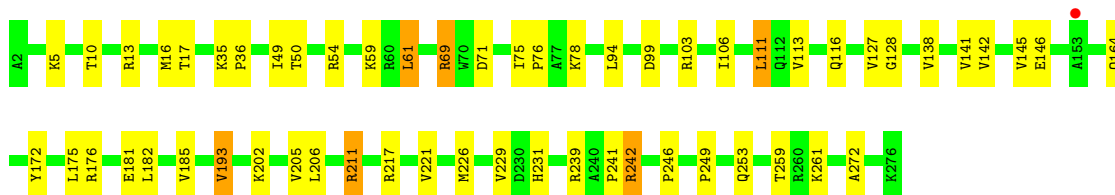
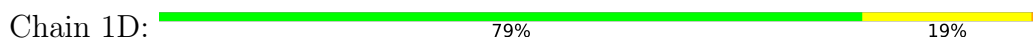
• Molecule 2: 5s ribosomal RNA



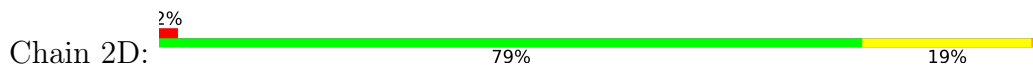
• Molecule 2: 5s ribosomal RNA

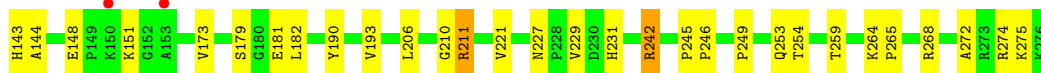


• Molecule 3: 50S ribosomal protein L2

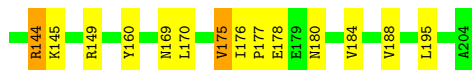
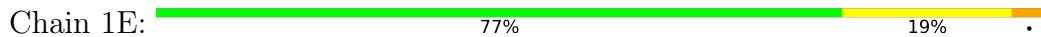


• Molecule 3: 50S ribosomal protein L2

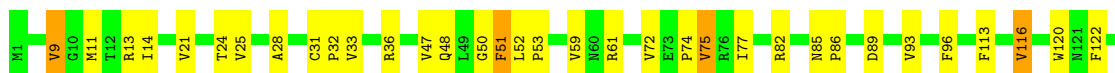
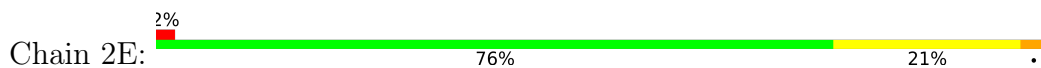




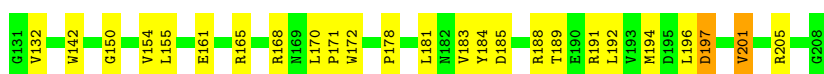
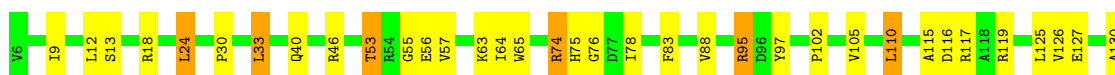
- Molecule 4: 50S ribosomal protein L3



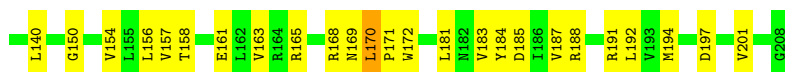
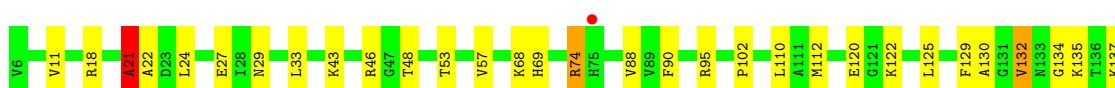
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

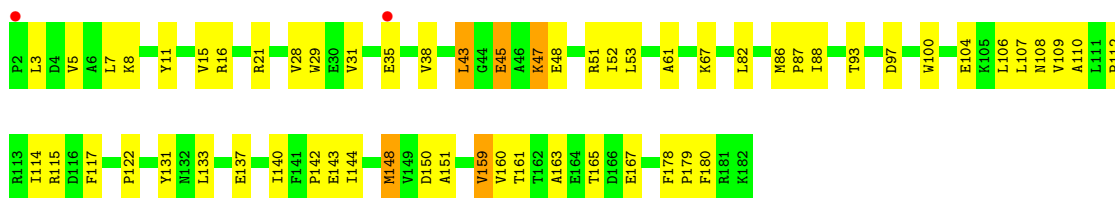


- Molecule 5: 50S ribosomal protein L4

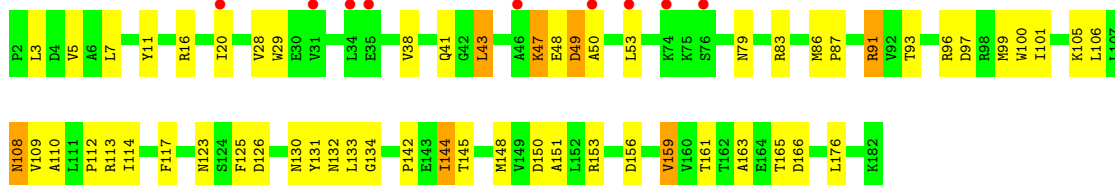


- Molecule 6: 50S ribosomal protein L5

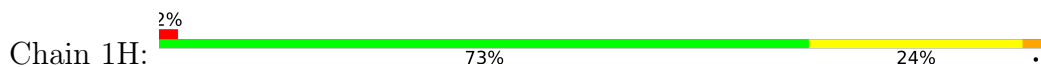




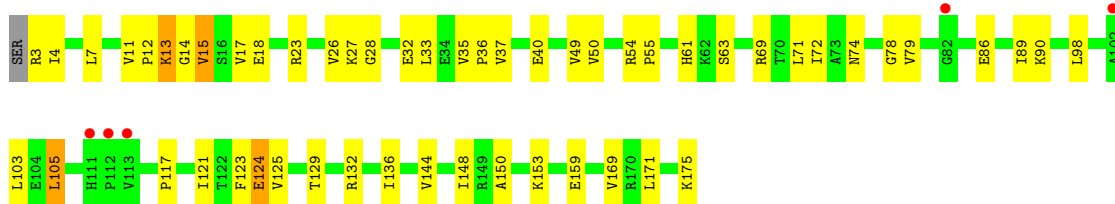
- Molecule 6: 50S ribosomal protein L5



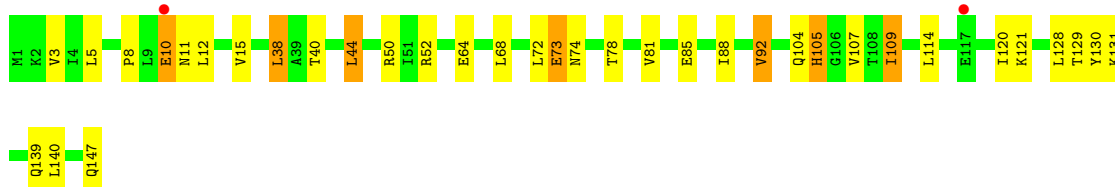
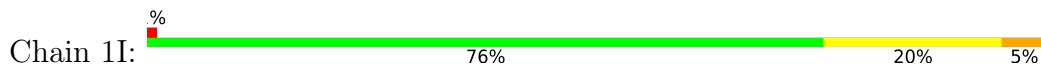
- Molecule 7: 50S ribosomal protein L6



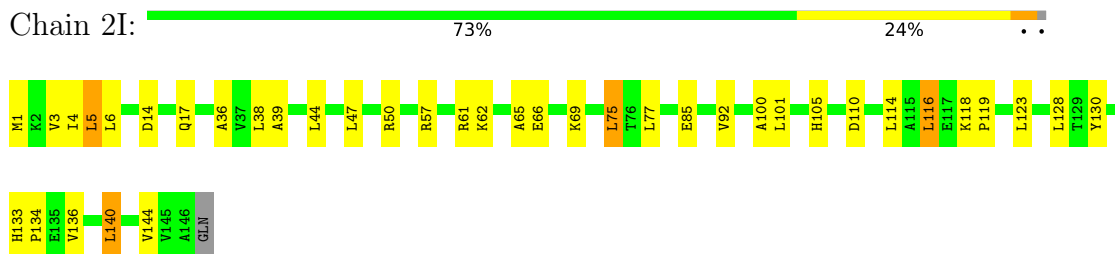
- Molecule 7: 50S ribosomal protein L6



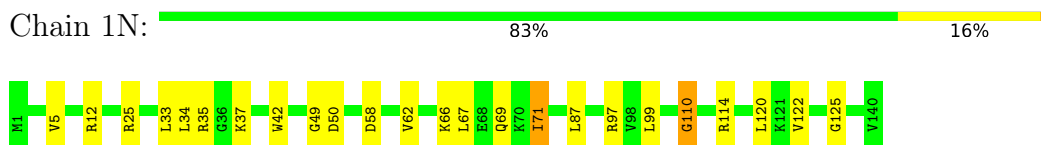
- Molecule 8: 50S ribosomal protein L9



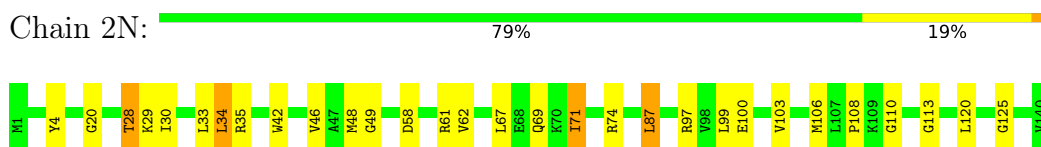
- Molecule 8: 50S ribosomal protein L9



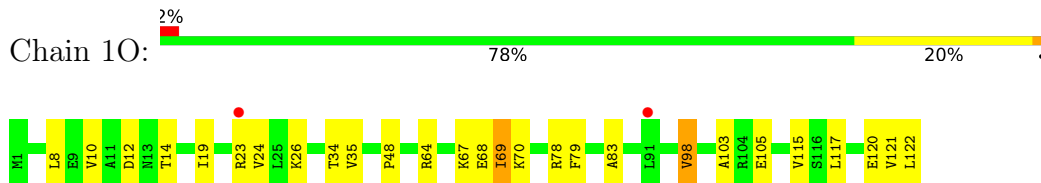
- Molecule 9: 50S ribosomal protein L13



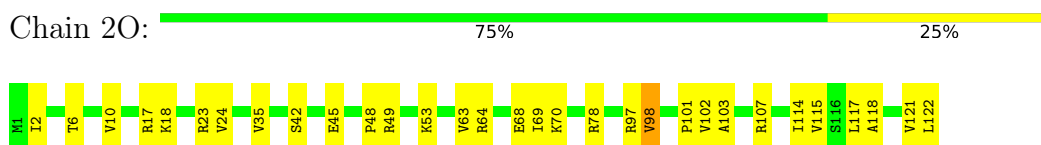
- Molecule 9: 50S ribosomal protein L13



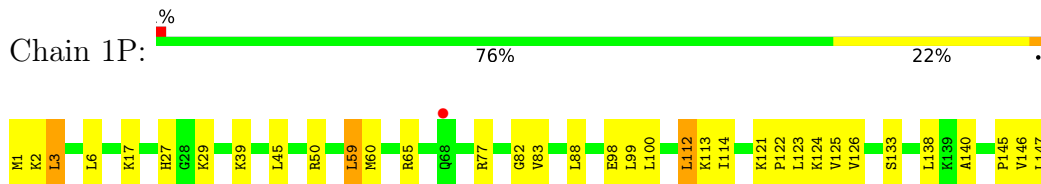
- Molecule 10: 50S ribosomal protein L14



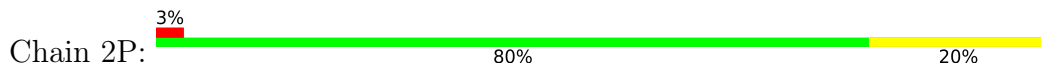
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15

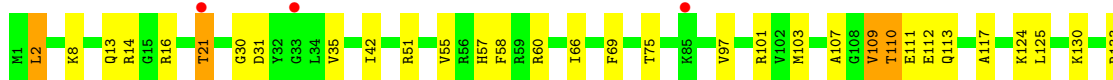
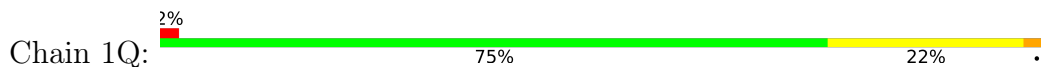


- Molecule 11: 50S ribosomal protein L15

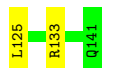
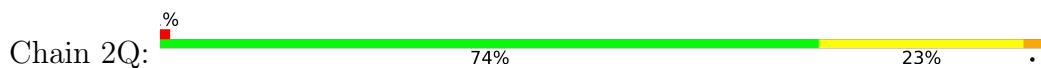




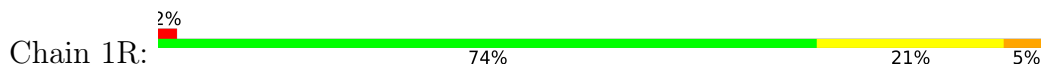
• Molecule 12: 50S ribosomal protein L16



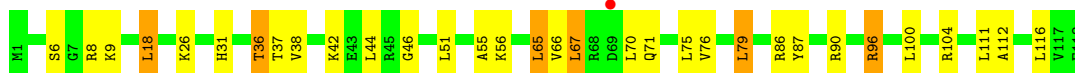
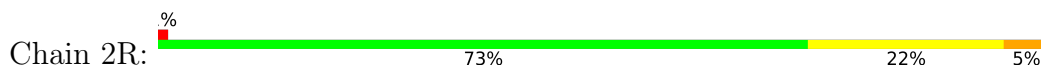
• Molecule 12: 50S ribosomal protein L16



• Molecule 13: 50S ribosomal protein L17



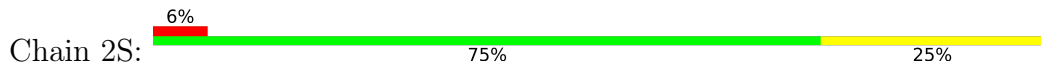
• Molecule 13: 50S ribosomal protein L17

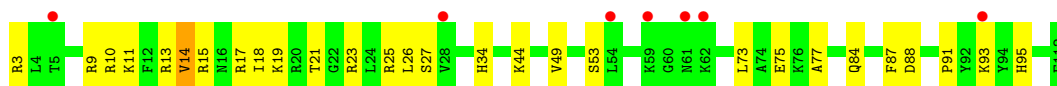


• Molecule 14: 50S ribosomal protein L18

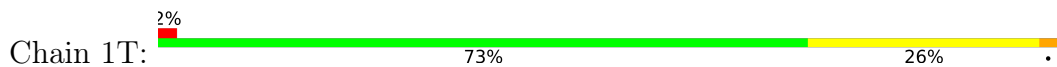


• Molecule 14: 50S ribosomal protein L18

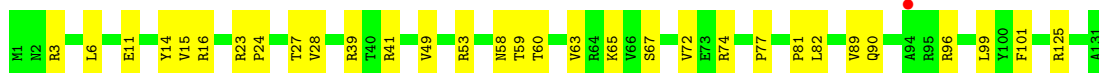
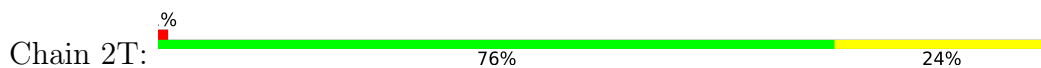




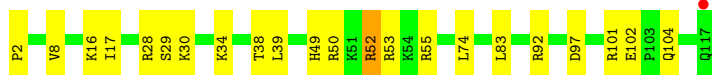
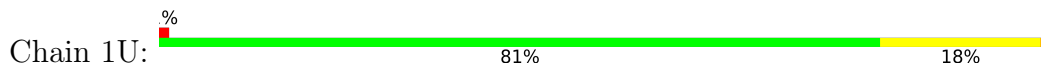
- Molecule 15: 50S ribosomal protein L19



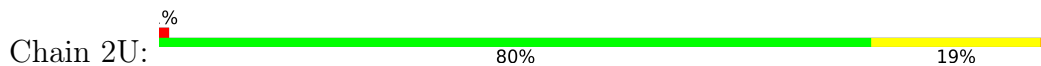
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



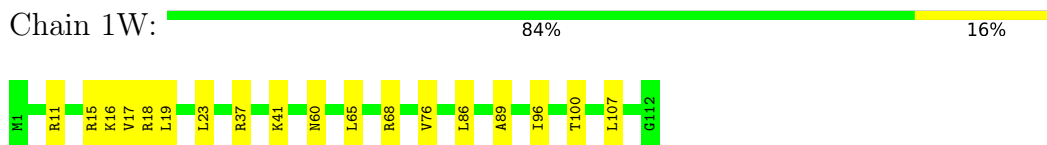
- Molecule 17: 50S ribosomal protein L21



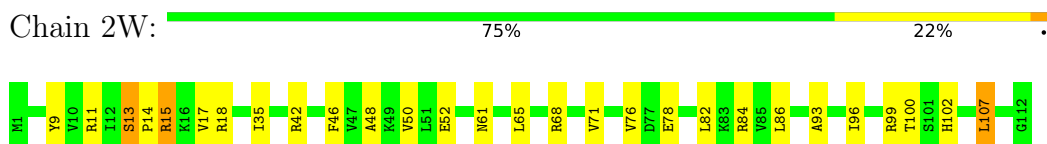
- Molecule 17: 50S ribosomal protein L21



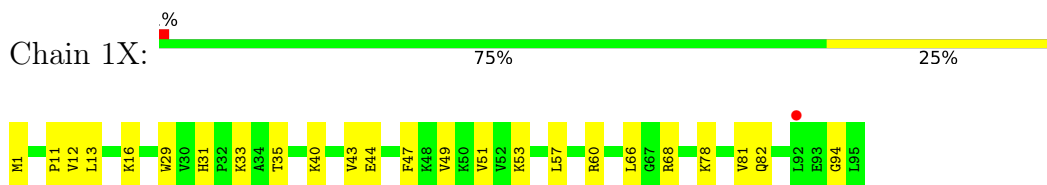
- Molecule 18: 50S ribosomal protein L22



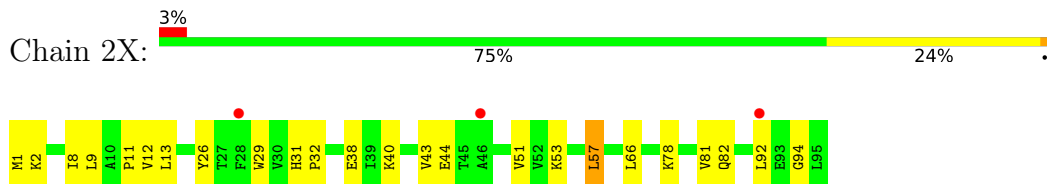
- Molecule 18: 50S ribosomal protein L22



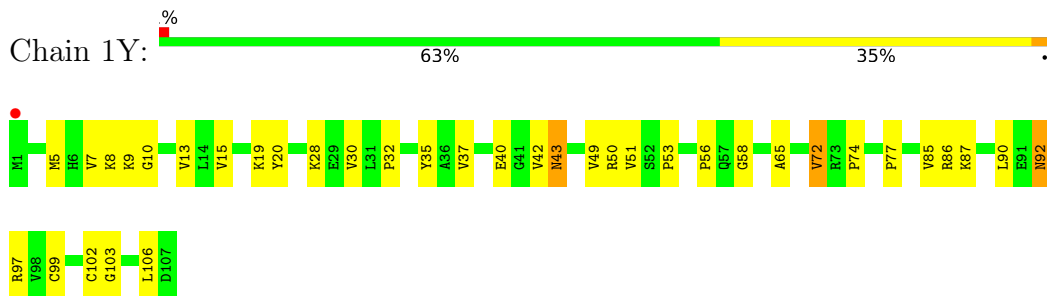
- Molecule 19: 50S ribosomal protein L23



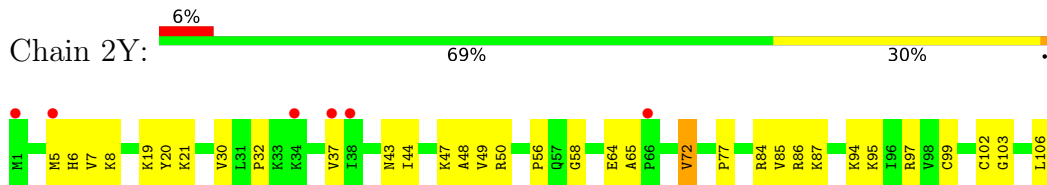
- Molecule 19: 50S ribosomal protein L23



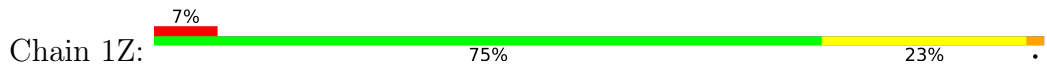
- Molecule 20: 50S ribosomal protein L24

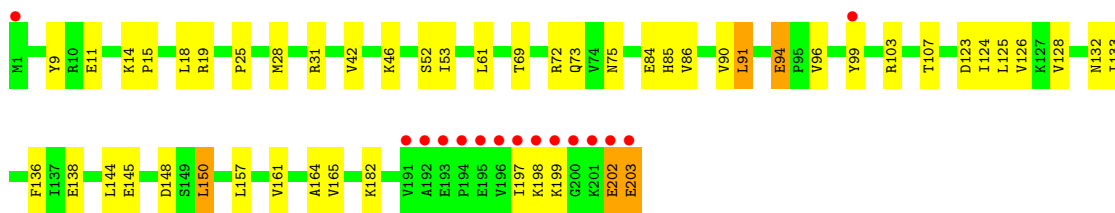


- Molecule 20: 50S ribosomal protein L24

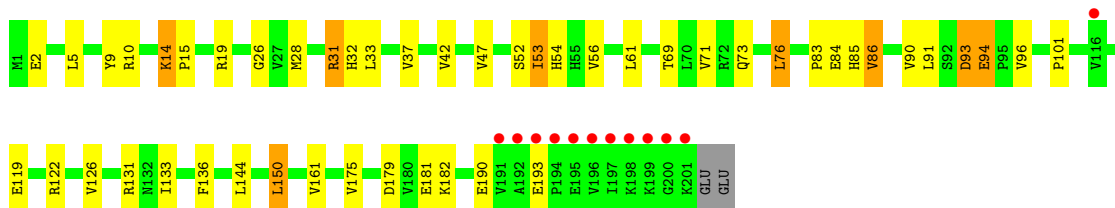
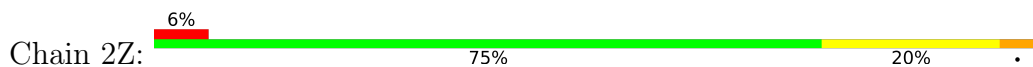


- Molecule 21: 50S ribosomal protein L25

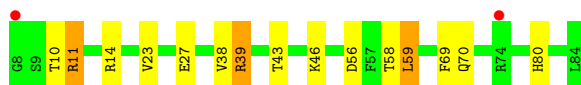
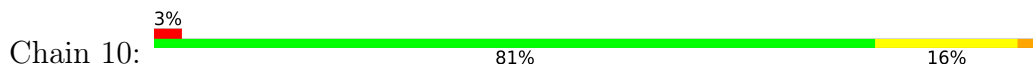




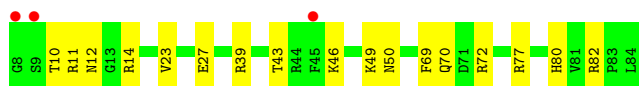
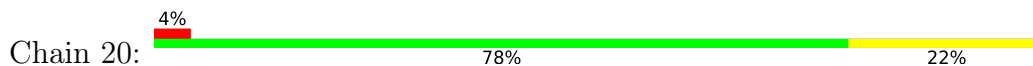
● Molecule 21: 50S ribosomal protein L25



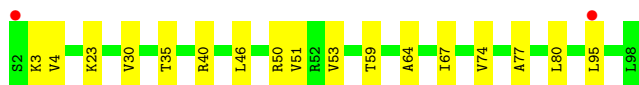
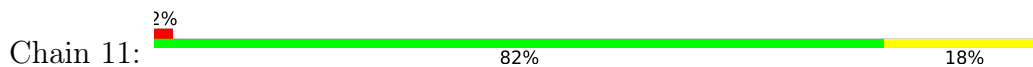
● Molecule 22: 50S ribosomal protein L27



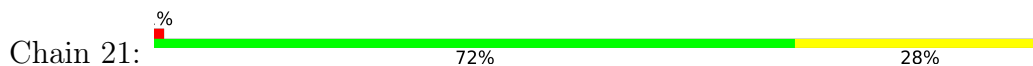
● Molecule 22: 50S ribosomal protein L27



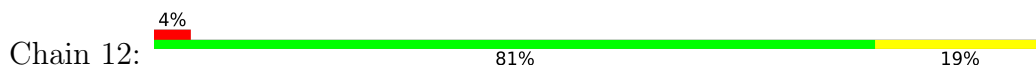
● Molecule 23: 50S ribosomal protein L28



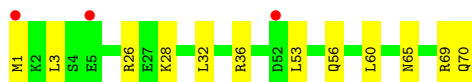
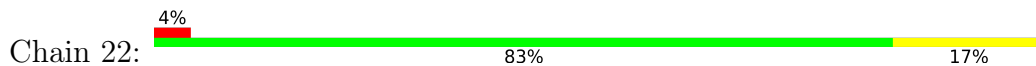
● Molecule 23: 50S ribosomal protein L28



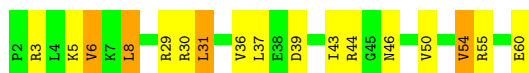
● Molecule 24: 50S ribosomal protein L29



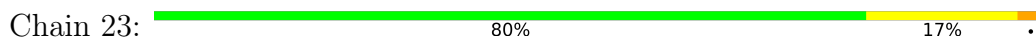
- Molecule 24: 50S ribosomal protein L29



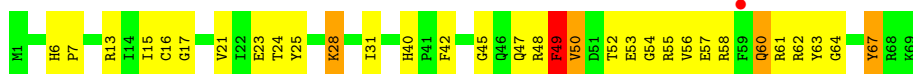
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



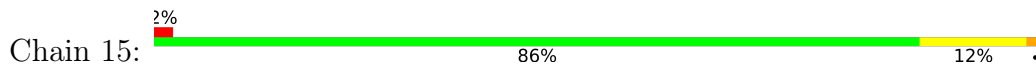
- Molecule 26: 50S ribosomal protein L31



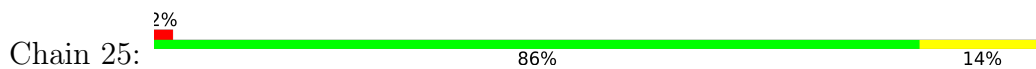
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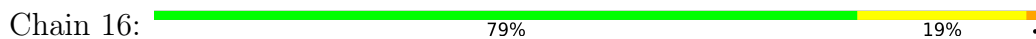
- Molecule 27: 50S ribosomal protein L32



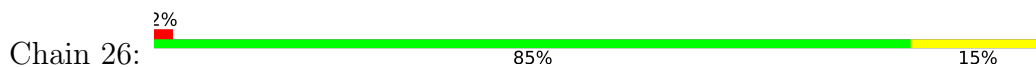
- Molecule 27: 50S ribosomal protein L32



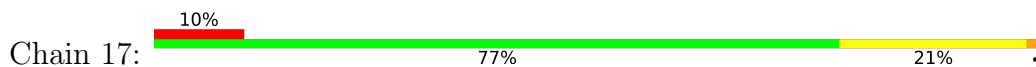
- Molecule 28: 50S ribosomal protein L33



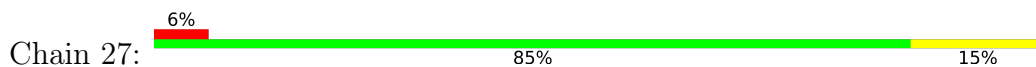
- Molecule 28: 50S ribosomal protein L33



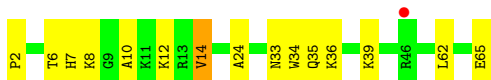
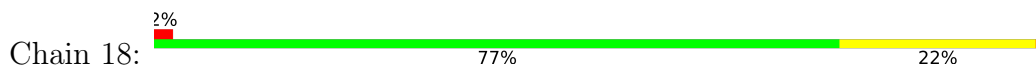
- Molecule 29: 50S ribosomal protein L34



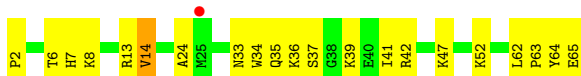
- Molecule 29: 50S ribosomal protein L34



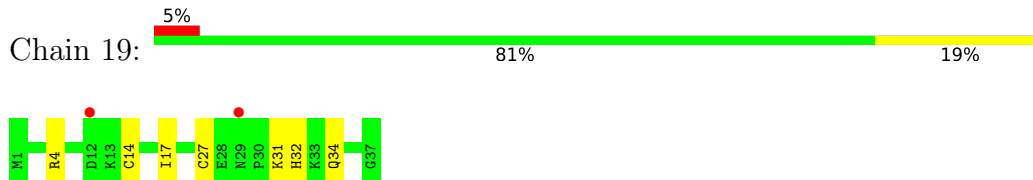
- Molecule 30: 50S ribosomal protein L35



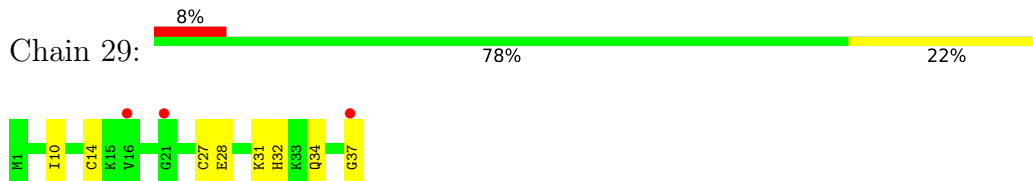
- Molecule 30: 50S ribosomal protein L35



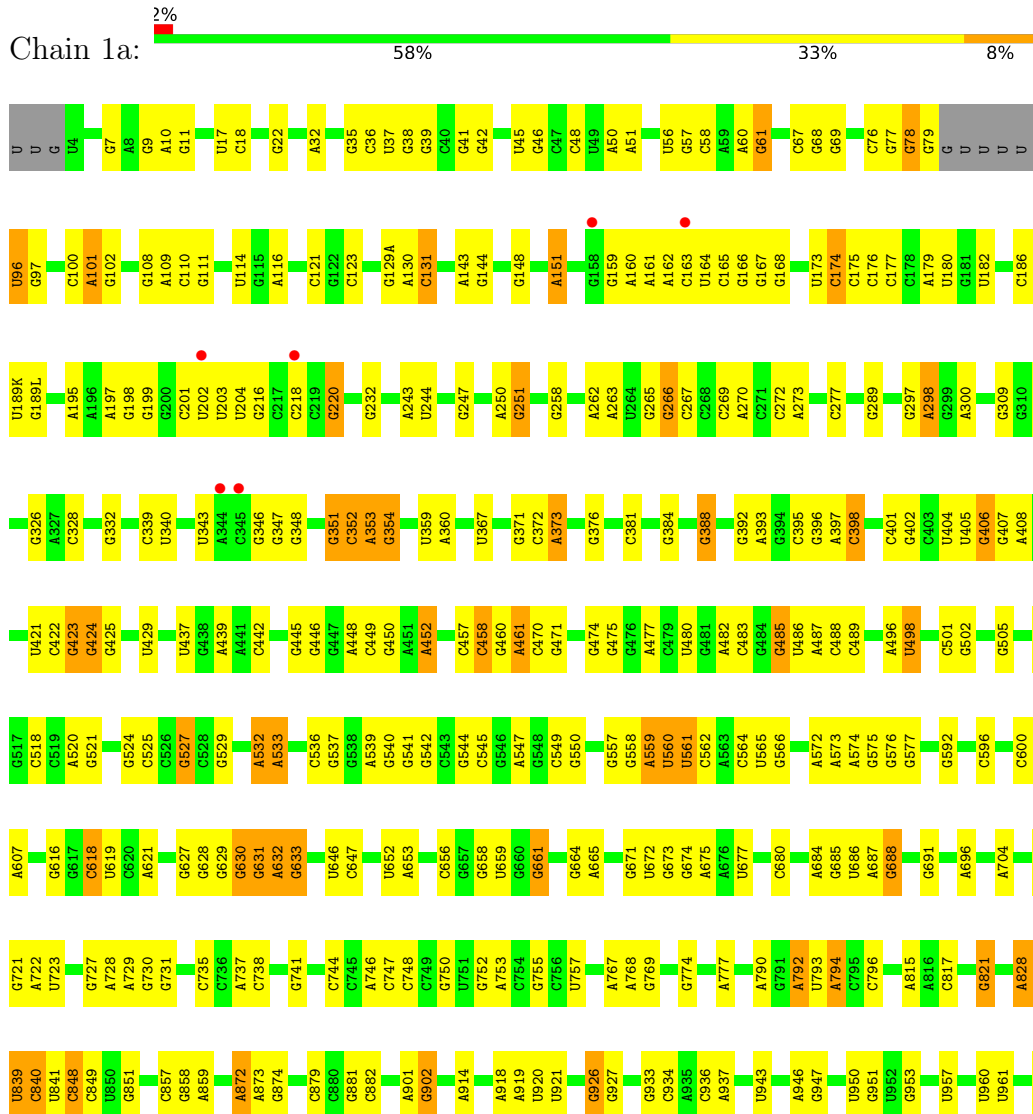
• Molecule 31: 50S ribosomal protein L36

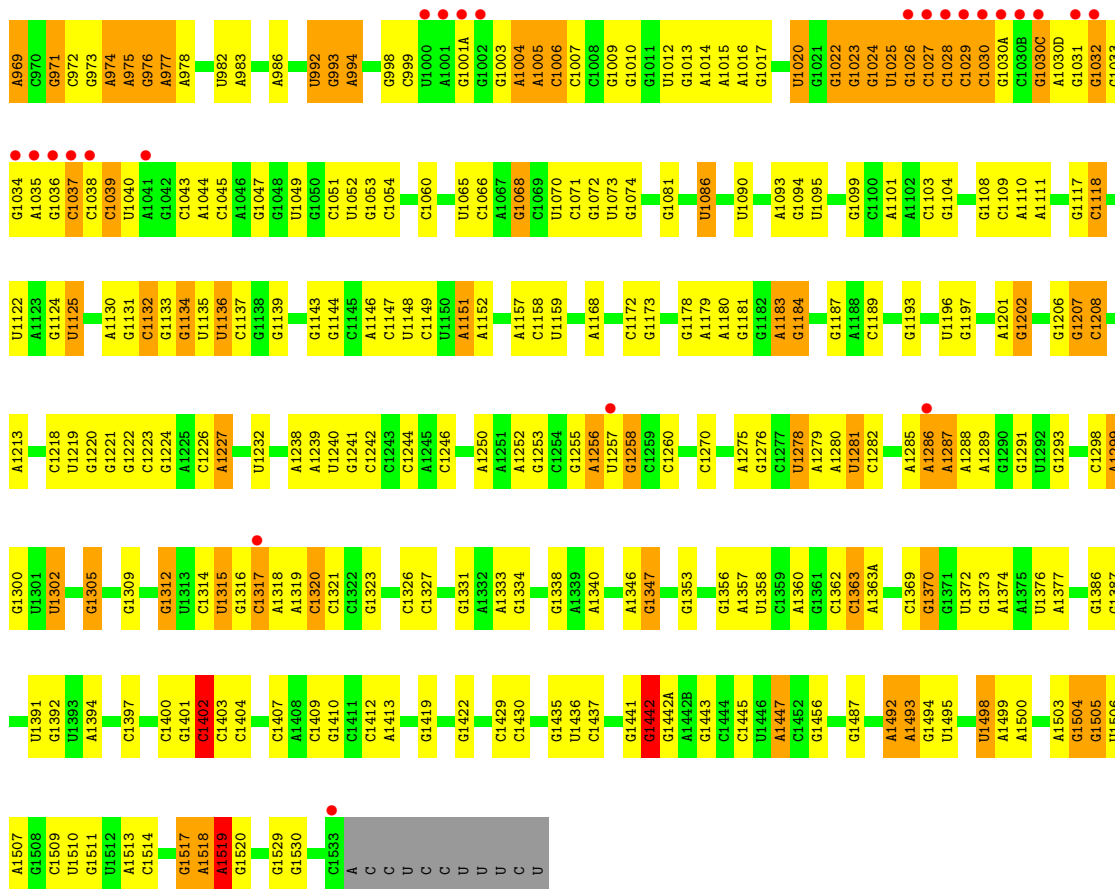


• Molecule 31: 50S ribosomal protein L36

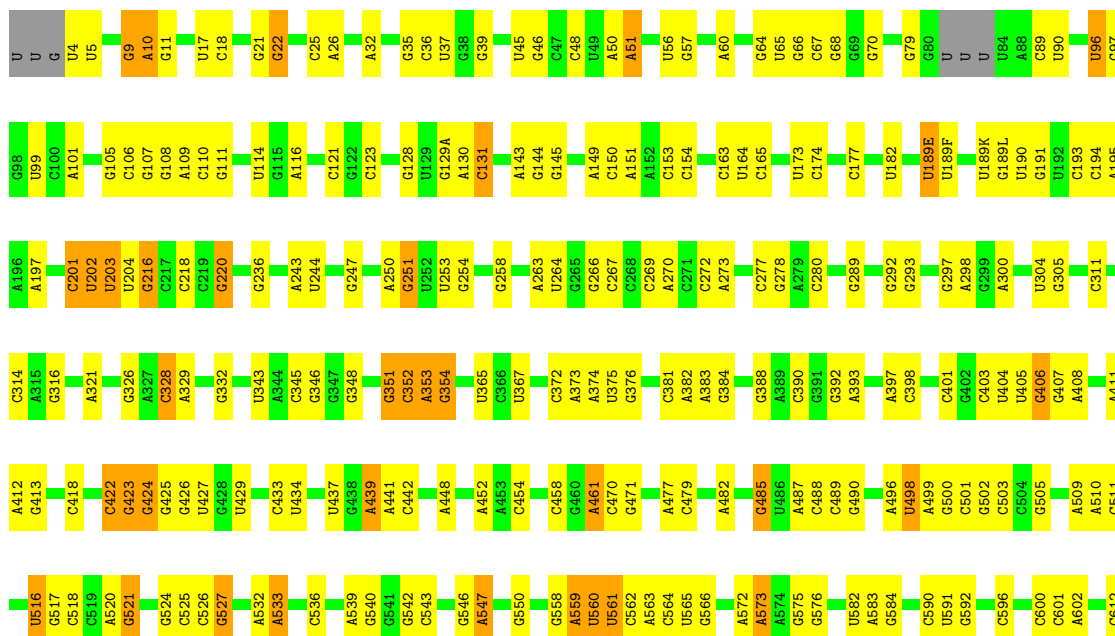


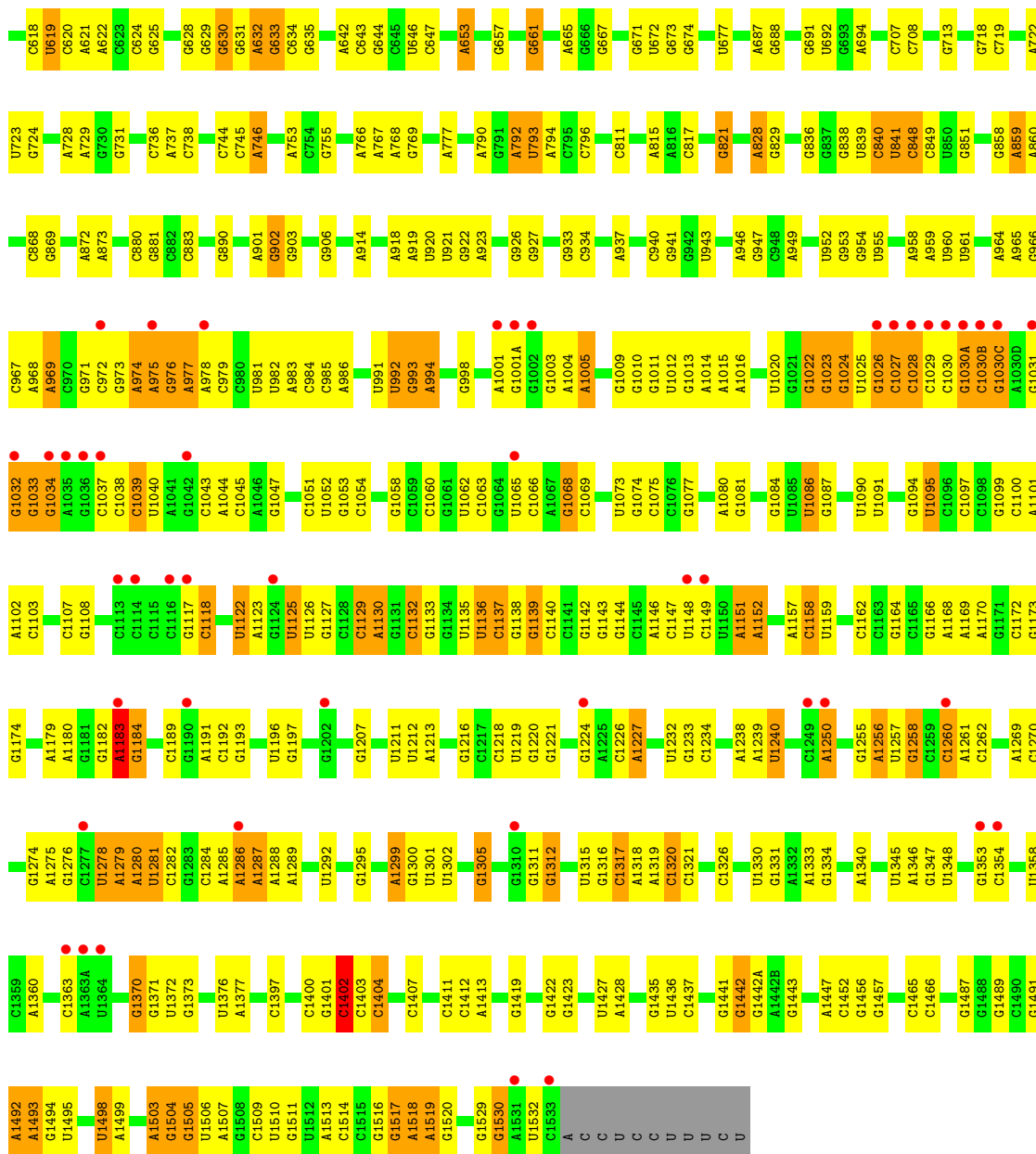
• Molecule 32: 16s ribosomal RNA



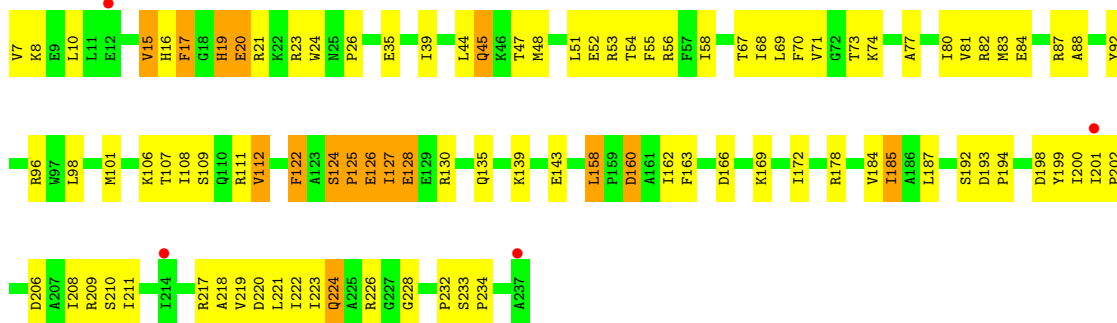


• Molecule 32: 16s ribosomal RNA

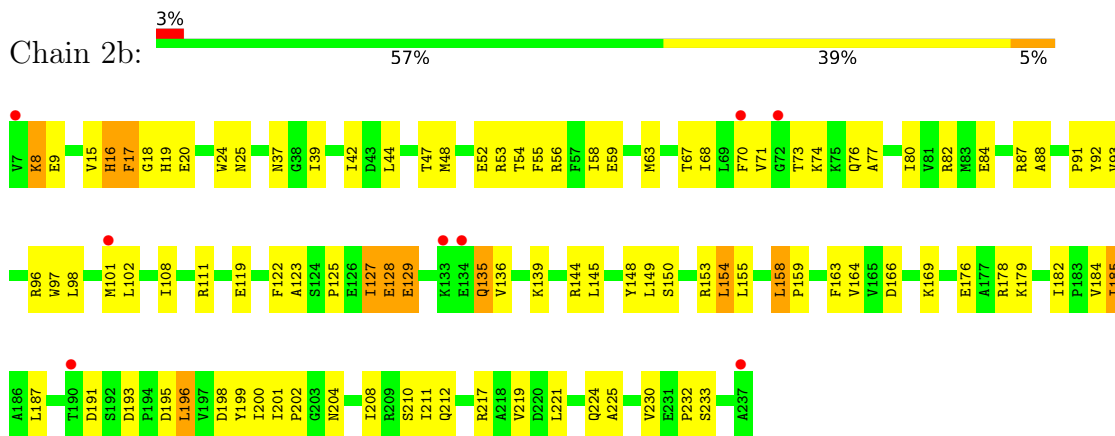




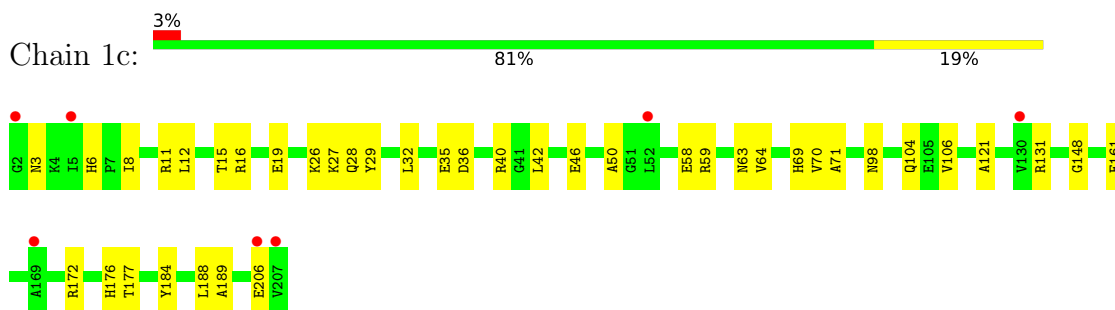
• Molecule 33: 30S ribosomal protein S2



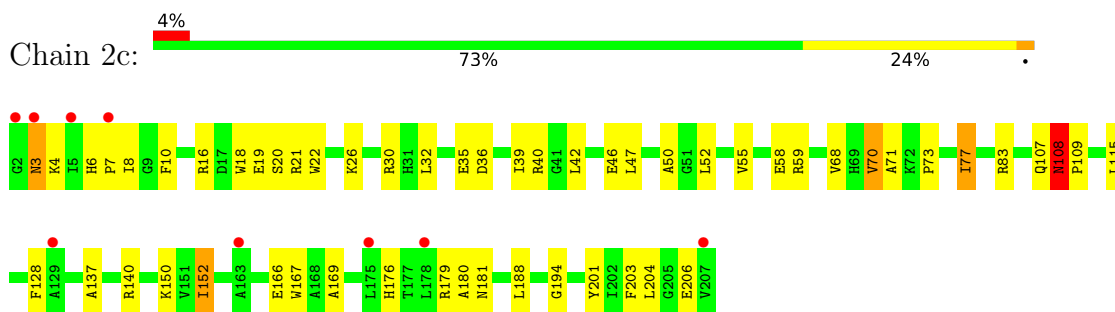
- Molecule 33: 30S ribosomal protein S2



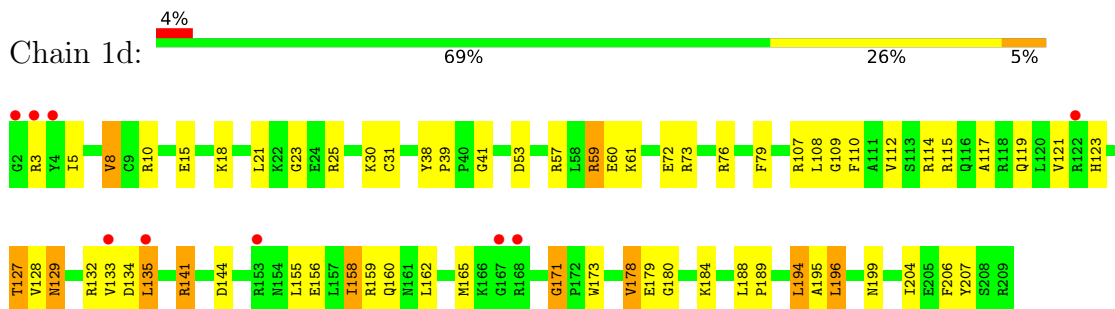
- Molecule 34: 30S ribosomal protein S3



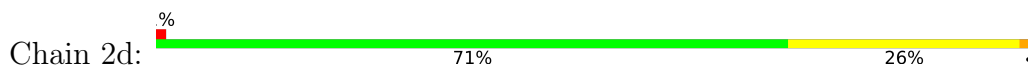
- Molecule 34: 30S ribosomal protein S3

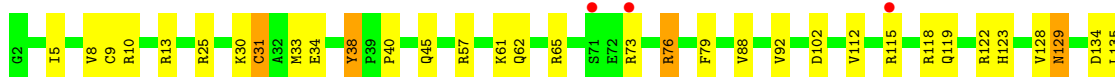


- Molecule 35: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S4

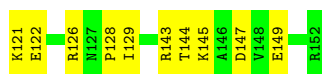
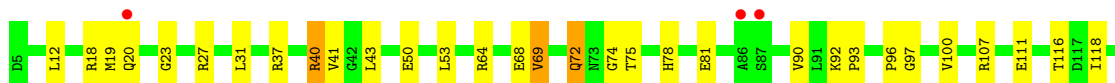
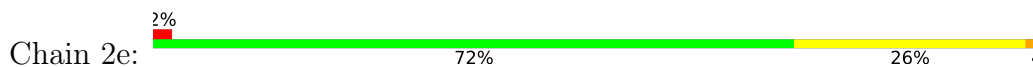




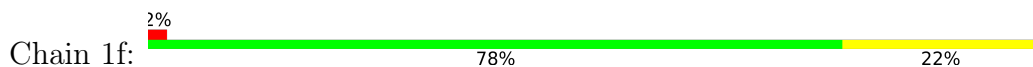
- Molecule 36: 30S ribosomal protein S5



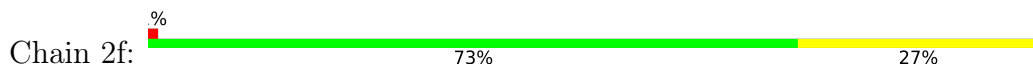
- Molecule 36: 30S ribosomal protein S5



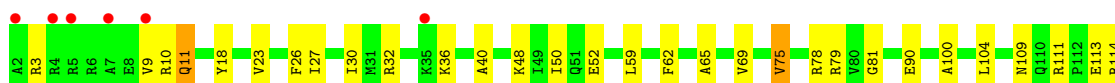
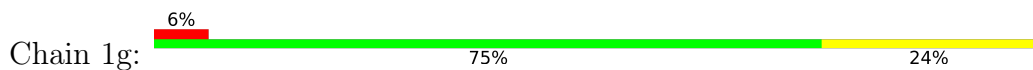
- Molecule 37: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S6

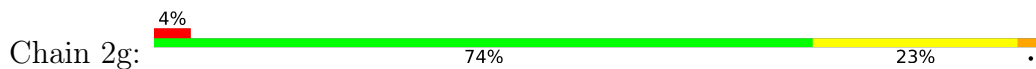


- Molecule 38: 30S ribosomal protein S7

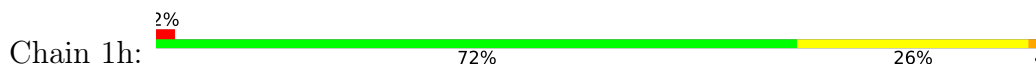




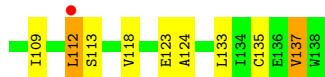
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8



- Molecule 39: 30S ribosomal protein S8

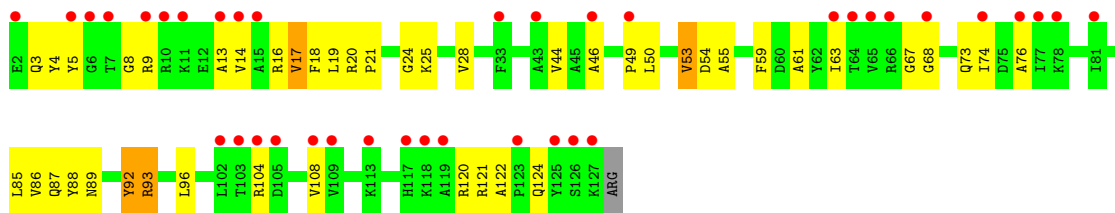


- Molecule 40: 30S ribosomal protein S9

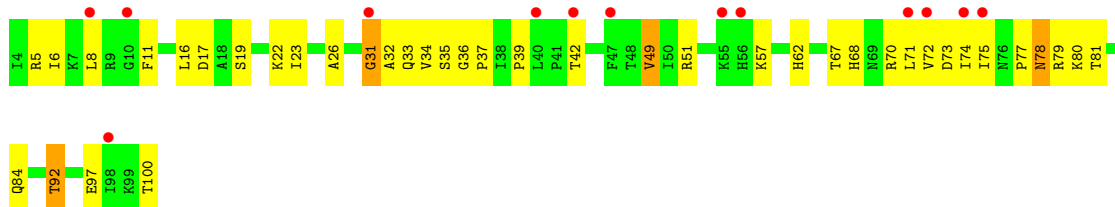


- Molecule 40: 30S ribosomal protein S9

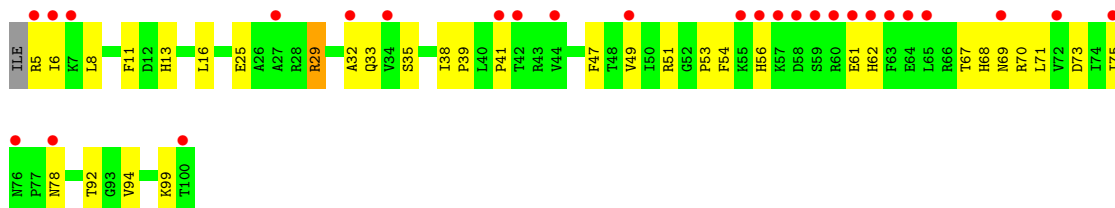




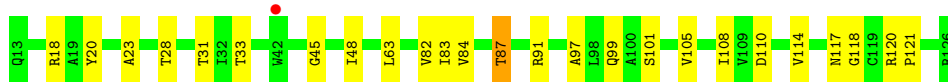
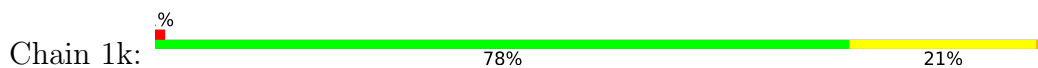
● Molecule 41: 30S ribosomal protein S10



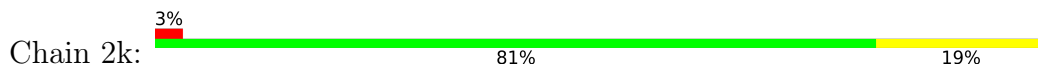
● Molecule 41: 30S ribosomal protein S10



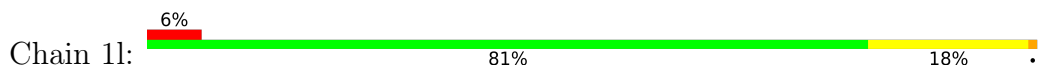
● Molecule 42: 30S ribosomal protein S11



● Molecule 42: 30S ribosomal protein S11

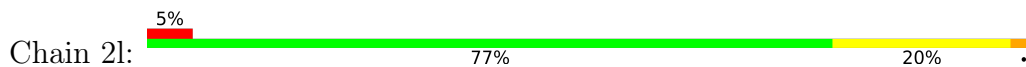


● Molecule 43: 30S ribosomal protein S12

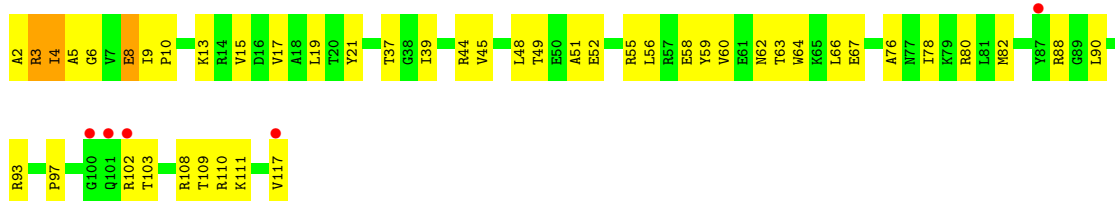




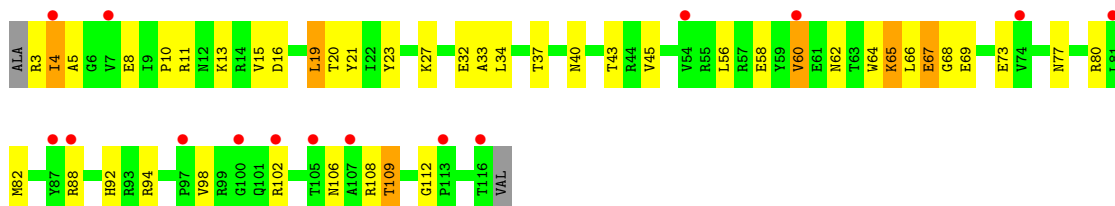
- Molecule 43: 30S ribosomal protein S12



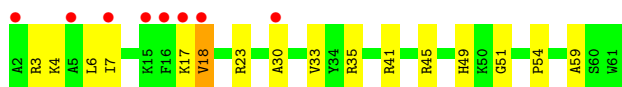
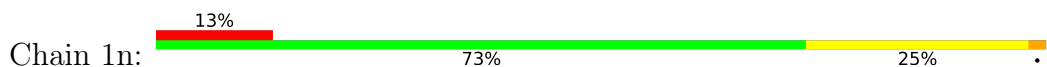
- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13



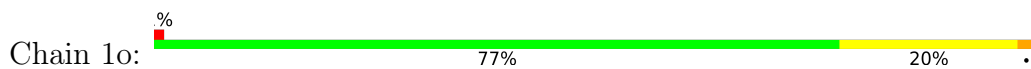
- Molecule 45: 30S ribosomal protein S14 type Z



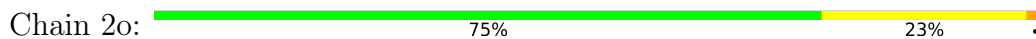
- Molecule 45: 30S ribosomal protein S14 type Z



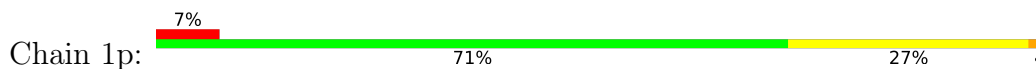
- Molecule 46: 30S ribosomal protein S15



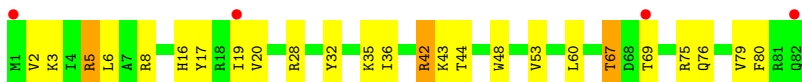
- Molecule 46: 30S ribosomal protein S15



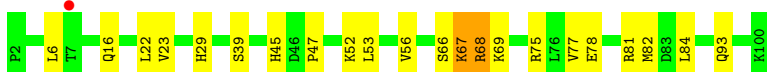
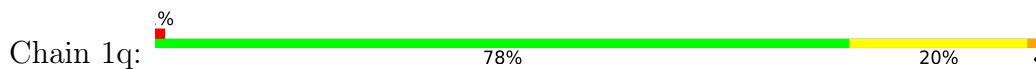
- Molecule 47: 30S ribosomal protein S16



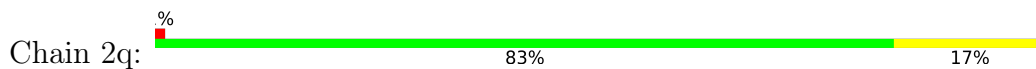
- Molecule 47: 30S ribosomal protein S16



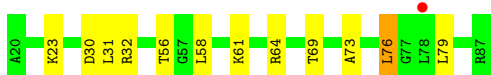
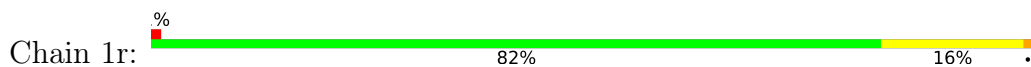
- Molecule 48: 30S ribosomal protein S17



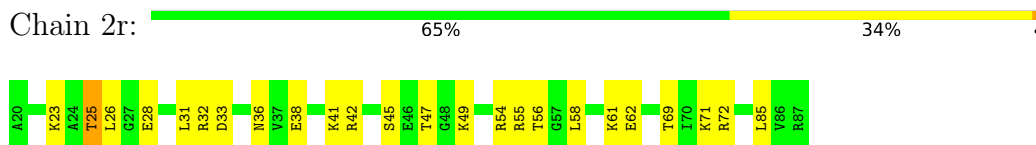
- Molecule 48: 30S ribosomal protein S17



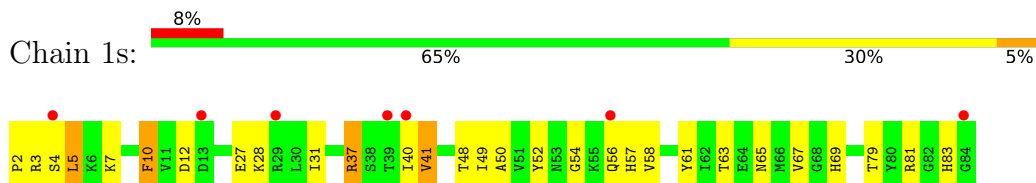
- Molecule 49: 30S ribosomal protein S18



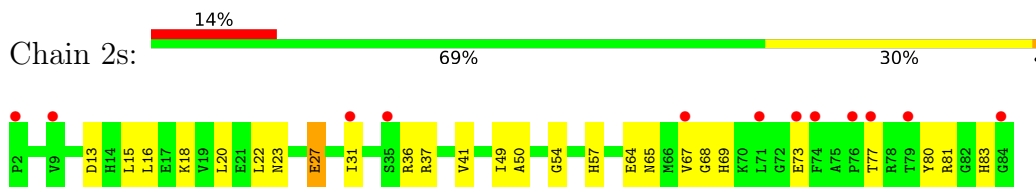
- Molecule 49: 30S ribosomal protein S18



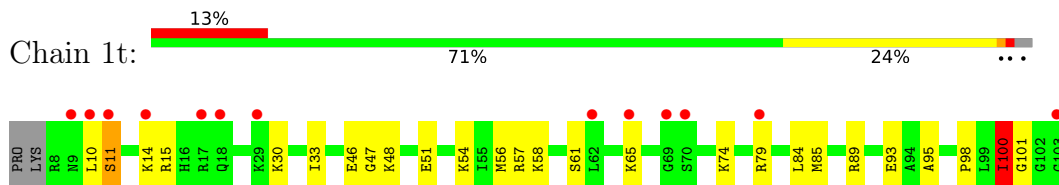
- Molecule 50: 30S ribosomal protein S19



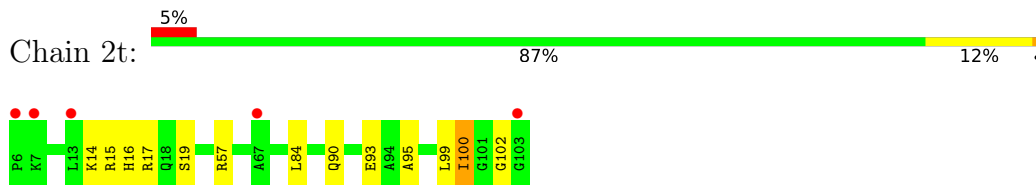
- Molecule 50: 30S ribosomal protein S19



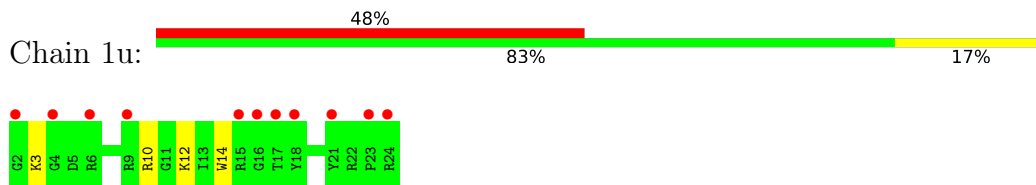
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

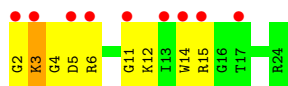


- Molecule 52: 30S ribosomal protein Thx

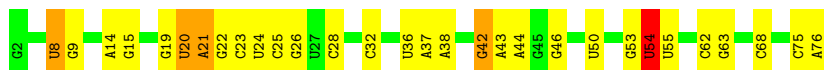


- Molecule 52: 30S ribosomal protein Thx





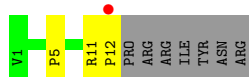
• Molecule 53: tRNA met



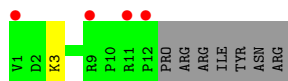
• Molecule 53: tRNA met



• Molecule 54: Onc112



• Molecule 54: Onc112



• Molecule 55: mRNA



• Molecule 55: mRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.30Å 452.29Å 625.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.10 49.72 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.72-3.10) 99.0 (49.72-3.10)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.12Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.231 , 0.271 0.230 , 0.269	Depositor DCC
R_{free} test set	52535 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtrriage
Anisotropy	0.244	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	293672	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ZN, 2MG, MA6, 0TD, OMU, OMG, MG, 4OC, OMC, K, M2G, G7M, PSU, UR3, 5MU, MPD, SF4, 5MC, UNX, 4SU, 2MA

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	0.25	1/67879 (0.0%)	0.39	4/105953 (0.0%)
1	2A	0.19	1/68951 (0.0%)	0.36	2/107627 (0.0%)
2	1B	0.23	0/2876	0.49	0/4486
2	2B	0.19	0/2878	0.34	0/4490
3	1D	0.42	0/2181	0.84	0/2940
3	2D	0.37	0/2186	0.84	1/2944 (0.0%)
4	1E	0.42	0/1592	0.86	4/2149 (0.2%)
4	2E	0.37	0/1592	0.87	1/2149 (0.0%)
5	1F	0.42	0/1619	0.82	2/2193 (0.1%)
5	2F	0.36	0/1615	0.86	2/2188 (0.1%)
6	1G	0.35	0/1451	0.84	2/1961 (0.1%)
6	2G	0.36	0/1449	0.85	1/1957 (0.1%)
7	1H	0.40	0/1356	0.90	5/1834 (0.3%)
7	2H	0.38	0/1350	0.93	5/1826 (0.3%)
8	1I	0.38	0/1109	0.87	0/1512
8	2I	0.36	0/1091	0.85	2/1490 (0.1%)
9	1N	0.39	0/1148	0.84	4/1547 (0.3%)
9	2N	0.33	0/1144	0.88	4/1543 (0.3%)
10	1O	0.44	0/943	0.80	0/1269
10	2O	0.38	0/943	0.80	0/1269
11	1P	0.42	0/1152	0.79	0/1533
11	2P	0.32	0/1152	0.79	0/1533
12	1Q	0.42	0/1143	0.77	0/1527
12	2Q	0.34	0/1143	0.73	0/1527
13	1R	0.43	0/982	0.76	0/1312
13	2R	0.36	0/982	0.72	0/1312
14	1S	0.36	0/887	0.83	1/1180 (0.1%)
14	2S	0.33	0/880	0.86	0/1172
15	1T	0.41	0/1105	0.82	0/1477
15	2T	0.33	0/1097	0.80	0/1468
16	1U	0.46	0/977	0.80	2/1301 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.35	0/977	0.78	1/1301 (0.1%)
17	1V	0.39	0/786	0.76	0/1053
17	2V	0.33	0/782	0.79	0/1049
18	1W	0.47	0/897	0.81	0/1205
18	2W	0.38	0/897	0.79	2/1205 (0.2%)
19	1X	0.41	0/764	0.78	0/1025
19	2X	0.33	0/764	0.78	0/1025
20	1Y	0.40	0/823	0.80	1/1099 (0.1%)
20	2Y	0.31	0/823	0.79	0/1100
21	1Z	0.38	0/1620	0.91	6/2200 (0.3%)
21	2Z	0.35	0/1590	0.89	3/2162 (0.1%)
22	10	0.39	0/616	0.81	0/821
22	20	0.34	0/616	0.89	5/821 (0.6%)
23	11	0.38	0/761	0.77	0/1013
23	21	0.36	0/766	0.79	0/1018
24	12	0.39	0/590	0.77	0/781
24	22	0.30	0/594	0.74	0/785
25	13	0.41	0/474	0.77	0/635
25	23	0.31	0/469	0.78	0/630
26	14	0.38	0/559	0.99	6/754 (0.8%)
26	24	0.47	0/549	1.03	6/741 (0.8%)
27	15	0.46	0/473	0.72	0/639
27	25	0.39	0/469	0.74	0/635
28	16	0.36	0/460	0.69	0/613
28	26	0.32	0/456	0.69	0/608
29	17	0.45	0/426	0.81	0/561
29	27	0.38	0/426	0.77	0/561
30	18	0.41	0/525	0.74	0/691
30	28	0.35	0/525	0.72	0/691
31	19	0.38	0/310	0.78	0/407
31	29	0.31	0/310	0.77	0/407
32	1a	0.19	1/35795 (0.0%)	0.37	2/55864 (0.0%)
32	2a	0.19	0/35890	0.36	1/56012 (0.0%)
33	1b	0.35	0/1876	0.94	6/2533 (0.2%)
33	2b	0.37	0/1860	0.89	7/2518 (0.3%)
34	1c	0.36	0/1582	0.84	0/2137
34	2c	0.38	0/1566	0.88	3/2119 (0.1%)
35	1d	0.37	0/1695	0.88	6/2274 (0.3%)
35	2d	0.34	0/1698	0.84	2/2277 (0.1%)
36	1e	0.34	0/1149	0.85	3/1548 (0.2%)
36	2e	0.34	0/1149	0.87	3/1548 (0.2%)
37	1f	0.32	0/827	0.77	2/1120 (0.2%)
37	2f	0.34	0/829	0.78	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.32	0/1254	0.83	0/1683
38	2g	0.33	0/1248	0.82	0/1676
39	1h	0.32	0/1118	0.84	3/1506 (0.2%)
39	2h	0.30	0/1108	0.82	0/1494
40	1i	0.37	0/1005	0.82	0/1351
40	2i	0.40	0/985	0.83	0/1329
41	1j	0.40	0/732	0.96	2/993 (0.2%)
41	2j	0.42	0/723	0.90	0/984
42	1k	0.36	0/849	0.76	0/1150
42	2k	0.38	0/848	0.87	1/1149 (0.1%)
43	1l	0.33	0/937	0.80	0/1260
43	2l	0.34	0/937	0.85	2/1260 (0.2%)
44	1m	0.33	0/924	0.84	1/1242 (0.1%)
44	2m	0.39	0/905	0.88	3/1217 (0.2%)
45	1n	0.32	0/501	0.77	0/664
45	2n	0.32	0/501	0.77	0/664
46	1o	0.34	0/739	0.80	0/985
46	2o	0.33	0/739	0.81	0/985
47	1p	0.36	0/697	0.78	0/939
47	2p	0.34	0/693	0.80	0/935
48	1q	0.31	0/836	0.81	3/1117 (0.3%)
48	2q	0.29	0/836	0.79	2/1117 (0.2%)
49	1r	0.34	0/560	0.78	0/746
49	2r	0.34	0/560	0.74	0/746
50	1s	0.35	0/663	0.88	1/895 (0.1%)
50	2s	0.38	0/660	0.91	1/893 (0.1%)
51	1t	0.33	0/734	0.86	1/969 (0.1%)
51	2t	0.34	0/736	0.81	0/976
52	1u	0.32	0/203	0.85	0/266
52	2u	0.35	0/203	0.80	0/266
53	1x	0.25	0/1725	0.45	0/2689
53	2x	0.25	1/1725 (0.1%)	0.43	0/2689
54	1y	0.41	0/106	1.01	0/146
54	2y	0.39	0/106	1.10	0/146
55	A	0.27	0/72	0.42	0/110
55	B	0.24	0/72	0.38	0/110
All	All	0.27	4/311106 (0.0%)	0.54	127/465325 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	O3'-P	5.15	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2564	OMU	O3'-P	5.13	1.61	1.56
32	1a	1498	UR3	O3'-P	5.09	1.61	1.56
53	2x	8	4SU	O3'-P	5.09	1.61	1.56

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1099	C	OP1-P-O3'	-11.84	72.47	108.00
1	1A	1099	C	OP2-P-O3'	-10.78	75.67	108.00
1	1A	1100	A	OP1-P-OP2	8.46	144.98	119.60
50	2s	67	VAL	N-CA-C	7.46	117.54	110.53
35	1d	38	TYR	CA-C-N	7.20	124.92	119.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	60842	0	30688	535	0
1	2A	61801	0	31173	620	0
2	1B	2572	0	1305	33	0
2	2B	2573	0	1306	28	0
3	1D	2131	0	2207	41	0
3	2D	2136	0	2218	46	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	33	0
5	1F	1584	0	1625	38	0
5	2F	1580	0	1619	34	0
6	1G	1426	0	1445	32	0
6	2G	1424	0	1441	37	0
7	1H	1330	0	1407	32	0
7	2H	1324	0	1402	31	0
8	1I	1094	0	1127	23	0
8	2I	1076	0	1094	23	0
9	1N	1121	0	1194	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	2N	1117	0	1184	20	0
10	1O	933	0	996	21	0
10	2O	933	0	996	23	0
11	1P	1135	0	1212	23	0
11	2P	1135	0	1212	18	0
12	1Q	1122	0	1179	23	0
12	2Q	1122	0	1179	25	0
13	1R	968	0	1033	19	0
13	2R	968	0	1033	20	0
14	1S	877	0	938	24	0
14	2S	870	0	923	22	0
15	1T	1091	0	1151	20	0
15	2T	1083	0	1136	20	0
16	1U	959	0	1019	13	0
16	2U	959	0	1019	12	0
17	1V	775	0	841	13	0
17	2V	771	0	829	13	0
18	1W	886	0	940	8	0
18	2W	886	0	940	19	0
19	1X	750	0	814	19	0
19	2X	750	0	814	14	0
20	1Y	810	0	892	25	0
20	2Y	810	0	887	23	0
21	1Z	1587	0	1598	34	0
21	2Z	1557	0	1564	30	0
22	10	608	0	622	10	0
22	20	608	0	622	10	0
23	11	754	0	823	10	0
23	21	759	0	837	17	0
24	12	588	0	643	11	0
24	22	592	0	654	7	0
25	13	469	0	518	12	0
25	23	464	0	514	7	0
26	14	546	0	522	23	0
26	24	536	0	514	22	0
27	15	459	0	476	6	0
27	25	455	0	465	6	0
28	16	453	0	473	8	0
28	26	449	0	469	6	0
29	17	418	0	467	10	0
29	27	418	0	467	6	0
30	18	517	0	582	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	28	517	0	582	16	0
31	19	307	0	335	4	0
31	29	307	0	335	6	0
32	1a	32246	0	16294	395	0
32	2a	32331	0	16338	423	0
33	1b	1842	0	1862	60	0
33	2b	1825	0	1828	66	0
34	1c	1558	0	1557	23	0
34	2c	1542	0	1517	34	0
35	1d	1665	0	1687	49	0
35	2d	1668	0	1703	53	0
36	1e	1133	0	1191	26	0
36	2e	1133	0	1191	30	0
37	1f	814	0	808	14	0
37	2f	816	0	808	23	0
38	1g	1235	0	1249	25	0
38	2g	1229	0	1238	24	0
39	1h	1098	0	1143	26	0
39	2h	1088	0	1126	31	0
40	1i	986	0	990	30	0
40	2i	966	0	953	33	0
41	1j	719	0	672	25	0
41	2j	710	0	661	26	0
42	1k	834	0	838	14	0
42	2k	833	0	836	11	0
43	1l	932	0	981	14	0
43	2l	932	0	981	18	0
44	1m	914	0	954	29	0
44	2m	895	0	920	27	0
45	1n	492	0	529	14	0
45	2n	492	0	529	24	0
46	1o	728	0	760	15	0
46	2o	728	0	760	15	0
47	1p	681	0	697	15	0
47	2p	677	0	686	15	0
48	1q	823	0	891	12	0
48	2q	823	0	891	10	0
49	1r	555	0	618	10	0
49	2r	555	0	618	21	0
50	1s	648	0	658	24	0
50	2s	645	0	635	22	0
51	1t	732	0	809	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	2t	733	0	795	6	0
52	1u	199	0	208	3	0
52	2u	199	0	208	6	0
53	1x	1625	0	829	24	0
53	2x	1625	0	829	17	0
54	1y	101	0	109	2	0
54	2y	101	0	109	1	0
55	A	65	0	33	4	0
55	B	65	0	33	4	0
56	10	7	0	0	0	0
56	11	3	0	0	0	0
56	13	3	0	0	0	0
56	15	3	0	0	0	0
56	17	2	0	0	0	0
56	18	1	0	0	0	0
56	19	2	0	0	0	0
56	1A	946	0	0	0	0
56	1B	29	0	0	0	0
56	1D	21	0	0	0	0
56	1E	6	0	0	0	0
56	1F	9	0	0	0	0
56	1G	4	0	0	0	0
56	1H	2	0	0	0	0
56	1N	3	0	0	0	0
56	1O	1	0	0	0	0
56	1P	2	0	0	0	0
56	1Q	4	0	0	0	0
56	1R	4	0	0	0	0
56	1T	2	0	0	0	0
56	1U	5	0	0	0	0
56	1V	3	0	0	0	0
56	1W	3	0	0	0	0
56	1X	1	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	1	0	0	0	0
56	1a	261	0	0	0	0
56	1b	1	0	0	0	0
56	1d	4	0	0	0	0
56	1e	4	0	0	0	0
56	1f	1	0	0	0	0
56	1g	1	0	0	0	0
56	1i	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1l	1	0	0	0	0
56	1n	1	0	0	0	0
56	1o	2	0	0	0	0
56	1r	1	0	0	0	0
56	1t	1	0	0	0	0
56	1x	12	0	0	0	0
56	20	1	0	0	0	0
56	21	1	0	0	0	0
56	23	1	0	0	0	0
56	28	2	0	0	0	0
56	2A	679	0	0	0	0
56	2B	17	0	0	0	0
56	2D	8	0	0	0	0
56	2E	7	0	0	0	0
56	2F	3	0	0	0	0
56	2G	2	0	0	0	0
56	2I	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	2	0	0	0	0
56	2R	1	0	0	0	0
56	2T	4	0	0	0	0
56	2U	2	0	0	0	0
56	2V	3	0	0	0	0
56	2W	1	0	0	0	0
56	2X	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2a	183	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2j	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	1	0	0	0	0
56	2n	1	0	0	0	0
56	2p	1	0	0	0	0
56	2q	1	0	0	0	0
56	2t	1	0	0	0	0
56	2x	10	0	0	0	0
57	1A	1	0	0	0	0
57	2A	1	0	0	0	0
58	1A	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1a	8	0	14	0	0
59	1B	12	0	12	1	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	2A	1	0	0	0	0
63	10	4	0	0	0	0
63	11	3	0	0	0	0
63	13	6	0	0	1	0
63	15	2	0	0	0	0
63	16	3	0	0	0	0
63	18	7	0	0	0	0
63	19	3	0	0	1	0
63	1A	1632	0	0	8	0
63	1B	50	0	0	0	0
63	1D	20	0	0	0	0
63	1E	17	0	0	0	0
63	1F	14	0	0	1	0
63	1G	5	0	0	0	0
63	1H	4	0	0	0	0
63	1N	7	0	0	0	0
63	1O	2	0	0	0	0
63	1P	18	0	0	0	0
63	1Q	5	0	0	0	0
63	1R	7	0	0	1	0
63	1T	4	0	0	0	0
63	1U	3	0	0	0	0
63	1V	3	0	0	0	0
63	1X	6	0	0	0	0
63	1Y	2	0	0	0	0
63	1a	369	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	1c	1	0	0	0	0
63	1d	6	0	0	0	0
63	1e	3	0	0	0	0
63	1f	1	0	0	0	0
63	1h	1	0	0	0	0
63	1l	3	0	0	0	0
63	1m	1	0	0	0	0
63	1n	1	0	0	0	0
63	1o	2	0	0	0	0
63	1p	1	0	0	0	0
63	1t	1	0	0	0	0
63	1x	2	0	0	0	0
63	20	2	0	0	0	0
63	21	2	0	0	0	0
63	23	2	0	0	0	0
63	25	1	0	0	0	0
63	26	2	0	0	0	0
63	28	5	0	0	0	0
63	2A	1221	0	0	6	0
63	2B	33	0	0	1	0
63	2D	13	0	0	0	0
63	2E	12	0	0	1	0
63	2F	4	0	0	0	0
63	2N	2	0	0	0	0
63	2O	4	0	0	0	0
63	2P	7	0	0	0	0
63	2Q	5	0	0	0	0
63	2R	2	0	0	0	0
63	2T	2	0	0	0	0
63	2U	3	0	0	0	0
63	2X	4	0	0	0	0
63	2Y	1	0	0	0	0
63	2a	305	0	0	6	0
63	2d	3	0	0	0	0
63	2e	1	0	0	0	0
63	2j	2	0	0	1	0
63	2l	1	0	0	0	0
63	2n	1	0	0	0	0
63	2p	1	0	0	0	0
63	2r	1	0	0	0	0
63	2t	1	0	0	0	0
63	2x	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	A	1	0	0	0	0
All	All	293672	0	194336	3566	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 3566 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2564:OMU:C4	1:1A:2564:OMU:C5	1.78	1.59
1:2A:2552:OMU:C5	1:2A:2552:OMU:C4	1.78	1.58
1:1A:1405:A:N6	1:1A:1418:U:H3	1.34	1.23
32:2a:516:PSU:HN3	32:2a:533:A:N6	1.44	1.13
1:1A:2159:C:N4	1:1A:2176:G:H1	1.52	1.07

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/275 (99%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/275 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	24	57
4	2E	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	24	57
5	1F	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	24	57
5	2F	201/203 (99%)	195 (97%)	4 (2%)	2 (1%)	12	41
6	1G	179/181 (99%)	167 (93%)	10 (6%)	2 (1%)	11	39
6	2G	179/181 (99%)	163 (91%)	13 (7%)	3 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	1H	172/174 (99%)	162 (94%)	10 (6%)	0	100	100
7	2H	171/174 (98%)	162 (95%)	9 (5%)	0	100	100
8	1I	145/147 (99%)	132 (91%)	9 (6%)	4 (3%)	4	20
8	2I	144/147 (98%)	134 (93%)	9 (6%)	1 (1%)	18	49
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	18	49
11	2P	147/149 (99%)	139 (95%)	7 (5%)	1 (1%)	18	49
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	14	44
14	2S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
15	1T	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
15	2T	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
16	1U	114/116 (98%)	114 (100%)	0	0	100	100
16	2U	114/116 (98%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	41
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	41
18	1W	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/95 (98%)	91 (98%)	1 (1%)	1 (1%)	11	39
19	2X	93/95 (98%)	90 (97%)	2 (2%)	1 (1%)	11	39
20	1Y	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
20	2Y	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
21	1Z	201/203 (99%)	187 (93%)	14 (7%)	0	100	100
21	2Z	199/203 (98%)	183 (92%)	16 (8%)	0	100	100
22	10	75/77 (97%)	73 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	20	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
23	11	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
23	21	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
24	12	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
24	22	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
25	13	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
25	23	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
26	14	67/69 (97%)	52 (78%)	12 (18%)	3 (4%)	2	12
26	24	67/69 (97%)	51 (76%)	12 (18%)	4 (6%)	1	7
27	15	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
27	25	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
28	16	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
28	26	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
29	17	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
29	27	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
30	18	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
30	28	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/231 (99%)	199 (87%)	21 (9%)	9 (4%)	2	14
33	2b	229/231 (99%)	200 (87%)	23 (10%)	6 (3%)	4	21
34	1c	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
34	2c	204/206 (99%)	191 (94%)	11 (5%)	2 (1%)	12	41
35	1d	206/208 (99%)	193 (94%)	11 (5%)	2 (1%)	12	41
35	2d	206/208 (99%)	196 (95%)	8 (4%)	2 (1%)	12	41
36	1e	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
36	2e	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
37	1f	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/155 (99%)	146 (95%)	7 (5%)	0	100	100
38	2g	153/155 (99%)	143 (94%)	8 (5%)	2 (1%)	9	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	1h	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/127 (98%)	115 (92%)	9 (7%)	1 (1%)	16	47
40	2i	124/127 (98%)	111 (90%)	11 (9%)	2 (2%)	7	30
41	1j	95/97 (98%)	82 (86%)	9 (10%)	4 (4%)	2	13
41	2j	94/97 (97%)	84 (89%)	9 (10%)	1 (1%)	11	39
42	1k	112/114 (98%)	105 (94%)	6 (5%)	1 (1%)	14	44
42	2k	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
43	1l	119/122 (98%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/122 (98%)	110 (92%)	9 (8%)	0	100	100
44	1m	114/116 (98%)	106 (93%)	7 (6%)	1 (1%)	14	44
44	2m	112/116 (97%)	105 (94%)	5 (4%)	2 (2%)	6	28
45	1n	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/88 (98%)	84 (98%)	1 (1%)	1 (1%)	10	37
46	2o	86/88 (98%)	81 (94%)	3 (4%)	2 (2%)	5	23
47	1p	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
47	2p	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
48	1q	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	12	41
48	2q	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
49	1r	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
50	2s	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
51	1t	94/98 (96%)	90 (96%)	1 (1%)	3 (3%)	3	18
51	2t	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	3	18
52	1u	21/23 (91%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/23 (91%)	19 (90%)	1 (5%)	1 (5%)	2	11
54	1y	10/19 (53%)	9 (90%)	1 (10%)	0	100	100
54	2y	10/19 (53%)	9 (90%)	1 (10%)	0	100	100
All	All	11460/11686 (98%)	10814 (94%)	571 (5%)	75 (1%)	18	49

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
8	1I	105	HIS
26	14	49	PHE
35	1d	171	GLY
40	1i	127	LYS

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	214/217 (99%)	199 (93%)	15 (7%)	14	41
3	2D	215/217 (99%)	201 (94%)	14 (6%)	15	44
4	1E	164/165 (99%)	150 (92%)	14 (8%)	10	35
4	2E	164/165 (99%)	152 (93%)	12 (7%)	13	40
5	1F	160/161 (99%)	145 (91%)	15 (9%)	8	31
5	2F	159/161 (99%)	144 (91%)	15 (9%)	8	31
6	1G	144/155 (93%)	130 (90%)	14 (10%)	8	30
6	2G	142/155 (92%)	132 (93%)	10 (7%)	14	41
7	1H	144/145 (99%)	136 (94%)	8 (6%)	19	49
7	2H	143/145 (99%)	135 (94%)	8 (6%)	19	49
8	1I	111/123 (90%)	101 (91%)	10 (9%)	9	33
8	2I	108/123 (88%)	99 (92%)	9 (8%)	10	35
9	1N	119/119 (100%)	111 (93%)	8 (7%)	15	43
9	2N	118/119 (99%)	111 (94%)	7 (6%)	18	48
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	60
10	2O	100/100 (100%)	95 (95%)	5 (5%)	22	53
11	1P	115/116 (99%)	106 (92%)	9 (8%)	11	38
11	2P	115/116 (99%)	111 (96%)	4 (4%)	32	62
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	16	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	45
13	1R	101/101 (100%)	89 (88%)	12 (12%)	5	21
13	2R	101/101 (100%)	88 (87%)	13 (13%)	4	18
14	1S	87/87 (100%)	83 (95%)	4 (5%)	24	55
14	2S	85/87 (98%)	81 (95%)	4 (5%)	23	55
15	1T	115/115 (100%)	108 (94%)	7 (6%)	17	46
15	2T	113/115 (98%)	109 (96%)	4 (4%)	32	62
16	1U	93/93 (100%)	88 (95%)	5 (5%)	20	50
16	2U	93/93 (100%)	87 (94%)	6 (6%)	15	44
17	1V	81/82 (99%)	73 (90%)	8 (10%)	7	29
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	29
18	1W	90/91 (99%)	83 (92%)	7 (8%)	11	38
18	2W	90/91 (99%)	85 (94%)	5 (6%)	19	49
19	1X	77/77 (100%)	76 (99%)	1 (1%)	61	77
19	2X	77/77 (100%)	74 (96%)	3 (4%)	28	60
20	1Y	86/88 (98%)	81 (94%)	5 (6%)	18	48
20	2Y	86/88 (98%)	83 (96%)	3 (4%)	32	62
21	1Z	169/176 (96%)	156 (92%)	13 (8%)	12	38
21	2Z	165/176 (94%)	152 (92%)	13 (8%)	11	37
22	10	61/62 (98%)	57 (93%)	4 (7%)	15	43
22	20	61/62 (98%)	59 (97%)	2 (3%)	33	63
23	11	79/82 (96%)	77 (98%)	2 (2%)	42	69
23	21	81/82 (99%)	78 (96%)	3 (4%)	30	61
24	12	65/66 (98%)	64 (98%)	1 (2%)	57	75
24	22	66/66 (100%)	64 (97%)	2 (3%)	36	65
25	13	51/51 (100%)	47 (92%)	4 (8%)	11	38
25	23	50/51 (98%)	47 (94%)	3 (6%)	17	47
26	14	58/62 (94%)	52 (90%)	6 (10%)	7	27
26	24	54/62 (87%)	51 (94%)	3 (6%)	19	49
27	15	51/51 (100%)	49 (96%)	2 (4%)	28	60
27	25	50/51 (98%)	49 (98%)	1 (2%)	48	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	16	51/51 (100%)	48 (94%)	3 (6%)	18	48
28	26	50/51 (98%)	48 (96%)	2 (4%)	28	60
29	17	41/41 (100%)	38 (93%)	3 (7%)	13	40
29	27	41/41 (100%)	40 (98%)	1 (2%)	43	69
30	18	54/54 (100%)	51 (94%)	3 (6%)	19	49
30	28	54/54 (100%)	52 (96%)	2 (4%)	30	61
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	66
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	191/199 (96%)	169 (88%)	22 (12%)	5	23
33	2b	187/199 (94%)	171 (91%)	16 (9%)	10	34
34	1c	144/160 (90%)	137 (95%)	7 (5%)	22	53
34	2c	140/160 (88%)	130 (93%)	10 (7%)	13	41
35	1d	171/180 (95%)	160 (94%)	11 (6%)	16	44
35	2d	172/180 (96%)	165 (96%)	7 (4%)	27	59
36	1e	114/114 (100%)	110 (96%)	4 (4%)	32	62
36	2e	114/114 (100%)	110 (96%)	4 (4%)	32	62
37	1f	85/90 (94%)	83 (98%)	2 (2%)	43	69
37	2f	85/90 (94%)	84 (99%)	1 (1%)	63	78
38	1g	120/126 (95%)	115 (96%)	5 (4%)	26	58
38	2g	119/126 (94%)	112 (94%)	7 (6%)	18	48
39	1h	116/118 (98%)	111 (96%)	5 (4%)	26	57
39	2h	114/118 (97%)	105 (92%)	9 (8%)	11	37
40	1i	91/98 (93%)	84 (92%)	7 (8%)	12	38
40	2i	88/98 (90%)	82 (93%)	6 (7%)	14	42
41	1j	68/87 (78%)	64 (94%)	4 (6%)	18	48
41	2j	68/87 (78%)	66 (97%)	2 (3%)	37	66
42	1k	83/86 (96%)	80 (96%)	3 (4%)	31	62
42	2k	83/86 (96%)	78 (94%)	5 (6%)	17	47
43	1l	96/102 (94%)	92 (96%)	4 (4%)	26	58
43	2l	96/102 (94%)	91 (95%)	5 (5%)	21	51
44	1m	90/94 (96%)	82 (91%)	8 (9%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	2m	87/94 (93%)	78 (90%)	9 (10%)	7	27
45	1n	49/49 (100%)	46 (94%)	3 (6%)	17	46
45	2n	49/49 (100%)	48 (98%)	1 (2%)	48	72
46	1o	78/79 (99%)	76 (97%)	2 (3%)	40	68
46	2o	78/79 (99%)	74 (95%)	4 (5%)	21	52
47	1p	69/71 (97%)	61 (88%)	8 (12%)	5	22
47	2p	68/71 (96%)	61 (90%)	7 (10%)	7	27
48	1q	94/94 (100%)	92 (98%)	2 (2%)	47	71
48	2q	94/94 (100%)	92 (98%)	2 (2%)	47	71
49	1r	59/59 (100%)	58 (98%)	1 (2%)	53	74
49	2r	59/59 (100%)	56 (95%)	3 (5%)	21	52
50	1s	68/72 (94%)	64 (94%)	4 (6%)	18	48
50	2s	67/72 (93%)	62 (92%)	5 (8%)	12	39
51	1t	71/76 (93%)	69 (97%)	2 (3%)	38	66
51	2t	70/76 (92%)	68 (97%)	2 (3%)	37	66
52	1u	18/18 (100%)	18 (100%)	0	100	100
52	2u	18/18 (100%)	18 (100%)	0	100	100
54	1y	12/19 (63%)	12 (100%)	0	100	100
54	2y	12/19 (63%)	12 (100%)	0	100	100
All	All	9387/9734 (96%)	8814 (94%)	573 (6%)	17	46

5 of 573 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	26	14	THR
33	2b	154	LEU
27	25	6	VAL
39	2h	135	CYS
31	19	17	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	129	ASN

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Mol	Chain	Res	Type
36	2e	78	HIS
41	2j	13	HIS
35	1d	119	GLN
35	1d	77	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2816/2915 (96%)	427 (15%)	31 (1%)
1	2A	2860/2915 (98%)	485 (16%)	28 (0%)
2	1B	119/120 (99%)	10 (8%)	0
2	2B	119/120 (99%)	12 (10%)	0
32	1a	1497/1521 (98%)	257 (17%)	0
32	2a	1501/1521 (98%)	252 (16%)	0
53	1x	75/76 (98%)	7 (9%)	0
53	2x	75/76 (98%)	8 (10%)	0
55	A	2/27 (7%)	0	0
55	B	2/27 (7%)	0	0
All	All	9066/9318 (97%)	1458 (16%)	59 (0%)

5 of 1458 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	54	G

5 of 59 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2597	U
1	2A	2172	U
1	2A	277	C
1	2A	2171	A
1	2A	1420	U

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

56 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	5MC	1a	1407	32	19,22,23	1.06	1 (5%)	26,32,35	1.20	4 (15%)
32	5MC	1a	1400	32	19,22,23	1.09	2 (10%)	26,32,35	1.32	3 (11%)
53	4SU	1x	8	53	18,21,22	1.24	2 (11%)	25,30,33	0.80	1 (4%)
1	PSU	2A	2605	1	18,21,22	1.40	3 (16%)	21,30,33	1.78	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.36	3 (16%)	21,30,33	1.69	5 (23%)
32	MA6	2a	1518	32	23,26,27	1.07	2 (8%)	33,38,41	4.52	14 (42%)
1	PSU	1A	1933	1	18,21,22	1.33	3 (16%)	21,30,33	1.62	6 (28%)
32	5MC	2a	1400	32	19,22,23	1.03	1 (5%)	26,32,35	1.32	4 (15%)
32	5MC	2a	1407	32	19,22,23	0.97	2 (10%)	26,32,35	1.23	4 (15%)
32	5MC	2a	967	32	19,22,23	0.96	2 (10%)	26,32,35	1.31	4 (15%)
32	MA6	1a	1518	32	23,26,27	1.07	3 (13%)	33,38,41	4.24	14 (42%)
53	5MU	2x	54	53	19,22,23	0.97	2 (10%)	27,32,35	1.11	2 (7%)
53	5MC	2x	32	53	19,22,23	1.06	2 (10%)	26,32,35	1.30	4 (15%)
1	2MA	1A	2515	56,1	22,25,26	2.74	8 (36%)	32,37,40	3.12	10 (31%)
1	PSU	1A	1939	56,1	18,21,22	1.18	3 (16%)	21,30,33	1.57	5 (23%)
32	M2G	1a	966	32	24,27,28	2.13	5 (20%)	33,40,43	1.61	7 (21%)
53	5MC	1x	32	53	19,22,23	1.05	3 (15%)	26,32,35	1.26	4 (15%)
1	5MU	1A	1961	1	19,22,23	0.79	1 (5%)	27,32,35	1.21	3 (11%)
53	PSU	1x	55	53	18,21,22	1.46	3 (16%)	21,30,33	1.69	3 (14%)
53	4SU	2x	8	53,56	18,21,22	1.25	2 (11%)	25,30,33	0.87	2 (8%)
43	0TD	2l	92	43	8,9,10	3.07	3 (37%)	6,11,13	2.47	3 (50%)
1	5MC	1A	1984	1	19,22,23	1.05	2 (10%)	26,32,35	1.33	4 (15%)
32	G7M	1a	527	56,32	23,26,27	2.79	8 (34%)	34,39,42	1.61	7 (20%)
32	5MC	1a	1404	32	19,22,23	0.91	0	26,32,35	1.23	4 (15%)
1	5MU	2A	1939	1	19,22,23	0.80	1 (5%)	27,32,35	1.16	2 (7%)
32	5MC	2a	1404	32	19,22,23	0.96	1 (5%)	26,32,35	1.22	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	1A	1942	56,1	19,22,23	2.45	7 (36%)	25,31,34	0.92	1 (4%)
1	5MC	2A	1962	56,1	19,22,23	1.01	1 (5%)	26,32,35	1.32	4 (15%)
32	G7M	2a	527	56,32	23,26,27	2.79	8 (34%)	34,39,42	1.62	9 (26%)
32	2MG	1a	1207	56,32	23,26,27	2.22	6 (26%)	33,38,41	2.39	14 (42%)
43	0TD	1l	92	43	8,9,10	2.77	3 (37%)	6,11,13	3.05	4 (66%)
32	2MG	2a	1207	32	23,26,27	2.14	5 (21%)	33,38,41	2.23	12 (36%)
32	UR3	2a	1498	32	19,22,23	1.99	3 (15%)	26,32,35	1.67	4 (15%)
32	M2G	2a	966	32	24,27,28	2.19	5 (20%)	33,40,43	1.67	7 (21%)
1	5MU	1A	1937	1	19,22,23	1.32	2 (10%)	27,32,35	1.49	5 (18%)
32	5MC	1a	967	32	19,22,23	1.09	2 (10%)	26,32,35	1.21	4 (15%)
32	4OC	2a	1402	32	20,23,24	2.64	8 (40%)	25,32,35	0.99	1 (4%)
32	PSU	1a	516	32	18,21,22	1.40	3 (16%)	21,30,33	2.09	5 (23%)
32	PSU	2a	516	32	18,21,22	1.39	2 (11%)	21,30,33	2.24	7 (33%)
1	5MC	2A	1942	1	19,22,23	0.99	1 (5%)	26,32,35	1.23	4 (15%)
32	MA6	2a	1519	32	23,26,27	1.07	2 (8%)	33,38,41	4.36	14 (42%)
32	MA6	1a	1519	32	23,26,27	1.07	2 (8%)	33,38,41	4.42	14 (42%)
1	OMC	2A	1920	1	19,22,23	2.50	7 (36%)	25,31,34	0.89	1 (4%)
1	OMU	2A	2552	56,1	19,22,23	6.85	10 (52%)	25,31,34	2.57	7 (28%)
1	2MA	2A	2503	56,1	22,25,26	2.71	7 (31%)	32,37,40	3.28	11 (34%)
1	5MC	1A	1964	1	19,22,23	1.03	1 (5%)	26,32,35	1.31	4 (15%)
1	5MU	2A	1915	1	19,22,23	1.22	2 (10%)	27,32,35	1.32	3 (11%)
1	PSU	1A	2617	1	18,21,22	1.18	3 (16%)	21,30,33	1.71	2 (9%)
32	UR3	1a	1498	32	19,22,23	2.00	4 (21%)	26,32,35	1.60	4 (15%)
1	OMG	1A	2263	53,56,1	23,26,27	1.75	4 (17%)	32,38,41	2.25	10 (31%)
53	PSU	2x	55	53	18,21,22	1.56	3 (16%)	21,30,33	1.79	5 (23%)
1	OMU	1A	2564	1	19,22,23	6.85	10 (52%)	25,31,34	2.75	8 (32%)
53	5MU	1x	54	53	19,22,23	1.09	2 (10%)	27,32,35	1.14	2 (7%)
1	OMG	2A	2251	53,56,1	23,26,27	1.72	2 (8%)	32,38,41	2.23	11 (34%)
1	PSU	2A	1917	1	18,21,22	1.31	3 (16%)	21,30,33	1.73	5 (23%)
32	4OC	1a	1402	32	20,23,24	2.63	8 (40%)	25,32,35	0.84	0

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	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
53	4SU	1x	8	53	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
53	5MU	2x	54	53	-	0/7/25/26	0/2/2/2
53	5MC	2x	32	53	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	56,1	-	2/7/25/26	0/3/3/3
1	PSU	1A	1939	56,1	-	1/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	1/11/29/30	0/3/3/3
53	5MC	1x	32	53	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1	-	0/7/25/26	0/2/2/2
53	PSU	1x	55	53	-	0/7/25/26	0/2/2/2
53	4SU	2x	8	53,56	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
1	5MC	1A	1984	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	56,32	-	3/7/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	OMC	1A	1942	56,1	-	3/9/27/28	0/2/2/2
1	5MC	2A	1962	56,1	-	2/7/25/26	0/2/2/2
32	G7M	2a	527	56,32	-	2/7/25/26	0/3/3/3
32	2MG	1a	1207	56,32	-	2/9/27/28	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	1A	1937	1	-	4/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	5/9/29/30	0/2/2/2
32	PSU	1a	516	32	-	1/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	1/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	OMU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
1	2MA	2A	2503	56,1	-	3/7/25/26	0/3/3/3
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	1/7/25/26	0/2/2/2
1	OMG	1A	2263	53,56,1	-	1/9/27/28	0/3/3/3
53	PSU	2x	55	53	-	0/7/25/26	0/2/2/2
1	OMU	1A	2564	1	-	1/9/27/28	0/2/2/2
53	5MU	1x	54	53	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	53,56,1	-	0/9/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2

The worst 5 of 194 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2564	OMU	C5-C4	15.99	1.78	1.43
1	2A	2552	OMU	C5-C4	15.94	1.78	1.43
1	1A	2564	OMU	C4-N3	-15.53	1.12	1.38
1	2A	2552	OMU	C4-N3	-15.22	1.12	1.38
1	1A	2564	OMU	C6-C5	-10.27	1.11	1.35

The worst 5 of 310 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1518	MA6	N1-C6-N6	-17.74	95.24	116.86
32	1a	1519	MA6	N1-C6-N6	-17.09	96.03	116.86
32	2a	1519	MA6	N1-C6-N6	-16.90	96.26	116.86
32	1a	1518	MA6	N1-C6-N6	-16.20	97.12	116.86
32	2a	1518	MA6	C5-C6-N6	12.79	145.57	125.33

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C1'-N1-C6
1	1A	1937	5MU	O4'-C4'-C5'-O5'
1	1A	2263	OMG	C1'-C2'-O2'-CM2
32	1a	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

26 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	1x	8	4SU	1	0
32	2a	1518	MA6	2	0
32	1a	1518	MA6	1	0
53	2x	54	5MU	1	0
1	1A	2515	2MA	2	0
1	1A	1961	5MU	2	0
53	2x	8	4SU	1	0
43	2l	92	0TD	1	0
32	2a	1404	5MC	1	0
1	1A	1942	OMC	1	0
1	2A	1962	5MC	1	0
32	1a	1207	2MG	3	0
32	2a	1498	UR3	1	0
32	2a	1402	4OC	2	0
32	1a	516	PSU	3	0
32	2a	516	PSU	2	0
32	2a	1519	MA6	2	0
32	1a	1519	MA6	1	0
1	2A	2552	OMU	1	0
1	2A	2503	2MA	2	0
32	1a	1498	UR3	1	0
1	1A	2263	OMG	1	0
1	1A	2564	OMU	2	0
53	1x	54	5MU	3	0
1	2A	2251	OMG	1	0
32	1a	1402	4OC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2322 ligands modelled in this entry, 2315 are monoatomic and 2 are unknown - leaving 5 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
61	SF4	1d	501	35	0,12,12	-	-	-		
61	SF4	2d	501	35	0,12,12	-	-	-		
59	ARG	1B	229	-	10,11,11	0.74	1 (10%)	9,13,13	1.00	1 (11%)
58	MPD	1a	1860	-	7,7,7	0.42	0	9,10,10	0.36	0
58	MPD	1A	3907	-	7,7,7	0.36	0	9,10,10	0.26	0

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
61	SF4	1d	501	35	-	-	0/6/5/5
61	SF4	2d	501	35	-	-	0/6/5/5
59	ARG	1B	229	-	-	2/11/11/11	-
58	MPD	1a	1860	-	-	4/5/5/5	-
58	MPD	1A	3907	-	-	1/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1B	229	ARG	OXT-C	-2.12	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1B	229	ARG	OXT-C-O	-2.91	117.49	124.08

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1a	1860	MPD	C2-C3-C4-O4
58	1a	1860	MPD	C2-C3-C4-C5
59	1B	229	ARG	NE-CD-CG-CB
58	1A	3907	MPD	O2-C2-C3-C4
58	1a	1860	MPD	C1-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1B	229	ARG	1	0
58	1A	3907	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1A	1151:U	O3'	1152:G	P	3.02

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	2813/2915 (96%)	-0.28	97 (3%) 48 28	23, 42, 82, 95	0
1	2A	2858/2915 (98%)	-0.12	115 (4%) 42 23	40, 59, 86, 96	0
2	1B	120/120 (100%)	-0.41	0 100 100	38, 57, 63, 76	0
2	2B	120/120 (100%)	0.29	0 100 100	62, 75, 81, 82	0
3	1D	275/275 (100%)	0.09	1 (0%) 88 76	30, 44, 54, 67	0
3	2D	275/275 (100%)	0.23	5 (1%) 67 47	43, 55, 62, 69	0
4	1E	204/204 (100%)	0.04	1 (0%) 87 73	28, 47, 60, 69	0
4	2E	204/204 (100%)	0.20	4 (1%) 65 44	43, 59, 67, 75	0
5	1F	203/203 (100%)	0.07	0 100 100	26, 48, 66, 73	0
5	2F	203/203 (100%)	0.11	1 (0%) 87 73	44, 65, 72, 79	0
6	1G	181/181 (100%)	0.10	2 (1%) 78 59	55, 64, 72, 80	0
6	2G	181/181 (100%)	0.68	9 (4%) 34 18	71, 75, 79, 85	0
7	1H	174/174 (100%)	0.08	3 (1%) 69 48	43, 54, 62, 65	0
7	2H	173/174 (99%)	0.46	5 (2%) 53 32	66, 75, 79, 85	0
8	1I	147/147 (100%)	0.03	2 (1%) 73 53	51, 67, 74, 76	0
8	2I	146/147 (99%)	0.15	0 100 100	59, 75, 79, 82	0
9	1N	140/140 (100%)	0.06	0 100 100	35, 45, 61, 67	0
9	2N	140/140 (100%)	0.14	0 100 100	52, 63, 71, 78	0
10	1O	122/122 (100%)	0.12	2 (1%) 70 49	38, 47, 58, 62	0
10	2O	122/122 (100%)	0.11	0 100 100	50, 57, 64, 69	0
11	1P	149/149 (100%)	-0.03	1 (0%) 84 68	28, 50, 61, 73	0
11	2P	149/149 (100%)	0.29	4 (2%) 56 35	46, 67, 75, 78	0
12	1Q	141/141 (100%)	0.24	3 (2%) 63 42	36, 49, 56, 63	0
12	2Q	141/141 (100%)	0.24	2 (1%) 73 53	51, 64, 69, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.15	2 (1%) 69 48	35, 42, 53, 65	0
13	2R	118/118 (100%)	0.17	1 (0%) 82 65	48, 56, 62, 69	0
14	1S	110/110 (100%)	0.00	0 100 100	45, 53, 60, 64	0
14	2S	110/110 (100%)	0.78	7 (6%) 25 14	65, 71, 74, 76	0
15	1T	131/131 (100%)	0.04	3 (2%) 61 39	42, 51, 67, 74	0
15	2T	131/131 (100%)	0.07	1 (0%) 82 65	55, 60, 70, 75	0
16	1U	116/116 (100%)	0.07	1 (0%) 81 63	30, 40, 52, 58	0
16	2U	116/116 (100%)	0.26	1 (0%) 81 63	50, 60, 69, 74	0
17	1V	101/101 (100%)	-0.21	0 100 100	27, 49, 59, 64	0
17	2V	101/101 (100%)	0.06	0 100 100	48, 67, 73, 76	0
18	1W	112/112 (100%)	-0.08	0 100 100	31, 38, 54, 71	0
18	2W	112/112 (100%)	0.15	0 100 100	46, 54, 64, 71	0
19	1X	95/95 (100%)	0.19	1 (1%) 78 59	34, 44, 60, 67	0
19	2X	95/95 (100%)	0.54	3 (3%) 50 30	53, 61, 68, 69	0
20	1Y	107/107 (100%)	0.19	1 (0%) 81 63	46, 53, 65, 68	0
20	2Y	107/107 (100%)	0.53	6 (5%) 30 16	62, 68, 73, 83	0
21	1Z	203/203 (100%)	0.49	15 (7%) 20 11	50, 61, 72, 81	0
21	2Z	201/203 (99%)	0.55	12 (5%) 27 15	66, 73, 79, 82	0
22	10	77/77 (100%)	0.25	2 (2%) 57 36	37, 45, 53, 57	0
22	20	77/77 (100%)	0.44	3 (3%) 43 24	57, 63, 68, 70	0
23	11	97/97 (100%)	0.18	2 (2%) 63 42	32, 48, 65, 71	0
23	21	97/97 (100%)	0.28	1 (1%) 79 61	47, 59, 70, 74	0
24	12	70/70 (100%)	0.18	3 (4%) 40 22	44, 52, 58, 71	0
24	22	70/70 (100%)	0.50	3 (4%) 40 22	61, 67, 72, 74	0
25	13	59/59 (100%)	0.10	0 100 100	36, 45, 62, 70	0
25	23	59/59 (100%)	0.04	0 100 100	57, 62, 69, 72	0
26	14	69/69 (100%)	0.31	1 (1%) 73 53	62, 73, 82, 84	0
26	24	69/69 (100%)	0.97	6 (8%) 16 9	75, 80, 84, 85	0
27	15	59/59 (100%)	-0.03	1 (1%) 69 48	28, 45, 57, 63	0
27	25	59/59 (100%)	0.06	1 (1%) 69 48	46, 57, 68, 73	0
28	16	53/53 (100%)	-0.21	0 100 100	45, 50, 58, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/53 (100%)	0.10	1 (1%) 66 45	59, 63, 67, 72	0
29	17	48/48 (100%)	0.31	5 (10%) 11 6	30, 33, 52, 56	0
29	27	48/48 (100%)	0.33	3 (6%) 26 14	43, 48, 61, 69	0
30	18	64/64 (100%)	0.19	1 (1%) 70 49	35, 41, 46, 48	0
30	28	64/64 (100%)	0.54	1 (1%) 70 49	52, 57, 62, 64	0
31	19	37/37 (100%)	0.35	2 (5%) 31 17	40, 48, 58, 62	0
31	29	37/37 (100%)	0.87	3 (8%) 18 10	62, 66, 70, 71	0
32	1a	1488/1521 (97%)	0.16	30 (2%) 65 44	45, 72, 87, 97	0
32	2a	1492/1521 (98%)	0.20	46 (3%) 51 30	52, 73, 88, 95	0
33	1b	231/231 (100%)	0.45	4 (1%) 69 48	69, 75, 81, 84	0
33	2b	231/231 (100%)	0.60	8 (3%) 47 27	72, 77, 82, 84	0
34	1c	206/206 (100%)	0.53	7 (3%) 48 28	70, 76, 79, 81	0
34	2c	206/206 (100%)	0.72	9 (4%) 39 21	73, 78, 81, 84	0
35	1d	208/208 (100%)	0.60	9 (4%) 40 22	65, 74, 78, 81	0
35	2d	208/208 (100%)	0.45	3 (1%) 73 53	64, 70, 75, 78	0
36	1e	148/148 (100%)	0.19	2 (1%) 73 53	61, 68, 73, 82	0
36	2e	148/148 (100%)	0.33	3 (2%) 65 44	65, 71, 76, 83	0
37	1f	100/100 (100%)	0.27	2 (2%) 65 44	63, 70, 73, 76	0
37	2f	100/100 (100%)	0.40	1 (1%) 79 61	67, 71, 75, 77	0
38	1g	155/155 (100%)	0.43	9 (5%) 29 16	67, 72, 80, 85	0
38	2g	155/155 (100%)	0.56	6 (3%) 43 24	74, 77, 80, 86	0
39	1h	137/137 (100%)	0.35	3 (2%) 62 41	64, 68, 72, 76	0
39	2h	137/137 (100%)	0.39	4 (2%) 53 32	67, 71, 74, 75	0
40	1i	127/127 (100%)	1.01	18 (14%) 6 3	69, 78, 81, 83	0
40	2i	126/127 (99%)	1.54	38 (30%) 1 1	72, 80, 83, 85	0
41	1j	97/97 (100%)	1.13	13 (13%) 7 4	71, 78, 80, 83	0
41	2j	96/97 (98%)	1.47	27 (28%) 1 1	74, 80, 83, 85	0
42	1k	114/114 (100%)	0.14	1 (0%) 81 63	56, 68, 72, 74	0
42	2k	114/114 (100%)	0.24	3 (2%) 57 36	63, 72, 75, 79	0
43	1l	121/122 (99%)	0.47	7 (5%) 29 16	58, 66, 70, 74	0
43	2l	121/122 (99%)	0.38	6 (4%) 34 18	60, 65, 70, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/116 (100%)	0.54	5 (4%) 40 22	64, 74, 78, 80	0
44	2m	114/116 (98%)	1.08	15 (13%) 7 4	73, 79, 82, 82	0
45	1n	60/60 (100%)	1.05	8 (13%) 7 4	71, 74, 77, 79	0
45	2n	60/60 (100%)	1.36	15 (25%) 2 1	74, 78, 81, 82	0
46	1o	88/88 (100%)	0.25	1 (1%) 78 59	57, 66, 73, 76	0
46	2o	88/88 (100%)	0.35	0 100 100	63, 69, 74, 76	0
47	1p	82/82 (100%)	0.99	6 (7%) 21 11	67, 73, 77, 79	0
47	2p	82/82 (100%)	0.68	4 (4%) 35 18	63, 69, 74, 76	0
48	1q	99/99 (100%)	0.45	1 (1%) 79 61	62, 66, 72, 73	0
48	2q	99/99 (100%)	0.33	1 (1%) 79 61	63, 69, 73, 75	0
49	1r	68/68 (100%)	0.19	1 (1%) 72 52	64, 69, 75, 77	0
49	2r	68/68 (100%)	0.14	0 100 100	68, 71, 76, 77	0
50	1s	83/83 (100%)	0.86	7 (8%) 17 9	70, 76, 79, 81	0
50	2s	83/83 (100%)	1.20	12 (14%) 6 3	71, 80, 82, 83	0
51	1t	96/98 (97%)	0.76	13 (13%) 7 4	65, 70, 75, 78	0
51	2t	98/98 (100%)	0.62	5 (5%) 33 18	62, 68, 75, 75	0
52	1u	23/23 (100%)	1.75	11 (47%) 0 0	70, 73, 76, 77	0
52	2u	23/23 (100%)	1.86	9 (39%) 1 0	76, 77, 79, 80	0
53	1x	72/76 (94%)	-0.40	0 100 100	41, 66, 76, 80	0
53	2x	72/76 (94%)	-0.09	1 (1%) 73 53	56, 73, 81, 90	0
54	1y	12/19 (63%)	0.84	1 (8%) 17 9	37, 48, 57, 59	0
54	2y	12/19 (63%)	1.44	4 (33%) 1 0	52, 59, 62, 69	0
55	A	3/27 (11%)	0.70	0 100 100	70, 70, 71, 74	0
55	B	3/27 (11%)	0.59	0 100 100	64, 64, 65, 69	0
All	All	20701/21004 (98%)	0.18	729 (3%) 47 27	23, 65, 82, 97	0

The worst 5 of 729 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	1Z	200	GLY	10.5
22	10	8	GLY	8.3
21	1Z	203	GLU	8.2
21	1Z	197	ILE	8.1
21	1Z	193	GLU	7.9

6.2 Non-standard residues in protein, DNA, RNA chains

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
53	PSU	2x	55	20/21	0.65	0.13	74,74,76,76	0
32	PSU	2a	516	20/21	0.79	0.12	73,74,78,78	0
32	PSU	1a	516	20/21	0.80	0.12	69,72,73,73	0
1	5MU	1A	1937	21/22	0.82	0.12	69,72,80,81	0
1	5MU	2A	1915	21/22	0.85	0.10	78,80,84,87	0
32	G7M	2a	527	24/25	0.87	0.13	69,70,71,72	0
53	5MU	2x	54	21/22	0.87	0.10	73,74,76,77	0
53	PSU	1x	55	20/21	0.87	0.09	66,67,69,69	0
43	0TD	1l	92	10/11	0.88	0.13	66,66,67,69	0
53	4SU	2x	8	20/21	0.88	0.09	72,75,76,77	0
53	5MC	1x	32	21/22	0.89	0.12	65,66,69,69	0
53	5MC	2x	32	21/22	0.89	0.11	70,71,72,73	0
53	5MU	1x	54	21/22	0.89	0.09	67,69,72,75	0
1	PSU	1A	1939	20/21	0.89	0.09	62,65,68,69	0
32	4OC	2a	1402	22/23	0.90	0.10	64,66,67,69	0
43	0TD	2l	92	10/11	0.90	0.12	65,65,66,67	0
32	2MG	1a	1207	24/25	0.90	0.09	72,75,78,79	0
53	4SU	1x	8	20/21	0.90	0.09	66,68,68,69	0
32	5MC	2a	967	21/22	0.90	0.13	70,71,74,77	0
32	2MG	2a	1207	24/25	0.90	0.09	75,77,78,79	0
1	PSU	2A	1917	20/21	0.91	0.09	67,70,73,74	0
1	PSU	1A	1933	20/21	0.92	0.09	58,61,63,64	0
32	M2G	2a	966	25/26	0.92	0.11	68,70,72,73	0
32	M2G	1a	966	25/26	0.92	0.12	66,67,69,70	0
1	2MA	2A	2503	23/24	0.92	0.14	41,43,46,48	0
1	PSU	2A	1911	20/21	0.92	0.08	67,68,69,69	0
32	G7M	1a	527	24/25	0.93	0.11	66,67,68,68	0
32	5MC	1a	1407	21/22	0.93	0.11	52,56,59,60	0
32	5MC	2a	1407	21/22	0.93	0.10	58,63,64,65	0
32	5MC	1a	967	21/22	0.93	0.11	67,68,69,70	0
32	5MC	1a	1404	21/22	0.94	0.10	57,59,61,61	0
32	5MC	2a	1400	21/22	0.94	0.09	67,69,71,71	0
1	OMC	1A	1942	21/22	0.94	0.12	54,57,58,59	0
32	5MC	1a	1400	21/22	0.94	0.09	62,64,65,65	0
32	UR3	2a	1498	21/22	0.94	0.09	60,61,63,64	0
32	4OC	1a	1402	22/23	0.95	0.09	60,61,62,62	0
32	5MC	2a	1404	21/22	0.95	0.08	59,60,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	OMC	2A	1920	21/22	0.95	0.08	62,64,66,66	0
1	5MC	1A	1964	21/22	0.95	0.09	40,43,44,45	0
32	MA6	2a	1518	24/25	0.95	0.10	60,61,62,62	0
1	OMU	1A	2564	21/22	0.96	0.09	35,37,38,39	0
1	5MU	1A	1961	21/22	0.96	0.10	37,39,40,40	0
32	UR3	1a	1498	21/22	0.96	0.09	56,57,60,61	0
32	MA6	2a	1519	24/25	0.96	0.09	58,59,60,60	0
32	MA6	1a	1518	24/25	0.96	0.10	53,54,56,57	0
1	5MC	2A	1942	21/22	0.96	0.06	55,56,57,57	0
1	OMG	2A	2251	24/25	0.96	0.09	45,46,50,51	0
32	MA6	1a	1519	24/25	0.96	0.10	51,55,55,56	0
1	PSU	2A	2605	20/21	0.96	0.09	42,45,45,45	0
1	5MC	1A	1984	21/22	0.97	0.09	42,43,46,49	0
1	PSU	1A	2617	20/21	0.97	0.11	36,37,38,39	0
1	OMU	2A	2552	21/22	0.97	0.08	45,46,48,48	0
1	OMG	1A	2263	24/25	0.97	0.08	31,33,36,36	0
1	5MU	2A	1939	21/22	0.97	0.08	46,49,50,50	0
1	2MA	1A	2515	23/24	0.97	0.09	24,26,28,30	0
1	5MC	2A	1962	21/22	0.97	0.10	53,54,57,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1765	1/1	0.32	0.27	80,80,80,80	0
56	MG	2A	3108	1/1	0.40	0.19	72,72,72,72	0
56	MG	1A	3658	1/1	0.45	0.21	50,50,50,50	0
56	MG	2a	1666	1/1	0.45	0.25	84,84,84,84	0
56	MG	1a	1764	1/1	0.46	0.17	70,70,70,70	0
56	MG	1a	1827	1/1	0.46	0.29	77,77,77,77	0
56	MG	2A	3292	1/1	0.51	0.19	60,60,60,60	0
56	MG	2a	1639	1/1	0.52	0.47	68,68,68,68	0
56	MG	2a	1684	1/1	0.52	0.26	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	2x	105	1/1	0.52	0.25	75,75,75,75	0
56	MG	2A	3600	1/1	0.53	0.13	80,80,80,80	0
56	MG	1a	1843	1/1	0.53	0.29	62,62,62,62	0
56	MG	2A	3078	1/1	0.53	0.15	67,67,67,67	0
56	MG	1a	1754	1/1	0.53	0.36	68,68,68,68	0
56	MG	1a	1667	1/1	0.53	0.49	83,83,83,83	0
56	MG	2A	3428	1/1	0.54	0.21	57,57,57,57	0
56	MG	1H	8001	1/1	0.56	0.33	61,61,61,61	0
56	MG	1B	215	1/1	0.57	0.18	71,71,71,71	0
56	MG	1A	3538	1/1	0.57	0.16	56,56,56,56	0
56	MG	1a	1641	1/1	0.57	0.20	75,75,75,75	0
56	MG	2A	3650	1/1	0.58	0.13	70,70,70,70	0
56	MG	2a	1668	1/1	0.58	0.19	60,60,60,60	0
56	MG	1a	1678	1/1	0.59	0.28	74,74,74,74	0
56	MG	1A	3584	1/1	0.59	0.29	61,61,61,61	0
56	MG	2A	3124	1/1	0.59	0.32	63,63,63,63	0
56	MG	1A	3583	1/1	0.59	0.09	65,65,65,65	0
56	MG	2A	3220	1/1	0.60	0.36	51,51,51,51	0
56	MG	2j	8001	1/1	0.61	0.13	79,79,79,79	0
56	MG	1a	1795	1/1	0.61	0.26	76,76,76,76	0
56	MG	2a	1715	1/1	0.62	0.13	75,75,75,75	0
56	MG	1A	3277	1/1	0.62	0.08	70,70,70,70	0
56	MG	2A	3249	1/1	0.62	0.17	76,76,76,76	0
56	MG	2a	1606	1/1	0.63	0.44	59,59,59,59	0
56	MG	2a	1608	1/1	0.63	0.70	69,69,69,69	0
56	MG	1a	1713	1/1	0.63	0.47	72,72,72,72	0
56	MG	1B	209	1/1	0.64	0.28	61,61,61,61	0
56	MG	2a	1641	1/1	0.64	0.26	76,76,76,76	0
56	MG	2a	1659	1/1	0.64	0.28	77,77,77,77	0
56	MG	1A	3258	1/1	0.64	0.19	71,71,71,71	0
56	MG	1x	111	1/1	0.64	0.35	72,72,72,72	0
56	MG	1a	1657	1/1	0.64	0.28	71,71,71,71	0
56	MG	2a	1701	1/1	0.64	0.39	61,61,61,61	0
56	MG	1a	1767	1/1	0.64	0.14	72,72,72,72	0
56	MG	1a	1732	1/1	0.64	0.65	74,74,74,74	0
56	MG	1a	1803	1/1	0.64	0.33	63,63,63,63	0
56	MG	1a	1659	1/1	0.65	0.37	64,64,64,64	0
56	MG	1e	202	1/1	0.65	0.26	64,64,64,64	0
56	MG	1A	3545	1/1	0.65	0.11	54,54,54,54	0
56	MG	1A	3607	1/1	0.65	0.15	45,45,45,45	0
56	MG	2A	3171	1/1	0.66	0.24	69,69,69,69	0
56	MG	1A	3873	1/1	0.66	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1671	1/1	0.66	0.38	71,71,71,71	0
56	MG	2A	3099	1/1	0.66	0.31	57,57,57,57	0
56	MG	1a	1819	1/1	0.66	0.19	69,69,69,69	0
56	MG	2a	1702	1/1	0.66	0.13	62,62,62,62	0
56	MG	2A	3349	1/1	0.66	0.14	55,55,55,55	0
56	MG	1A	3598	1/1	0.66	0.14	55,55,55,55	0
56	MG	2n	101	1/1	0.66	0.23	77,77,77,77	0
56	MG	2A	3452	1/1	0.66	0.10	66,66,66,66	0
56	MG	2B	3002	1/1	0.67	0.18	72,72,72,72	0
56	MG	2a	1646	1/1	0.67	0.33	66,66,66,66	0
56	MG	2a	1649	1/1	0.67	0.25	68,68,68,68	0
56	MG	2A	3322	1/1	0.67	0.19	71,71,71,71	0
56	MG	2a	1754	1/1	0.67	0.11	69,69,69,69	0
56	MG	1A	3203	1/1	0.67	0.17	65,65,65,65	0
56	MG	2a	1638	1/1	0.67	0.21	71,71,71,71	0
56	MG	2A	3158	1/1	0.67	0.17	78,78,78,78	0
56	MG	1a	1685	1/1	0.68	0.35	67,67,67,67	0
56	MG	1a	1737	1/1	0.68	0.15	74,74,74,74	0
56	MG	2G	201	1/1	0.68	0.12	72,72,72,72	0
56	MG	2a	1714	1/1	0.68	0.26	62,62,62,62	0
56	MG	1A	3613	1/1	0.68	0.24	68,68,68,68	0
56	MG	2A	3121	1/1	0.68	0.26	68,68,68,68	0
56	MG	2a	1756	1/1	0.68	0.21	73,73,73,73	0
56	MG	2a	1766	1/1	0.68	0.17	70,70,70,70	0
56	MG	2a	1618	1/1	0.68	0.20	80,80,80,80	0
56	MG	2a	1635	1/1	0.68	0.26	73,73,73,73	0
56	MG	1a	1823	1/1	0.68	0.16	54,54,54,54	0
56	MG	2A	3183	1/1	0.69	0.36	54,54,54,54	0
56	MG	1A	3116	1/1	0.69	0.13	40,40,40,40	0
56	MG	2a	1643	1/1	0.69	0.15	67,67,67,67	0
56	MG	1A	3914	1/1	0.69	0.17	57,57,57,57	0
56	MG	1a	1804	1/1	0.69	0.15	67,67,67,67	0
56	MG	1a	1604	1/1	0.69	0.29	72,72,72,72	0
56	MG	2A	3157	1/1	0.69	0.22	47,47,47,47	0
56	MG	2A	3022	1/1	0.69	0.26	59,59,59,59	0
56	MG	1A	3612	1/1	0.69	0.13	65,65,65,65	0
56	MG	2A	3466	1/1	0.69	0.17	57,57,57,57	0
56	MG	2A	3206	1/1	0.70	0.17	57,57,57,57	0
56	MG	2a	1703	1/1	0.70	0.33	77,77,77,77	0
56	MG	1a	1766	1/1	0.70	0.27	72,72,72,72	0
56	MG	1a	1682	1/1	0.70	0.10	55,55,55,55	0
56	MG	2a	1720	1/1	0.70	0.20	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	3289	1/1	0.70	0.14	55,55,55,55	0
56	MG	1A	3340	1/1	0.70	0.22	53,53,53,53	0
56	MG	1a	1862	1/1	0.70	0.28	70,70,70,70	0
56	MG	2a	1675	1/1	0.70	0.47	69,69,69,69	0
56	MG	2B	3013	1/1	0.70	0.10	72,72,72,72	0
56	MG	2A	3191	1/1	0.70	0.19	50,50,50,50	0
56	MG	1a	1674	1/1	0.71	0.23	74,74,74,74	0
56	MG	2a	1677	1/1	0.71	0.27	76,76,76,76	0
56	MG	2A	3051	1/1	0.71	0.28	49,49,49,49	0
56	MG	1A	3488	1/1	0.71	0.16	46,46,46,46	0
56	MG	2a	1636	1/1	0.71	0.17	81,81,81,81	0
56	MG	2A	3431	1/1	0.71	0.17	61,61,61,61	0
56	MG	2A	3187	1/1	0.71	0.25	57,57,57,57	0
56	MG	1A	3392	1/1	0.71	0.26	57,57,57,57	0
56	MG	2A	3482	1/1	0.71	0.17	74,74,74,74	0
56	MG	1B	216	1/1	0.71	0.13	49,49,49,49	0
56	MG	1d	502	1/1	0.71	0.15	68,68,68,68	0
56	MG	2A	3226	1/1	0.71	0.30	56,56,56,56	0
56	MG	2A	3123	1/1	0.71	0.23	69,69,69,69	0
56	MG	1a	1693	1/1	0.71	0.15	75,75,75,75	0
56	MG	1a	1711	1/1	0.71	0.15	77,77,77,77	0
56	MG	1a	1849	1/1	0.72	0.20	62,62,62,62	0
56	MG	2a	1693	1/1	0.72	0.36	63,63,63,63	0
56	MG	2A	3258	1/1	0.72	0.20	58,58,58,58	0
56	MG	2A	3264	1/1	0.72	0.12	49,49,49,49	0
56	MG	2A	3272	1/1	0.72	0.18	54,54,54,54	0
56	MG	2A	3126	1/1	0.72	0.25	57,57,57,57	0
56	MG	1A	3275	1/1	0.72	0.20	70,70,70,70	0
56	MG	2A	3299	1/1	0.72	0.24	66,66,66,66	0
56	MG	1a	1706	1/1	0.72	0.34	66,66,66,66	0
56	MG	1A	3905	1/1	0.72	0.20	54,54,54,54	0
56	MG	2A	3368	1/1	0.72	0.18	55,55,55,55	0
56	MG	2A	3404	1/1	0.72	0.20	55,55,55,55	0
56	MG	2A	3410	1/1	0.72	0.18	63,63,63,63	0
56	MG	2A	3175	1/1	0.72	0.16	58,58,58,58	0
56	MG	2A	3097	1/1	0.73	0.35	62,62,62,62	0
56	MG	1a	1739	1/1	0.73	0.34	65,65,65,65	0
56	MG	1A	3741	1/1	0.73	0.14	31,31,31,31	0
56	MG	1A	3246	1/1	0.73	0.38	59,59,59,59	0
56	MG	1n	101	1/1	0.73	0.32	71,71,71,71	0
56	MG	1A	3171	1/1	0.73	0.27	42,42,42,42	0
56	MG	1B	226	1/1	0.73	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3418	1/1	0.73	0.16	65,65,65,65	0
56	MG	2A	3231	1/1	0.73	0.14	64,64,64,64	0
56	MG	1a	1733	1/1	0.73	0.25	65,65,65,65	0
56	MG	2A	3061	1/1	0.73	0.28	61,61,61,61	0
56	MG	2A	3159	1/1	0.73	0.18	53,53,53,53	0
56	MG	2A	3168	1/1	0.73	0.09	52,52,52,52	0
56	MG	2a	1644	1/1	0.73	0.33	69,69,69,69	0
56	MG	2A	3504	1/1	0.73	0.08	64,64,64,64	0
56	MG	2a	1647	1/1	0.73	0.26	73,73,73,73	0
56	MG	2A	3518	1/1	0.73	0.15	63,63,63,63	0
56	MG	2l	201	1/1	0.73	0.18	71,71,71,71	0
56	MG	1A	3693	1/1	0.73	0.13	34,34,34,34	0
56	MG	2p	101	1/1	0.73	0.41	58,58,58,58	0
56	MG	2a	1663	1/1	0.73	0.29	65,65,65,65	0
58	MPD	1a	1860	8/8	0.73	0.20	65,70,76,77	0
56	MG	2A	3041	1/1	0.74	0.23	63,63,63,63	0
56	MG	2A	3203	1/1	0.74	0.19	71,71,71,71	0
56	MG	1a	1619	1/1	0.74	0.25	74,74,74,74	0
56	MG	2a	1609	1/1	0.74	0.28	67,67,67,67	0
56	MG	2a	1721	1/1	0.74	0.17	71,71,71,71	0
56	MG	2A	3055	1/1	0.74	0.23	62,62,62,62	0
56	MG	2A	3314	1/1	0.74	0.21	65,65,65,65	0
56	MG	1o	101	1/1	0.74	0.37	66,66,66,66	0
56	MG	2A	3336	1/1	0.74	0.14	78,78,78,78	0
56	MG	1A	3460	1/1	0.74	0.12	44,44,44,44	0
56	MG	2A	3080	1/1	0.74	0.31	61,61,61,61	0
56	MG	2A	3374	1/1	0.74	0.12	74,74,74,74	0
56	MG	1A	3624	1/1	0.74	0.08	62,62,62,62	0
56	MG	2A	3188	1/1	0.74	0.36	55,55,55,55	0
62	K	2A	3665	1/1	0.74	0.22	60,60,60,60	0
56	MG	1A	3751	1/1	0.75	0.18	43,43,43,43	0
56	MG	2A	3069	1/1	0.75	0.22	41,41,41,41	0
56	MG	1a	1637	1/1	0.75	0.32	52,52,52,52	0
56	MG	2A	3519	1/1	0.75	0.19	44,44,44,44	0
56	MG	2a	1673	1/1	0.75	0.24	65,65,65,65	0
56	MG	1b	3001	1/1	0.75	0.20	73,73,73,73	0
56	MG	1a	1724	1/1	0.75	0.30	78,78,78,78	0
56	MG	2A	3312	1/1	0.75	0.18	69,69,69,69	0
56	MG	1a	1725	1/1	0.75	0.30	59,59,59,59	0
56	MG	1A	3146	1/1	0.75	0.31	52,52,52,52	0
56	MG	2A	3334	1/1	0.75	0.12	61,61,61,61	0
56	MG	2x	109	1/1	0.75	0.21	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3263	1/1	0.75	0.12	52,52,52,52	0
56	MG	2A	3475	1/1	0.75	0.13	48,48,48,48	0
56	MG	2A	3488	1/1	0.76	0.22	74,74,74,74	0
56	MG	1a	1698	1/1	0.76	0.19	72,72,72,72	0
56	MG	1a	1859	1/1	0.76	0.17	62,62,62,62	0
56	MG	1a	1651	1/1	0.76	0.21	52,52,52,52	0
56	MG	2A	3526	1/1	0.76	0.14	60,60,60,60	0
56	MG	2a	1670	1/1	0.76	0.23	58,58,58,58	0
56	MG	2A	3563	1/1	0.76	0.18	45,45,45,45	0
56	MG	1A	3236	1/1	0.76	0.18	47,47,47,47	0
56	MG	1Q	203	1/1	0.76	0.19	47,47,47,47	0
56	MG	2A	3204	1/1	0.76	0.19	56,56,56,56	0
56	MG	2B	3004	1/1	0.76	0.21	64,64,64,64	0
56	MG	2A	3337	1/1	0.76	0.16	60,60,60,60	0
56	MG	2D	302	1/1	0.76	0.44	48,48,48,48	0
56	MG	1A	3243	1/1	0.76	0.11	55,55,55,55	0
56	MG	1f	8001	1/1	0.76	0.12	63,63,63,63	0
56	MG	1l	201	1/1	0.76	0.08	63,63,63,63	0
56	MG	2A	3398	1/1	0.76	0.11	64,64,64,64	0
56	MG	2a	1610	1/1	0.76	0.16	72,72,72,72	0
56	MG	1A	3795	1/1	0.76	0.18	39,39,39,39	0
56	MG	2a	1621	1/1	0.76	0.22	60,60,60,60	0
56	MG	1a	1627	1/1	0.76	0.29	57,57,57,57	0
56	MG	1a	1814	1/1	0.76	0.26	64,64,64,64	0
56	MG	2A	3419	1/1	0.76	0.35	44,44,44,44	0
56	MG	1a	1635	1/1	0.76	0.35	75,75,75,75	0
56	MG	2a	1640	1/1	0.76	0.42	71,71,71,71	0
56	MG	1A	3412	1/1	0.76	0.13	28,28,28,28	0
56	MG	2t	3001	1/1	0.76	0.40	66,66,66,66	0
56	MG	2x	101	1/1	0.76	0.20	70,70,70,70	0
56	MG	1a	1687	1/1	0.76	0.25	71,71,71,71	0
56	MG	2A	3273	1/1	0.76	0.15	61,61,61,61	0
56	MG	1a	1831	1/1	0.76	0.13	69,69,69,69	0
56	MG	1A	3123	1/1	0.76	0.13	41,41,41,41	0
56	MG	2A	3181	1/1	0.77	0.32	57,57,57,57	0
56	MG	1B	208	1/1	0.77	0.14	54,54,54,54	0
56	MG	1D	307	1/1	0.77	0.17	45,45,45,45	0
56	MG	1a	1773	1/1	0.77	0.39	82,82,82,82	0
56	MG	2A	3190	1/1	0.77	0.18	52,52,52,52	0
56	MG	1a	1777	1/1	0.77	0.11	74,74,74,74	0
56	MG	1a	1631	1/1	0.77	0.38	72,72,72,72	0
56	MG	1A	3591	1/1	0.77	0.28	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3060	1/1	0.77	0.22	48,48,48,48	0
56	MG	1A	3025	1/1	0.77	0.28	55,55,55,55	0
56	MG	1A	3930	1/1	0.77	0.37	32,32,32,32	0
56	MG	2a	1614	1/1	0.77	0.28	65,65,65,65	0
56	MG	2A	3160	1/1	0.77	0.15	63,63,63,63	0
56	MG	2A	3237	1/1	0.77	0.31	58,58,58,58	0
56	MG	2a	1630	1/1	0.77	0.46	76,76,76,76	0
56	MG	2x	104	1/1	0.77	0.17	72,72,72,72	0
56	MG	1a	1756	1/1	0.77	0.19	58,58,58,58	0
56	MG	1a	1644	1/1	0.77	0.22	62,62,62,62	0
56	MG	2A	3539	1/1	0.77	0.18	57,57,57,57	0
56	MG	1a	1683	1/1	0.77	0.27	67,67,67,67	0
56	MG	1D	304	1/1	0.78	0.17	49,49,49,49	0
56	MG	1a	1634	1/1	0.78	0.19	63,63,63,63	0
56	MG	1A	3361	1/1	0.78	0.21	47,47,47,47	0
56	MG	1F	304	1/1	0.78	0.28	32,32,32,32	0
56	MG	1a	1752	1/1	0.78	0.21	67,67,67,67	0
56	MG	2a	1676	1/1	0.78	0.20	68,68,68,68	0
56	MG	1r	3001	1/1	0.78	0.31	70,70,70,70	0
56	MG	2A	3411	1/1	0.78	0.20	58,58,58,58	0
56	MG	1A	3511	1/1	0.78	0.20	47,47,47,47	0
56	MG	2a	1698	1/1	0.78	0.23	77,77,77,77	0
56	MG	2A	3009	1/1	0.78	0.21	59,59,59,59	0
56	MG	1A	3868	1/1	0.78	0.15	56,56,56,56	0
56	MG	1a	1759	1/1	0.78	0.18	69,69,69,69	0
56	MG	2A	3445	1/1	0.78	0.13	61,61,61,61	0
56	MG	1a	1603	1/1	0.78	0.26	64,64,64,64	0
56	MG	2A	3052	1/1	0.78	0.27	62,62,62,62	0
56	MG	2a	1633	1/1	0.78	0.14	54,54,54,54	0
56	MG	2a	1745	1/1	0.78	0.08	71,71,71,71	0
56	MG	1A	3711	1/1	0.78	0.09	45,45,45,45	0
56	MG	2A	3479	1/1	0.78	0.22	49,49,49,49	0
56	MG	1a	1858	1/1	0.78	0.24	62,62,62,62	0
56	MG	2a	1774	1/1	0.78	0.19	68,68,68,68	0
56	MG	2a	1776	1/1	0.78	0.13	65,65,65,65	0
56	MG	2A	3176	1/1	0.78	0.14	52,52,52,52	0
56	MG	1a	1606	1/1	0.78	0.26	62,62,62,62	0
56	MG	1A	3740	1/1	0.78	0.12	47,47,47,47	0
56	MG	1a	1668	1/1	0.78	0.27	70,70,70,70	0
56	MG	1A	3143	1/1	0.78	0.17	63,63,63,63	0
56	MG	2A	3081	1/1	0.78	0.47	62,62,62,62	0
56	MG	2A	3088	1/1	0.78	0.35	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3581	1/1	0.78	0.21	67,67,67,67	0
56	MG	2A	3201	1/1	0.78	0.21	53,53,53,53	0
56	MG	2A	3621	1/1	0.78	0.11	76,76,76,76	0
56	MG	2A	3644	1/1	0.78	0.18	56,56,56,56	0
56	MG	2a	1603	1/1	0.79	0.13	60,60,60,60	0
56	MG	1a	1625	1/1	0.79	0.18	71,71,71,71	0
56	MG	1a	1852	1/1	0.79	0.26	63,63,63,63	0
56	MG	2A	3459	1/1	0.79	0.11	56,56,56,56	0
56	MG	2a	1689	1/1	0.79	0.12	75,75,75,75	0
56	MG	1a	1728	1/1	0.79	0.34	75,75,75,75	0
56	MG	1a	1729	1/1	0.79	0.20	52,52,52,52	0
56	MG	1A	3622	1/1	0.79	0.14	56,56,56,56	0
56	MG	1a	1785	1/1	0.79	0.33	71,71,71,71	0
56	MG	1a	1789	1/1	0.79	0.22	74,74,74,74	0
56	MG	2a	1632	1/1	0.79	0.28	60,60,60,60	0
56	MG	1a	1646	1/1	0.79	0.27	72,72,72,72	0
56	MG	1a	1647	1/1	0.79	0.40	66,66,66,66	0
56	MG	1A	3822	1/1	0.79	0.20	37,37,37,37	0
56	MG	1a	1806	1/1	0.79	0.30	68,68,68,68	0
56	MG	2A	3112	1/1	0.79	0.30	56,56,56,56	0
56	MG	2A	3116	1/1	0.79	0.33	73,73,73,73	0
56	MG	2A	3565	1/1	0.79	0.14	48,48,48,48	0
56	MG	1a	1809	1/1	0.79	0.13	62,62,62,62	0
56	MG	1A	3510	1/1	0.79	0.10	52,52,52,52	0
56	MG	1a	1613	1/1	0.79	0.12	75,75,75,75	0
56	MG	2A	3628	1/1	0.79	0.17	58,58,58,58	0
56	MG	2A	3405	1/1	0.79	0.12	66,66,66,66	0
56	MG	1B	213	1/1	0.79	0.14	49,49,49,49	0
56	MG	2a	1660	1/1	0.79	0.20	81,81,81,81	0
56	MG	2A	3142	1/1	0.79	0.23	61,61,61,61	0
56	MG	1a	1639	1/1	0.79	0.30	61,61,61,61	0
56	MG	2B	3007	1/1	0.79	0.21	63,63,63,63	0
56	MG	1a	1670	1/1	0.79	0.20	59,59,59,59	0
56	MG	1a	1640	1/1	0.79	0.22	71,71,71,71	0
56	MG	1a	1845	1/1	0.79	0.28	61,61,61,61	0
56	MG	1A	3662	1/1	0.80	0.13	39,39,39,39	0
56	MG	1a	1632	1/1	0.80	0.19	63,63,63,63	0
56	MG	1A	3208	1/1	0.80	0.11	45,45,45,45	0
56	MG	2A	3057	1/1	0.80	0.22	53,53,53,53	0
56	MG	1a	1793	1/1	0.80	0.15	71,71,71,71	0
56	MG	1A	3579	1/1	0.80	0.35	37,37,37,37	0
56	MG	1a	1652	1/1	0.80	0.21	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3308	1/1	0.80	0.11	51,51,51,51	0
56	MG	2A	3441	1/1	0.80	0.18	65,65,65,65	0
56	MG	2B	3001	1/1	0.80	0.13	71,71,71,71	0
56	MG	2A	3140	1/1	0.80	0.31	65,65,65,65	0
56	MG	1a	1616	1/1	0.80	0.12	73,73,73,73	0
56	MG	1t	3001	1/1	0.80	0.39	69,69,69,69	0
56	MG	2A	3462	1/1	0.80	0.21	66,66,66,66	0
56	MG	2A	3328	1/1	0.80	0.15	71,71,71,71	0
56	MG	2a	1654	1/1	0.80	0.32	62,62,62,62	0
56	MG	2D	308	1/1	0.80	0.14	47,47,47,47	0
56	MG	1A	3606	1/1	0.80	0.12	40,40,40,40	0
56	MG	2G	202	1/1	0.80	0.19	74,74,74,74	0
56	MG	1a	1689	1/1	0.80	0.32	69,69,69,69	0
56	MG	2A	3089	1/1	0.80	0.34	69,69,69,69	0
56	MG	2A	3162	1/1	0.80	0.35	57,57,57,57	0
56	MG	2A	3357	1/1	0.80	0.16	51,51,51,51	0
56	MG	2A	3092	1/1	0.80	0.31	61,61,61,61	0
56	MG	2a	1674	1/1	0.80	0.12	64,64,64,64	0
56	MG	1A	3834	1/1	0.80	0.12	47,47,47,47	0
56	MG	1A	3947	1/1	0.80	0.19	56,56,56,56	0
56	MG	2a	1620	1/1	0.80	0.48	56,56,56,56	0
56	MG	2A	3083	1/1	0.81	0.22	76,76,76,76	0
56	MG	2A	3455	1/1	0.81	0.11	53,53,53,53	0
56	MG	2A	3457	1/1	0.81	0.09	63,63,63,63	0
56	MG	2a	1601	1/1	0.81	0.24	58,58,58,58	0
56	MG	2A	3085	1/1	0.81	0.23	62,62,62,62	0
56	MG	1a	1786	1/1	0.81	0.14	65,65,65,65	0
56	MG	1x	110	1/1	0.81	0.12	58,58,58,58	0
56	MG	1A	3523	1/1	0.81	0.25	57,57,57,57	0
56	MG	1A	3802	1/1	0.81	0.09	54,54,54,54	0
56	MG	2a	1612	1/1	0.81	0.25	66,66,66,66	0
56	MG	2A	3014	1/1	0.81	0.33	76,76,76,76	0
56	MG	1A	3300	1/1	0.81	0.19	45,45,45,45	0
56	MG	2A	3031	1/1	0.81	0.24	56,56,56,56	0
56	MG	2A	3039	1/1	0.81	0.27	56,56,56,56	0
56	MG	2a	1624	1/1	0.81	0.43	64,64,64,64	0
56	MG	1a	1761	1/1	0.81	0.25	68,68,68,68	0
56	MG	2a	1719	1/1	0.81	0.21	63,63,63,63	0
56	MG	2A	3205	1/1	0.81	0.29	51,51,51,51	0
56	MG	2A	3045	1/1	0.81	0.10	56,56,56,56	0
56	MG	2A	3207	1/1	0.81	0.33	68,68,68,68	0
56	MG	1A	3717	1/1	0.81	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3216	1/1	0.81	0.79	34,34,34,34	0
56	MG	1a	1808	1/1	0.81	0.14	66,66,66,66	0
56	MG	1a	1664	1/1	0.81	0.15	71,71,71,71	0
56	MG	1F	309	1/1	0.81	0.12	43,43,43,43	0
56	MG	1a	1817	1/1	0.81	0.19	72,72,72,72	0
56	MG	2A	3065	1/1	0.81	0.36	47,47,47,47	0
56	MG	2A	3651	1/1	0.81	0.13	65,65,65,65	0
56	MG	2A	3658	1/1	0.81	0.11	49,49,49,49	0
56	MG	2A	3679	1/1	0.81	0.13	53,53,53,53	0
56	MG	2A	3420	1/1	0.81	0.09	64,64,64,64	0
56	MG	1G	3004	1/1	0.81	0.15	59,59,59,59	0
56	MG	1A	3272	1/1	0.81	0.11	52,52,52,52	0
56	MG	2A	3439	1/1	0.81	0.39	70,70,70,70	0
56	MG	1a	1783	1/1	0.81	0.12	63,63,63,63	0
56	MG	1A	3690	1/1	0.81	0.11	42,42,42,42	0
56	MG	1A	3220	1/1	0.82	0.18	28,28,28,28	0
56	MG	1A	3416	1/1	0.82	0.10	44,44,44,44	0
56	MG	2A	3233	1/1	0.82	0.13	49,49,49,49	0
56	MG	2A	3091	1/1	0.82	0.28	54,54,54,54	0
56	MG	1A	3692	1/1	0.82	0.15	58,58,58,58	0
56	MG	1a	1774	1/1	0.82	0.23	70,70,70,70	0
56	MG	1a	1696	1/1	0.82	0.29	58,58,58,58	0
56	MG	2a	1708	1/1	0.82	0.18	56,56,56,56	0
56	MG	1a	1820	1/1	0.82	0.22	63,63,63,63	0
56	MG	1A	3166	1/1	0.82	0.33	36,36,36,36	0
56	MG	2A	3520	1/1	0.82	0.17	46,46,46,46	0
56	MG	2U	202	1/1	0.82	0.29	59,59,59,59	0
56	MG	1a	1703	1/1	0.82	0.14	72,72,72,72	0
56	MG	2A	3119	1/1	0.82	0.18	49,49,49,49	0
56	MG	2a	1604	1/1	0.82	0.12	72,72,72,72	0
56	MG	2a	1657	1/1	0.82	0.23	69,69,69,69	0
56	MG	2a	1763	1/1	0.82	0.16	82,82,82,82	0
56	MG	2a	1658	1/1	0.82	0.33	58,58,58,58	0
56	MG	2A	3555	1/1	0.82	0.09	59,59,59,59	0
56	MG	1B	206	1/1	0.82	0.21	49,49,49,49	0
56	MG	2a	1778	1/1	0.82	0.17	77,77,77,77	0
56	MG	2a	1662	1/1	0.82	0.42	77,77,77,77	0
56	MG	1a	1840	1/1	0.82	0.20	67,67,67,67	0
56	MG	1A	3705	1/1	0.82	0.15	45,45,45,45	0
56	MG	1A	3555	1/1	0.82	0.21	38,38,38,38	0
56	MG	2A	3130	1/1	0.82	0.17	62,62,62,62	0
56	MG	1A	3855	1/1	0.82	0.27	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1619	1/1	0.82	0.20	65,65,65,65	0
56	MG	1a	1762	1/1	0.82	0.13	71,71,71,71	0
56	MG	2x	107	1/1	0.82	0.17	69,69,69,69	0
56	MG	2A	3156	1/1	0.82	0.34	58,58,58,58	0
56	MG	1A	3559	1/1	0.82	0.09	39,39,39,39	0
56	MG	1A	3567	1/1	0.82	0.11	52,52,52,52	0
56	MG	1A	3586	1/1	0.83	0.15	36,36,36,36	0
56	MG	2A	3636	1/1	0.83	0.11	52,52,52,52	0
56	MG	2A	3169	1/1	0.83	0.26	50,50,50,50	0
56	MG	1A	3703	1/1	0.83	0.18	43,43,43,43	0
56	MG	2A	3172	1/1	0.83	0.16	68,68,68,68	0
56	MG	1A	3078	1/1	0.83	0.24	45,45,45,45	0
56	MG	2A	3068	1/1	0.83	0.11	51,51,51,51	0
56	MG	2a	1664	1/1	0.83	0.37	65,65,65,65	0
56	MG	2a	1665	1/1	0.83	0.20	81,81,81,81	0
56	MG	1A	3922	1/1	0.83	0.38	31,31,31,31	0
56	MG	1a	1781	1/1	0.83	0.15	58,58,58,58	0
56	MG	1a	1782	1/1	0.83	0.28	58,58,58,58	0
56	MG	1A	3927	1/1	0.83	0.13	50,50,50,50	0
56	MG	1A	3229	1/1	0.83	0.14	32,32,32,32	0
56	MG	1A	3316	1/1	0.83	0.16	45,45,45,45	0
56	MG	2A	3195	1/1	0.83	0.29	43,43,43,43	0
56	MG	2E	305	1/1	0.83	0.26	45,45,45,45	0
56	MG	1a	1660	1/1	0.83	0.14	68,68,68,68	0
56	MG	2a	1683	1/1	0.83	0.15	71,71,71,71	0
56	MG	1A	3317	1/1	0.83	0.10	45,45,45,45	0
56	MG	1A	3469	1/1	0.83	0.11	39,39,39,39	0
56	MG	2A	3437	1/1	0.83	0.29	62,62,62,62	0
56	MG	1a	1801	1/1	0.83	0.08	85,85,85,85	0
56	MG	2a	1699	1/1	0.83	0.15	59,59,59,59	0
56	MG	1A	3474	1/1	0.83	0.10	56,56,56,56	0
56	MG	1a	1736	1/1	0.83	0.11	73,73,73,73	0
56	MG	1x	106	1/1	0.83	0.29	62,62,62,62	0
56	MG	1A	3179	1/1	0.83	0.14	57,57,57,57	0
56	MG	2A	3115	1/1	0.83	0.14	46,46,46,46	0
56	MG	1A	3576	1/1	0.83	0.09	43,43,43,43	0
56	MG	1A	3816	1/1	0.83	0.19	42,42,42,42	0
56	MG	1a	1633	1/1	0.83	0.29	51,51,51,51	0
56	MG	1B	224	1/1	0.83	0.19	54,54,54,54	0
56	MG	2A	3476	1/1	0.83	0.13	57,57,57,57	0
56	MG	2a	1751	1/1	0.83	0.11	77,77,77,77	0
56	MG	2A	3027	1/1	0.83	0.25	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3125	1/1	0.83	0.38	68,68,68,68	0
56	MG	1a	1758	1/1	0.83	0.11	70,70,70,70	0
56	MG	2a	1631	1/1	0.83	0.38	64,64,64,64	0
56	MG	2A	3038	1/1	0.83	0.25	49,49,49,49	0
56	MG	2A	3275	1/1	0.83	0.20	55,55,55,55	0
56	MG	2a	1634	1/1	0.83	0.22	69,69,69,69	0
56	MG	1a	1684	1/1	0.83	0.55	56,56,56,56	0
56	MG	2A	3040	1/1	0.83	0.30	42,42,42,42	0
56	MG	2A	3148	1/1	0.83	0.26	66,66,66,66	0
56	MG	1A	3490	1/1	0.83	0.14	44,44,44,44	0
56	MG	2q	201	1/1	0.83	0.20	62,62,62,62	0
56	MG	1A	3507	1/1	0.83	0.16	52,52,52,52	0
56	MG	1a	1828	1/1	0.83	0.13	60,60,60,60	0
56	MG	1A	3187	1/1	0.83	0.18	41,41,41,41	0
56	MG	2A	3579	1/1	0.83	0.13	50,50,50,50	0
56	MG	1A	3585	1/1	0.83	0.07	39,39,39,39	0
56	MG	2A	3331	1/1	0.83	0.10	57,57,57,57	0
56	MG	1A	3870	1/1	0.83	0.11	35,35,35,35	0
56	MG	2a	1650	1/1	0.83	0.35	61,61,61,61	0
56	MG	2A	3677	1/1	0.84	0.12	57,57,57,57	0
56	MG	1A	3345	1/1	0.84	0.11	45,45,45,45	0
56	MG	1A	3729	1/1	0.84	0.14	32,32,32,32	0
56	MG	2A	3218	1/1	0.84	0.25	55,55,55,55	0
56	MG	2B	3003	1/1	0.84	0.17	68,68,68,68	0
56	MG	1a	1630	1/1	0.84	0.19	64,64,64,64	0
56	MG	2B	3006	1/1	0.84	0.25	69,69,69,69	0
56	MG	2A	3222	1/1	0.84	0.11	57,57,57,57	0
56	MG	2B	3009	1/1	0.84	0.14	66,66,66,66	0
56	MG	2B	3012	1/1	0.84	0.09	64,64,64,64	0
56	MG	2A	3047	1/1	0.84	0.23	56,56,56,56	0
56	MG	2A	3434	1/1	0.84	0.14	58,58,58,58	0
56	MG	2a	1672	1/1	0.84	0.41	52,52,52,52	0
56	MG	1A	3629	1/1	0.84	0.15	64,64,64,64	0
56	MG	1A	3654	1/1	0.84	0.19	49,49,49,49	0
56	MG	2E	307	1/1	0.84	0.18	52,52,52,52	0
56	MG	1D	309	1/1	0.84	0.26	42,42,42,42	0
56	MG	2A	3240	1/1	0.84	0.28	60,60,60,60	0
56	MG	1A	3437	1/1	0.84	0.16	26,26,26,26	0
56	MG	2A	3144	1/1	0.84	0.10	49,49,49,49	0
56	MG	1F	308	1/1	0.84	0.27	56,56,56,56	0
56	MG	1A	3926	1/1	0.84	0.10	45,45,45,45	0
56	MG	2a	1605	1/1	0.84	0.12	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1740	1/1	0.84	0.16	70,70,70,70	0
56	MG	2A	3463	1/1	0.84	0.15	52,52,52,52	0
56	MG	1a	1744	1/1	0.84	0.13	62,62,62,62	0
56	MG	2A	3470	1/1	0.84	0.14	57,57,57,57	0
56	MG	1A	3781	1/1	0.84	0.08	66,66,66,66	0
56	MG	2a	1713	1/1	0.84	0.08	67,67,67,67	0
56	MG	2a	1613	1/1	0.84	0.33	61,61,61,61	0
56	MG	1A	3010	1/1	0.84	0.26	45,45,45,45	0
56	MG	2A	3079	1/1	0.84	0.25	51,51,51,51	0
56	MG	1A	3560	1/1	0.84	0.10	35,35,35,35	0
56	MG	1A	3198	1/1	0.84	0.32	60,60,60,60	0
56	MG	1x	101	1/1	0.84	0.23	69,69,69,69	0
56	MG	1a	1691	1/1	0.84	0.11	67,67,67,67	0
56	MG	2a	1626	1/1	0.84	0.35	61,61,61,61	0
56	MG	2A	3086	1/1	0.84	0.27	58,58,58,58	0
56	MG	2A	3323	1/1	0.84	0.32	50,50,50,50	0
56	MG	1A	3520	1/1	0.84	0.19	40,40,40,40	0
56	MG	1a	1694	1/1	0.84	0.16	64,64,64,64	0
56	MG	1A	3401	1/1	0.84	0.12	56,56,56,56	0
56	MG	2A	3184	1/1	0.84	0.39	59,59,59,59	0
56	MG	2e	201	1/1	0.84	0.30	57,57,57,57	0
56	MG	1A	3842	1/1	0.84	0.10	47,47,47,47	0
56	MG	1A	3535	1/1	0.84	0.14	34,34,34,34	0
56	MG	2A	3023	1/1	0.84	0.18	53,53,53,53	0
56	MG	2A	3361	1/1	0.84	0.20	60,60,60,60	0
56	MG	2A	3107	1/1	0.84	0.15	66,66,66,66	0
56	MG	1a	1653	1/1	0.84	0.34	56,56,56,56	0
56	MG	2A	3383	1/1	0.84	0.14	57,57,57,57	0
56	MG	1a	1771	1/1	0.84	0.10	71,71,71,71	0
56	MG	2A	3649	1/1	0.84	0.25	57,57,57,57	0
56	MG	2x	106	1/1	0.84	0.16	63,63,63,63	0
56	MG	2a	1648	1/1	0.84	0.12	70,70,70,70	0
56	MG	2x	108	1/1	0.84	0.52	57,57,57,57	0
56	MG	2A	3033	1/1	0.84	0.20	58,58,58,58	0
56	MG	1a	1617	1/1	0.84	0.13	69,69,69,69	0
56	MG	1A	3059	1/1	0.84	0.32	60,60,60,60	0
56	MG	1a	1638	1/1	0.85	0.17	68,68,68,68	0
56	MG	2a	1669	1/1	0.85	0.15	63,63,63,63	0
56	MG	1a	1671	1/1	0.85	0.25	57,57,57,57	0
56	MG	1a	1614	1/1	0.85	0.24	51,51,51,51	0
56	MG	1a	1769	1/1	0.85	0.10	68,68,68,68	0
56	MG	2A	3067	1/1	0.85	0.29	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3548	1/1	0.85	0.13	46,46,46,46	0
56	MG	1A	3725	1/1	0.85	0.14	46,46,46,46	0
56	MG	2A	3384	1/1	0.85	0.16	48,48,48,48	0
56	MG	2A	3133	1/1	0.85	0.15	52,52,52,52	0
56	MG	2a	1682	1/1	0.85	0.30	58,58,58,58	0
56	MG	1A	3878	1/1	0.85	0.14	51,51,51,51	0
56	MG	2A	3074	1/1	0.85	0.17	48,48,48,48	0
56	MG	2A	3228	1/1	0.85	0.29	46,46,46,46	0
56	MG	1a	1824	1/1	0.85	0.31	54,54,54,54	0
56	MG	2A	3413	1/1	0.85	0.30	62,62,62,62	0
56	MG	2a	1625	1/1	0.85	0.29	72,72,72,72	0
56	MG	2A	3147	1/1	0.85	0.17	54,54,54,54	0
56	MG	1A	3890	1/1	0.85	0.10	32,32,32,32	0
56	MG	1a	1621	1/1	0.85	0.14	71,71,71,71	0
56	MG	1a	1624	1/1	0.85	0.23	51,51,51,51	0
56	MG	1A	3727	1/1	0.85	0.10	67,67,67,67	0
56	MG	1A	3314	1/1	0.85	0.15	32,32,32,32	0
56	MG	1a	1742	1/1	0.85	0.20	71,71,71,71	0
56	MG	2a	1717	1/1	0.85	0.21	67,67,67,67	0
56	MG	2A	3270	1/1	0.85	0.14	50,50,50,50	0
56	MG	1A	3098	1/1	0.85	0.10	51,51,51,51	0
56	MG	1A	3234	1/1	0.85	0.08	41,41,41,41	0
56	MG	2a	1723	1/1	0.85	0.17	62,62,62,62	0
56	MG	2A	3090	1/1	0.85	0.16	58,58,58,58	0
56	MG	1a	1855	1/1	0.85	0.29	52,52,52,52	0
56	MG	2a	1642	1/1	0.85	0.28	75,75,75,75	0
56	MG	1a	1658	1/1	0.85	0.36	67,67,67,67	0
56	MG	2a	1761	1/1	0.85	0.19	63,63,63,63	0
56	MG	1V	201	1/1	0.85	0.13	45,45,45,45	0
56	MG	2A	3098	1/1	0.85	0.34	59,59,59,59	0
56	MG	2B	3010	1/1	0.85	0.17	69,69,69,69	0
56	MG	1a	1799	1/1	0.85	0.08	66,66,66,66	0
56	MG	2A	3465	1/1	0.85	0.21	57,57,57,57	0
56	MG	2a	1782	1/1	0.85	0.13	63,63,63,63	0
56	MG	2B	3015	1/1	0.85	0.07	76,76,76,76	0
56	MG	2a	1651	1/1	0.85	0.50	62,62,62,62	0
56	MG	2a	1652	1/1	0.85	0.39	58,58,58,58	0
56	MG	2B	3016	1/1	0.85	0.08	71,71,71,71	0
56	MG	2a	1655	1/1	0.85	0.11	68,68,68,68	0
56	MG	2a	1656	1/1	0.85	0.19	68,68,68,68	0
56	MG	2A	3100	1/1	0.85	0.32	60,60,60,60	0
56	MG	1A	3224	1/1	0.85	0.23	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2x	103	1/1	0.85	0.18	73,73,73,73	0
56	MG	2A	3046	1/1	0.85	0.31	61,61,61,61	0
56	MG	2A	3111	1/1	0.85	0.19	48,48,48,48	0
56	MG	2a	1661	1/1	0.85	0.20	65,65,65,65	0
56	MG	1a	1661	1/1	0.85	0.14	66,66,66,66	0
56	MG	1B	228	1/1	0.85	0.10	67,67,67,67	0
56	MG	1A	3587	1/1	0.85	0.12	45,45,45,45	0
56	MG	1A	3259	1/1	0.85	0.15	71,71,71,71	0
56	MG	2A	3517	1/1	0.85	0.07	60,60,60,60	0
56	MG	1A	3749	1/1	0.86	0.14	45,45,45,45	0
56	MG	2A	3199	1/1	0.86	0.23	56,56,56,56	0
56	MG	1Z	8001	1/1	0.86	0.10	60,60,60,60	0
56	MG	2a	1637	1/1	0.86	0.25	60,60,60,60	0
56	MG	10	101	1/1	0.86	0.12	48,48,48,48	0
56	MG	2A	3072	1/1	0.86	0.17	54,54,54,54	0
56	MG	15	104	1/1	0.86	0.15	63,63,63,63	0
56	MG	1a	1830	1/1	0.86	0.08	68,68,68,68	0
56	MG	1A	3678	1/1	0.86	0.13	44,44,44,44	0
56	MG	1A	3763	1/1	0.86	0.09	33,33,33,33	0
56	MG	1a	1841	1/1	0.86	0.16	67,67,67,67	0
56	MG	2A	3493	1/1	0.86	0.09	61,61,61,61	0
56	MG	1A	3269	1/1	0.86	0.22	41,41,41,41	0
56	MG	2A	3223	1/1	0.86	0.35	60,60,60,60	0
56	MG	1a	1609	1/1	0.86	0.12	68,68,68,68	0
56	MG	1A	3601	1/1	0.86	0.18	31,31,31,31	0
56	MG	2A	3087	1/1	0.86	0.09	51,51,51,51	0
56	MG	1a	1757	1/1	0.86	0.23	55,55,55,55	0
56	MG	2A	3528	1/1	0.86	0.33	51,51,51,51	0
56	MG	1a	1854	1/1	0.86	0.11	72,72,72,72	0
56	MG	2A	3239	1/1	0.86	0.12	63,63,63,63	0
56	MG	1B	202	1/1	0.86	0.27	61,61,61,61	0
56	MG	2A	3557	1/1	0.86	0.11	51,51,51,51	0
56	MG	2A	3559	1/1	0.86	0.12	47,47,47,47	0
56	MG	1B	205	1/1	0.86	0.18	57,57,57,57	0
56	MG	1a	1760	1/1	0.86	0.37	65,65,65,65	0
56	MG	2A	3571	1/1	0.86	0.15	57,57,57,57	0
56	MG	1A	3797	1/1	0.86	0.12	45,45,45,45	0
56	MG	1a	1672	1/1	0.86	0.11	61,61,61,61	0
56	MG	1a	1763	1/1	0.86	0.21	82,82,82,82	0
56	MG	2A	3602	1/1	0.86	0.17	47,47,47,47	0
56	MG	1A	3180	1/1	0.86	0.12	51,51,51,51	0
56	MG	1e	204	1/1	0.86	0.12	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	1A	3811	1/1	0.86	0.13	30,30,30,30	0
56	MG	1a	1679	1/1	0.86	0.18	81,81,81,81	0
56	MG	1A	3479	1/1	0.86	0.16	33,33,33,33	0
56	MG	2A	3114	1/1	0.86	0.15	50,50,50,50	0
56	MG	1a	1768	1/1	0.86	0.11	68,68,68,68	0
56	MG	2A	3654	1/1	0.86	0.23	50,50,50,50	0
56	MG	2A	3309	1/1	0.86	0.17	61,61,61,61	0
56	MG	2A	3661	1/1	0.86	0.18	62,62,62,62	0
56	MG	2a	1678	1/1	0.86	0.22	64,64,64,64	0
56	MG	2A	3663	1/1	0.86	0.16	55,55,55,55	0
56	MG	1o	102	1/1	0.86	0.10	49,49,49,49	0
56	MG	1A	3273	1/1	0.86	0.08	41,41,41,41	0
56	MG	2A	3316	1/1	0.86	0.11	67,67,67,67	0
56	MG	1a	1770	1/1	0.86	0.40	65,65,65,65	0
56	MG	2a	1697	1/1	0.86	0.17	65,65,65,65	0
56	MG	1A	3182	1/1	0.86	0.27	60,60,60,60	0
56	MG	1B	219	1/1	0.86	0.09	42,42,42,42	0
56	MG	1A	3712	1/1	0.86	0.11	48,48,48,48	0
56	MG	1A	3854	1/1	0.86	0.21	59,59,59,59	0
56	MG	2A	3127	1/1	0.86	0.20	61,61,61,61	0
56	MG	2a	1704	1/1	0.86	0.14	70,70,70,70	0
56	MG	2A	3002	1/1	0.86	0.28	59,59,59,59	0
56	MG	2a	1712	1/1	0.86	0.17	66,66,66,66	0
56	MG	2A	3348	1/1	0.86	0.11	41,41,41,41	0
56	MG	1B	227	1/1	0.86	0.10	51,51,51,51	0
56	MG	2A	3353	1/1	0.86	0.25	53,53,53,53	0
56	MG	2A	3010	1/1	0.86	0.13	43,43,43,43	0
56	MG	1A	3716	1/1	0.86	0.18	60,60,60,60	0
56	MG	1A	3491	1/1	0.86	0.12	35,35,35,35	0
56	MG	1a	1695	1/1	0.86	0.20	67,67,67,67	0
56	MG	2A	3024	1/1	0.86	0.21	45,45,45,45	0
56	MG	2A	3154	1/1	0.86	0.12	48,48,48,48	0
56	MG	2A	3387	1/1	0.86	0.11	69,69,69,69	0
56	MG	2Q	201	1/1	0.86	0.25	59,59,59,59	0
56	MG	2T	3004	1/1	0.86	0.07	50,50,50,50	0
56	MG	2A	3393	1/1	0.86	0.24	54,54,54,54	0
56	MG	2A	3397	1/1	0.86	0.09	48,48,48,48	0
56	MG	1a	1636	1/1	0.86	0.54	60,60,60,60	0
56	MG	2A	3028	1/1	0.86	0.07	51,51,51,51	0
56	MG	1a	1697	1/1	0.86	0.15	55,55,55,55	0
56	MG	1A	3548	1/1	0.86	0.10	47,47,47,47	0
56	MG	2A	3036	1/1	0.86	0.20	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3872	1/1	0.86	0.11	58,58,58,58	0
56	MG	1D	316	1/1	0.86	0.13	34,34,34,34	0
56	MG	1A	3550	1/1	0.86	0.13	51,51,51,51	0
56	MG	1A	3154	1/1	0.86	0.19	45,45,45,45	0
56	MG	2A	3426	1/1	0.86	0.20	60,60,60,60	0
56	MG	2a	1616	1/1	0.86	0.14	57,57,57,57	0
56	MG	1a	1718	1/1	0.86	0.10	73,73,73,73	0
56	MG	1a	1723	1/1	0.86	0.07	69,69,69,69	0
56	MG	1A	3075	1/1	0.86	0.12	37,37,37,37	0
56	MG	1a	1645	1/1	0.86	0.39	59,59,59,59	0
56	MG	1a	1813	1/1	0.86	0.10	72,72,72,72	0
56	MG	1A	3593	1/1	0.86	0.12	52,52,52,52	0
56	MG	2A	3185	1/1	0.86	0.36	56,56,56,56	0
56	MG	1A	3911	1/1	0.86	0.09	28,28,28,28	0
56	MG	1a	1818	1/1	0.86	0.23	73,73,73,73	0
56	MG	1a	1649	1/1	0.86	0.13	70,70,70,70	0
56	MG	1A	3745	1/1	0.86	0.17	49,49,49,49	0
56	MG	1A	3399	1/1	0.87	0.11	49,49,49,49	0
56	MG	2A	3509	1/1	0.87	0.11	59,59,59,59	0
56	MG	1D	319	1/1	0.87	0.08	66,66,66,66	0
56	MG	2A	3021	1/1	0.87	0.24	67,67,67,67	0
56	MG	2A	3246	1/1	0.87	0.13	54,54,54,54	0
56	MG	2A	3248	1/1	0.87	0.11	51,51,51,51	0
56	MG	2A	3522	1/1	0.87	0.13	50,50,50,50	0
56	MG	1D	321	1/1	0.87	0.15	46,46,46,46	0
56	MG	1A	3527	1/1	0.87	0.18	49,49,49,49	0
56	MG	2A	3118	1/1	0.87	0.12	47,47,47,47	0
56	MG	1A	3142	1/1	0.87	0.12	34,34,34,34	0
56	MG	2A	3025	1/1	0.87	0.20	56,56,56,56	0
56	MG	1A	3881	1/1	0.87	0.15	53,53,53,53	0
56	MG	1A	3061	1/1	0.87	0.20	43,43,43,43	0
56	MG	2a	1653	1/1	0.87	0.45	67,67,67,67	0
56	MG	2A	3029	1/1	0.87	0.15	50,50,50,50	0
56	MG	1a	1816	1/1	0.87	0.11	57,57,57,57	0
56	MG	2A	3570	1/1	0.87	0.13	43,43,43,43	0
56	MG	1A	3893	1/1	0.87	0.76	39,39,39,39	0
56	MG	2A	3575	1/1	0.87	0.12	65,65,65,65	0
56	MG	1A	3230	1/1	0.87	0.16	36,36,36,36	0
56	MG	1A	3737	1/1	0.87	0.21	31,31,31,31	0
56	MG	2A	3584	1/1	0.87	0.14	64,64,64,64	0
56	MG	2A	3134	1/1	0.87	0.15	68,68,68,68	0
56	MG	2A	3135	1/1	0.87	0.47	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1743	1/1	0.87	0.20	73,73,73,73	0
56	MG	1A	3064	1/1	0.87	0.19	46,46,46,46	0
56	MG	1a	1746	1/1	0.87	0.16	69,69,69,69	0
56	MG	2A	3043	1/1	0.87	0.31	61,61,61,61	0
56	MG	1A	3455	1/1	0.87	0.13	37,37,37,37	0
56	MG	10	107	1/1	0.87	0.13	54,54,54,54	0
56	MG	2A	3332	1/1	0.87	0.19	43,43,43,43	0
56	MG	1A	3552	1/1	0.87	0.19	32,32,32,32	0
56	MG	1a	1602	1/1	0.87	0.12	82,82,82,82	0
56	MG	1A	3623	1/1	0.87	0.22	53,53,53,53	0
56	MG	2A	3054	1/1	0.87	0.58	66,66,66,66	0
56	MG	1A	3928	1/1	0.87	0.34	35,35,35,35	0
56	MG	1a	1842	1/1	0.87	0.16	62,62,62,62	0
56	MG	2A	3355	1/1	0.87	0.19	53,53,53,53	0
56	MG	2A	3167	1/1	0.87	0.17	66,66,66,66	0
56	MG	1A	3069	1/1	0.87	0.57	30,30,30,30	0
56	MG	1A	3934	1/1	0.87	0.13	44,44,44,44	0
56	MG	2B	3005	1/1	0.87	0.27	77,77,77,77	0
56	MG	1A	3944	1/1	0.87	0.16	31,31,31,31	0
56	MG	2a	1695	1/1	0.87	0.24	58,58,58,58	0
56	MG	2A	3379	1/1	0.87	0.12	55,55,55,55	0
56	MG	2B	3008	1/1	0.87	0.25	64,64,64,64	0
56	MG	1A	3753	1/1	0.87	0.12	51,51,51,51	0
56	MG	2A	3173	1/1	0.87	0.16	56,56,56,56	0
56	MG	2A	3174	1/1	0.87	0.28	55,55,55,55	0
56	MG	1A	3948	1/1	0.87	0.29	44,44,44,44	0
56	MG	1A	3165	1/1	0.87	0.14	36,36,36,36	0
56	MG	2A	3177	1/1	0.87	0.22	54,54,54,54	0
56	MG	2A	3180	1/1	0.87	0.18	65,65,65,65	0
56	MG	1A	3764	1/1	0.87	0.20	47,47,47,47	0
56	MG	1a	1620	1/1	0.87	0.14	60,60,60,60	0
56	MG	1A	3244	1/1	0.87	0.07	31,31,31,31	0
56	MG	1A	3121	1/1	0.87	0.25	68,68,68,68	0
56	MG	1A	3250	1/1	0.87	0.10	48,48,48,48	0
56	MG	2O	202	1/1	0.87	0.11	63,63,63,63	0
56	MG	1A	3665	1/1	0.87	0.10	46,46,46,46	0
56	MG	2A	3082	1/1	0.87	0.09	47,47,47,47	0
56	MG	1a	1629	1/1	0.87	0.19	54,54,54,54	0
56	MG	1A	3329	1/1	0.87	0.16	49,49,49,49	0
56	MG	2A	3196	1/1	0.87	0.20	52,52,52,52	0
56	MG	1a	1776	1/1	0.87	0.08	80,80,80,80	0
56	MG	1A	3581	1/1	0.87	0.15	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3202	1/1	0.87	0.18	52,52,52,52	0
56	MG	2A	3440	1/1	0.87	0.08	55,55,55,55	0
56	MG	1A	3331	1/1	0.87	0.13	40,40,40,40	0
56	MG	2A	3442	1/1	0.87	0.18	64,64,64,64	0
56	MG	1B	223	1/1	0.87	0.12	43,43,43,43	0
56	MG	1A	3494	1/1	0.87	0.10	42,42,42,42	0
56	MG	1A	3256	1/1	0.87	0.36	48,48,48,48	0
56	MG	1A	3849	1/1	0.87	0.08	60,60,60,60	0
56	MG	2A	3209	1/1	0.87	0.22	61,61,61,61	0
56	MG	2A	3213	1/1	0.87	0.21	53,53,53,53	0
56	MG	2A	3216	1/1	0.87	0.13	52,52,52,52	0
56	MG	2A	3094	1/1	0.87	0.09	55,55,55,55	0
56	MG	2A	3096	1/1	0.87	0.24	62,62,62,62	0
56	MG	1x	104	1/1	0.87	0.21	69,69,69,69	0
56	MG	1A	3056	1/1	0.87	0.24	55,55,55,55	0
56	MG	1A	3130	1/1	0.87	0.39	31,31,31,31	0
56	MG	2A	3477	1/1	0.87	0.08	50,50,50,50	0
56	MG	1D	306	1/1	0.87	0.21	35,35,35,35	0
56	MG	1A	3260	1/1	0.87	0.27	42,42,42,42	0
56	MG	1A	3714	1/1	0.87	0.18	52,52,52,52	0
56	MG	2A	3234	1/1	0.87	0.13	55,55,55,55	0
58	MPD	1A	3907	8/8	0.87	0.34	51,53,55,56	0
56	MG	2A	3499	1/1	0.87	0.15	41,41,41,41	0
56	MG	2A	3502	1/1	0.87	0.10	70,70,70,70	0
56	MG	1A	3942	1/1	0.88	0.15	55,55,55,55	0
56	MG	1a	1669	1/1	0.88	0.37	57,57,57,57	0
56	MG	1a	1851	1/1	0.88	0.09	78,78,78,78	0
56	MG	1A	3070	1/1	0.88	0.09	31,31,31,31	0
56	MG	1a	1607	1/1	0.88	0.38	60,60,60,60	0
56	MG	1A	3759	1/1	0.88	0.09	53,53,53,53	0
56	MG	1a	1856	1/1	0.88	0.23	62,62,62,62	0
56	MG	1a	1612	1/1	0.88	0.21	56,56,56,56	0
56	MG	1A	3108	1/1	0.88	0.18	40,40,40,40	0
56	MG	1A	3294	1/1	0.88	0.13	42,42,42,42	0
56	MG	1a	1681	1/1	0.88	0.24	56,56,56,56	0
56	MG	2A	3364	1/1	0.88	0.13	58,58,58,58	0
56	MG	1a	1615	1/1	0.88	0.17	71,71,71,71	0
56	MG	2A	3372	1/1	0.88	0.14	58,58,58,58	0
56	MG	2A	3641	1/1	0.88	0.11	61,61,61,61	0
56	MG	1d	503	1/1	0.88	0.11	70,70,70,70	0
56	MG	1e	201	1/1	0.88	0.45	68,68,68,68	0
56	MG	2A	3381	1/1	0.88	0.16	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3424	1/1	0.88	0.19	51,51,51,51	0
56	MG	1e	203	1/1	0.88	0.15	63,63,63,63	0
56	MG	1A	3792	1/1	0.88	0.12	34,34,34,34	0
56	MG	2A	3389	1/1	0.88	0.17	49,49,49,49	0
56	MG	2A	3662	1/1	0.88	0.18	63,63,63,63	0
56	MG	1A	3223	1/1	0.88	0.12	46,46,46,46	0
56	MG	2A	3396	1/1	0.88	0.26	58,58,58,58	0
56	MG	1A	3308	1/1	0.88	0.15	58,58,58,58	0
56	MG	1A	3255	1/1	0.88	0.18	30,30,30,30	0
56	MG	1A	3467	1/1	0.88	0.11	48,48,48,48	0
56	MG	1A	3671	1/1	0.88	0.10	62,62,62,62	0
56	MG	1A	3821	1/1	0.88	0.18	37,37,37,37	0
56	MG	2A	3093	1/1	0.88	0.17	61,61,61,61	0
56	MG	1A	3557	1/1	0.88	0.15	42,42,42,42	0
56	MG	1A	3679	1/1	0.88	0.19	32,32,32,32	0
56	MG	1x	103	1/1	0.88	0.32	63,63,63,63	0
56	MG	2a	1680	1/1	0.88	0.54	58,58,58,58	0
56	MG	1A	3034	1/1	0.88	0.28	45,45,45,45	0
56	MG	2A	3422	1/1	0.88	0.16	54,54,54,54	0
56	MG	1A	3228	1/1	0.88	0.23	40,40,40,40	0
56	MG	2A	3427	1/1	0.88	0.08	63,63,63,63	0
56	MG	1x	109	1/1	0.88	0.25	63,63,63,63	0
56	MG	1A	3477	1/1	0.88	0.21	49,49,49,49	0
56	MG	2a	1696	1/1	0.88	0.35	63,63,63,63	0
56	MG	1a	1792	1/1	0.88	0.10	68,68,68,68	0
56	MG	2A	3219	1/1	0.88	0.16	45,45,45,45	0
56	MG	2A	3001	1/1	0.88	0.28	60,60,60,60	0
56	MG	1A	3119	1/1	0.88	0.23	30,30,30,30	0
56	MG	2F	302	1/1	0.88	0.13	47,47,47,47	0
56	MG	2A	3008	1/1	0.88	0.15	45,45,45,45	0
56	MG	1a	1708	1/1	0.88	0.08	64,64,64,64	0
56	MG	2A	3227	1/1	0.88	0.17	58,58,58,58	0
56	MG	1A	3482	1/1	0.88	0.13	28,28,28,28	0
56	MG	2A	3230	1/1	0.88	0.26	55,55,55,55	0
56	MG	1a	1712	1/1	0.88	0.19	70,70,70,70	0
56	MG	2W	201	1/1	0.88	0.15	62,62,62,62	0
56	MG	1A	3710	1/1	0.88	0.15	30,30,30,30	0
56	MG	1A	3486	1/1	0.88	0.20	46,46,46,46	0
56	MG	1D	313	1/1	0.88	0.11	41,41,41,41	0
56	MG	1A	3487	1/1	0.88	0.09	51,51,51,51	0
56	MG	1A	3713	1/1	0.88	0.38	59,59,59,59	0
56	MG	2a	1743	1/1	0.88	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3243	1/1	0.88	0.24	50,50,50,50	0
56	MG	2A	3472	1/1	0.88	0.08	68,68,68,68	0
56	MG	1a	1812	1/1	0.88	0.22	67,67,67,67	0
56	MG	1A	3032	1/1	0.88	0.13	35,35,35,35	0
56	MG	2A	3128	1/1	0.88	0.27	51,51,51,51	0
56	MG	1A	3263	1/1	0.88	0.23	36,36,36,36	0
56	MG	2a	1615	1/1	0.88	0.18	63,63,63,63	0
56	MG	1A	3080	1/1	0.88	0.42	33,33,33,33	0
56	MG	2A	3483	1/1	0.88	0.18	51,51,51,51	0
56	MG	1A	3270	1/1	0.88	0.06	49,49,49,49	0
56	MG	1A	3504	1/1	0.88	0.07	44,44,44,44	0
56	MG	2A	3139	1/1	0.88	0.32	57,57,57,57	0
56	MG	2A	3037	1/1	0.88	0.20	66,66,66,66	0
56	MG	2k	201	1/1	0.88	0.19	64,64,64,64	0
56	MG	2A	3274	1/1	0.88	0.13	54,54,54,54	0
56	MG	1A	3366	1/1	0.88	0.20	44,44,44,44	0
56	MG	2a	1628	1/1	0.88	0.25	58,58,58,58	0
56	MG	1N	201	1/1	0.88	0.41	41,41,41,41	0
56	MG	1A	3917	1/1	0.88	0.14	40,40,40,40	0
56	MG	1A	3920	1/1	0.88	0.19	47,47,47,47	0
56	MG	1a	1655	1/1	0.88	0.34	51,51,51,51	0
56	MG	1A	3371	1/1	0.88	0.12	30,30,30,30	0
56	MG	1A	3383	1/1	0.88	0.09	33,33,33,33	0
56	MG	10	105	1/1	0.88	0.09	49,49,49,49	0
56	MG	2A	3531	1/1	0.88	0.23	65,65,65,65	0
56	MG	2A	3533	1/1	0.88	0.09	60,60,60,60	0
56	MG	1A	3204	1/1	0.88	0.18	45,45,45,45	0
56	MG	1A	3522	1/1	0.88	0.15	39,39,39,39	0
56	MG	1A	3088	1/1	0.88	0.33	32,32,32,32	0
56	MG	1A	3526	1/1	0.88	0.10	36,36,36,36	0
56	MG	1A	3282	1/1	0.89	0.13	67,67,67,67	0
56	MG	1a	1802	1/1	0.89	0.10	71,71,71,71	0
56	MG	2A	3131	1/1	0.89	0.29	63,63,63,63	0
56	MG	1A	3426	1/1	0.89	0.13	32,32,32,32	0
56	MG	2A	3283	1/1	0.89	0.07	56,56,56,56	0
56	MG	2A	3285	1/1	0.89	0.12	49,49,49,49	0
56	MG	1B	201	1/1	0.89	0.16	53,53,53,53	0
56	MG	2A	3521	1/1	0.89	0.14	49,49,49,49	0
56	MG	1A	3614	1/1	0.89	0.10	42,42,42,42	0
56	MG	1a	1807	1/1	0.89	0.21	56,56,56,56	0
56	MG	2A	3301	1/1	0.89	0.09	52,52,52,52	0
56	MG	2A	3305	1/1	0.89	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3117	1/1	0.89	0.23	45,45,45,45	0
56	MG	1A	3760	1/1	0.89	0.09	58,58,58,58	0
56	MG	2A	3311	1/1	0.89	0.15	45,45,45,45	0
56	MG	2A	3143	1/1	0.89	0.18	56,56,56,56	0
56	MG	1A	3005	1/1	0.89	0.18	40,40,40,40	0
56	MG	2A	3558	1/1	0.89	0.15	50,50,50,50	0
56	MG	2A	3146	1/1	0.89	0.32	55,55,55,55	0
56	MG	1A	3012	1/1	0.89	0.17	35,35,35,35	0
56	MG	2A	3035	1/1	0.89	0.21	70,70,70,70	0
56	MG	2A	3326	1/1	0.89	0.15	55,55,55,55	0
56	MG	1A	3778	1/1	0.89	0.10	53,53,53,53	0
56	MG	2A	3573	1/1	0.89	0.16	59,59,59,59	0
56	MG	1A	3181	1/1	0.89	0.07	45,45,45,45	0
56	MG	2A	3577	1/1	0.89	0.09	48,48,48,48	0
56	MG	2A	3578	1/1	0.89	0.14	51,51,51,51	0
56	MG	1A	3632	1/1	0.89	0.10	34,34,34,34	0
56	MG	1A	3793	1/1	0.89	0.08	37,37,37,37	0
56	MG	2A	3335	1/1	0.89	0.14	63,63,63,63	0
56	MG	1A	3636	1/1	0.89	0.10	42,42,42,42	0
56	MG	1A	3640	1/1	0.89	0.21	43,43,43,43	0
56	MG	1A	3084	1/1	0.89	0.14	49,49,49,49	0
56	MG	1A	3472	1/1	0.89	0.11	42,42,42,42	0
56	MG	1a	1826	1/1	0.89	0.19	68,68,68,68	0
56	MG	1A	3659	1/1	0.89	0.16	38,38,38,38	0
56	MG	1D	302	1/1	0.89	0.48	34,34,34,34	0
56	MG	1A	3818	1/1	0.89	0.12	29,29,29,29	0
56	MG	1A	3554	1/1	0.89	0.23	45,45,45,45	0
56	MG	1a	1832	1/1	0.89	0.15	73,73,73,73	0
56	MG	1a	1642	1/1	0.89	0.33	68,68,68,68	0
56	MG	1A	3249	1/1	0.89	0.11	48,48,48,48	0
56	MG	1A	3826	1/1	0.89	0.10	47,47,47,47	0
56	MG	1D	311	1/1	0.89	0.23	47,47,47,47	0
56	MG	1A	3323	1/1	0.89	0.14	42,42,42,42	0
56	MG	2a	1681	1/1	0.89	0.25	69,69,69,69	0
56	MG	2A	3672	1/1	0.89	0.18	64,64,64,64	0
56	MG	2A	3674	1/1	0.89	0.38	50,50,50,50	0
56	MG	1a	1648	1/1	0.89	0.21	57,57,57,57	0
56	MG	2a	1687	1/1	0.89	0.13	62,62,62,62	0
56	MG	2A	3386	1/1	0.89	0.28	48,48,48,48	0
56	MG	2a	1690	1/1	0.89	0.17	65,65,65,65	0
56	MG	1a	1745	1/1	0.89	0.15	54,54,54,54	0
56	MG	2A	3071	1/1	0.89	0.25	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3325	1/1	0.89	0.18	42,42,42,42	0
56	MG	1A	3086	1/1	0.89	0.14	52,52,52,52	0
56	MG	1A	3684	1/1	0.89	0.07	50,50,50,50	0
56	MG	1a	1755	1/1	0.89	0.20	68,68,68,68	0
56	MG	2A	3194	1/1	0.89	0.09	54,54,54,54	0
56	MG	1A	3190	1/1	0.89	0.12	44,44,44,44	0
56	MG	1A	3569	1/1	0.89	0.11	30,30,30,30	0
56	MG	1a	1656	1/1	0.89	0.14	73,73,73,73	0
56	MG	1A	3574	1/1	0.89	0.11	32,32,32,32	0
56	MG	2a	1709	1/1	0.89	0.16	63,63,63,63	0
56	MG	1A	3134	1/1	0.89	0.21	38,38,38,38	0
56	MG	1A	3015	1/1	0.89	0.15	37,37,37,37	0
56	MG	1A	3707	1/1	0.89	0.13	52,52,52,52	0
56	MG	2A	3421	1/1	0.89	0.11	61,61,61,61	0
56	MG	1Q	201	1/1	0.89	0.16	41,41,41,41	0
56	MG	1A	3089	1/1	0.89	0.09	41,41,41,41	0
56	MG	1a	1665	1/1	0.89	0.22	55,55,55,55	0
56	MG	1U	204	1/1	0.89	0.32	35,35,35,35	0
56	MG	2F	303	1/1	0.89	0.14	50,50,50,50	0
56	MG	2A	3430	1/1	0.89	0.06	56,56,56,56	0
56	MG	1A	3021	1/1	0.89	0.25	36,36,36,36	0
56	MG	1A	3149	1/1	0.89	0.34	35,35,35,35	0
56	MG	2a	1752	1/1	0.89	0.13	64,64,64,64	0
56	MG	1A	3500	1/1	0.89	0.13	39,39,39,39	0
56	MG	1A	3910	1/1	0.89	0.26	39,39,39,39	0
56	MG	1A	3373	1/1	0.89	0.11	60,60,60,60	0
56	MG	1A	3104	1/1	0.89	0.36	32,32,32,32	0
56	MG	1A	3155	1/1	0.89	0.17	32,32,32,32	0
56	MG	1A	3721	1/1	0.89	0.13	53,53,53,53	0
56	MG	2A	3448	1/1	0.89	0.11	47,47,47,47	0
56	MG	2A	3102	1/1	0.89	0.24	48,48,48,48	0
56	MG	2A	3454	1/1	0.89	0.10	60,60,60,60	0
56	MG	1a	1680	1/1	0.89	0.12	45,45,45,45	0
56	MG	1A	3158	1/1	0.89	0.10	42,42,42,42	0
56	MG	1x	108	1/1	0.89	0.29	65,65,65,65	0
56	MG	1A	3515	1/1	0.89	0.09	46,46,46,46	0
56	MG	1A	3600	1/1	0.89	0.10	38,38,38,38	0
56	MG	1A	3072	1/1	0.89	0.12	43,43,43,43	0
56	MG	1A	3022	1/1	0.89	0.08	43,43,43,43	0
56	MG	1A	3932	1/1	0.89	0.17	51,51,51,51	0
56	MG	2A	3005	1/1	0.89	0.15	53,53,53,53	0
56	MG	2A	3120	1/1	0.89	0.20	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3006	1/1	0.89	0.28	52,52,52,52	0
56	MG	2A	3007	1/1	0.89	0.18	51,51,51,51	0
56	MG	2A	3250	1/1	0.89	0.13	48,48,48,48	0
56	MG	2A	3251	1/1	0.89	0.23	53,53,53,53	0
56	MG	1A	3168	1/1	0.89	0.16	39,39,39,39	0
56	MG	1A	3609	1/1	0.89	0.09	43,43,43,43	0
57	UNX	2A	3667	1/1	0.89	0.35	45,45,45,45	0
56	MG	2A	3489	1/1	0.89	0.22	55,55,55,55	0
56	MG	1a	1692	1/1	0.89	0.15	70,70,70,70	0
56	MG	1A	3746	1/1	0.89	0.10	40,40,40,40	0
56	MG	1A	3445	1/1	0.90	0.09	42,42,42,42	0
56	MG	1A	3935	1/1	0.90	0.16	38,38,38,38	0
56	MG	2A	3352	1/1	0.90	0.11	49,49,49,49	0
56	MG	1A	3936	1/1	0.90	0.14	32,32,32,32	0
56	MG	1A	3036	1/1	0.90	0.10	58,58,58,58	0
56	MG	2A	3564	1/1	0.90	0.08	68,68,68,68	0
56	MG	1A	3301	1/1	0.90	0.09	40,40,40,40	0
56	MG	2A	3358	1/1	0.90	0.10	43,43,43,43	0
56	MG	1a	1779	1/1	0.90	0.07	66,66,66,66	0
56	MG	1A	3551	1/1	0.90	0.42	54,54,54,54	0
56	MG	1A	3779	1/1	0.90	0.08	46,46,46,46	0
56	MG	2A	3370	1/1	0.90	0.14	62,62,62,62	0
56	MG	1A	3657	1/1	0.90	0.10	41,41,41,41	0
56	MG	1a	1688	1/1	0.90	0.32	58,58,58,58	0
56	MG	1A	3782	1/1	0.90	0.13	44,44,44,44	0
56	MG	1A	3040	1/1	0.90	0.20	49,49,49,49	0
56	MG	1A	3241	1/1	0.90	0.22	30,30,30,30	0
56	MG	1A	3183	1/1	0.90	0.16	42,42,42,42	0
56	MG	2A	3614	1/1	0.90	0.10	64,64,64,64	0
56	MG	1a	1794	1/1	0.90	0.35	69,69,69,69	0
56	MG	1A	3122	1/1	0.90	0.11	37,37,37,37	0
56	MG	2A	3212	1/1	0.90	0.27	53,53,53,53	0
56	MG	2A	3105	1/1	0.90	0.18	42,42,42,42	0
56	MG	2A	3394	1/1	0.90	0.07	62,62,62,62	0
56	MG	1A	3189	1/1	0.90	0.35	43,43,43,43	0
56	MG	2A	3217	1/1	0.90	0.21	53,53,53,53	0
56	MG	1A	3247	1/1	0.90	0.14	36,36,36,36	0
56	MG	2A	3399	1/1	0.90	0.14	53,53,53,53	0
56	MG	1A	3041	1/1	0.90	0.19	46,46,46,46	0
56	MG	2A	3659	1/1	0.90	0.07	60,60,60,60	0
56	MG	1A	3681	1/1	0.90	0.07	47,47,47,47	0
56	MG	2A	3113	1/1	0.90	0.19	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1700	1/1	0.90	0.12	50,50,50,50	0
56	MG	2A	3666	1/1	0.90	0.14	54,54,54,54	0
56	MG	2A	3668	1/1	0.90	0.13	62,62,62,62	0
56	MG	2A	3224	1/1	0.90	0.43	46,46,46,46	0
56	MG	2A	3416	1/1	0.90	0.16	62,62,62,62	0
56	MG	2A	3676	1/1	0.90	0.10	54,54,54,54	0
56	MG	2A	3225	1/1	0.90	0.18	57,57,57,57	0
56	MG	1A	3484	1/1	0.90	0.21	43,43,43,43	0
56	MG	2A	3011	1/1	0.90	0.17	59,59,59,59	0
56	MG	2A	3013	1/1	0.90	0.09	57,57,57,57	0
56	MG	1A	3160	1/1	0.90	0.12	40,40,40,40	0
56	MG	1A	3201	1/1	0.90	0.19	25,25,25,25	0
56	MG	1A	3106	1/1	0.90	0.13	39,39,39,39	0
56	MG	1A	3580	1/1	0.90	0.18	48,48,48,48	0
56	MG	2A	3235	1/1	0.90	0.28	49,49,49,49	0
56	MG	1A	3043	1/1	0.90	0.31	29,29,29,29	0
56	MG	1A	3851	1/1	0.90	0.08	63,63,63,63	0
56	MG	1A	3363	1/1	0.90	0.14	54,54,54,54	0
56	MG	2B	3011	1/1	0.90	0.11	78,78,78,78	0
56	MG	1A	3138	1/1	0.90	0.05	50,50,50,50	0
56	MG	1D	308	1/1	0.90	0.08	42,42,42,42	0
56	MG	1A	3496	1/1	0.90	0.13	40,40,40,40	0
56	MG	1A	3170	1/1	0.90	0.24	42,42,42,42	0
56	MG	1A	3218	1/1	0.90	0.15	35,35,35,35	0
56	MG	1A	3506	1/1	0.90	0.07	44,44,44,44	0
56	MG	1D	317	1/1	0.90	0.30	35,35,35,35	0
56	MG	2A	3260	1/1	0.90	0.13	63,63,63,63	0
56	MG	1A	3876	1/1	0.90	0.18	32,32,32,32	0
56	MG	1A	3115	1/1	0.90	0.21	41,41,41,41	0
56	MG	2A	3458	1/1	0.90	0.17	42,42,42,42	0
56	MG	2a	1716	1/1	0.90	0.25	72,72,72,72	0
56	MG	2A	3266	1/1	0.90	0.10	50,50,50,50	0
56	MG	1A	3508	1/1	0.90	0.13	53,53,53,53	0
56	MG	1A	3882	1/1	0.90	0.16	57,57,57,57	0
56	MG	1A	3388	1/1	0.90	0.10	42,42,42,42	0
56	MG	1G	3002	1/1	0.90	0.11	57,57,57,57	0
56	MG	1a	1654	1/1	0.90	0.16	71,71,71,71	0
56	MG	2A	3279	1/1	0.90	0.17	60,60,60,60	0
56	MG	2a	1602	1/1	0.90	0.12	64,64,64,64	0
56	MG	2A	3280	1/1	0.90	0.09	42,42,42,42	0
56	MG	1A	3221	1/1	0.90	0.38	29,29,29,29	0
56	MG	1a	1751	1/1	0.90	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1759	1/1	0.90	0.08	78,78,78,78	0
56	MG	1A	3222	1/1	0.90	0.09	62,62,62,62	0
56	MG	1H	8002	1/1	0.90	0.16	44,44,44,44	0
56	MG	2a	1764	1/1	0.90	0.09	66,66,66,66	0
56	MG	1A	3174	1/1	0.90	0.11	56,56,56,56	0
56	MG	2A	3484	1/1	0.90	0.09	53,53,53,53	0
56	MG	2A	3486	1/1	0.90	0.28	54,54,54,54	0
56	MG	1A	3274	1/1	0.90	0.09	41,41,41,41	0
56	MG	1A	3413	1/1	0.90	0.15	24,24,24,24	0
56	MG	1T	202	1/1	0.90	0.07	51,51,51,51	0
56	MG	2A	3494	1/1	0.90	0.14	60,60,60,60	0
56	MG	1a	1663	1/1	0.90	0.15	74,74,74,74	0
56	MG	1A	3175	1/1	0.90	0.26	57,57,57,57	0
56	MG	1A	3743	1/1	0.90	0.09	41,41,41,41	0
56	MG	1A	3921	1/1	0.90	0.12	55,55,55,55	0
56	MG	1A	3176	1/1	0.90	0.43	33,33,33,33	0
56	MG	1A	3925	1/1	0.90	0.16	42,42,42,42	0
56	MG	1A	3616	1/1	0.90	0.07	67,67,67,67	0
56	MG	2x	102	1/1	0.90	0.13	73,73,73,73	0
56	MG	2a	1627	1/1	0.90	0.23	58,58,58,58	0
56	MG	2A	3076	1/1	0.90	0.42	49,49,49,49	0
56	MG	2A	3077	1/1	0.90	0.12	56,56,56,56	0
56	MG	1A	3529	1/1	0.90	0.14	44,44,44,44	0
56	MG	1A	3035	1/1	0.90	0.10	33,33,33,33	0
56	MG	1A	3057	1/1	0.90	0.22	32,32,32,32	0
56	MG	1a	1675	1/1	0.90	0.14	46,46,46,46	0
56	MG	2x	110	1/1	0.90	0.20	70,70,70,70	0
56	MG	1A	3544	1/1	0.90	0.08	59,59,59,59	0
56	MG	1g	3001	1/1	0.90	0.24	62,62,62,62	0
56	MG	2A	3340	1/1	0.90	0.17	50,50,50,50	0
56	MG	2A	3551	1/1	0.90	0.12	48,48,48,48	0
56	MG	2A	3254	1/1	0.91	0.24	42,42,42,42	0
56	MG	2a	1611	1/1	0.91	0.15	59,59,59,59	0
56	MG	2A	3256	1/1	0.91	0.17	56,56,56,56	0
56	MG	1A	3326	1/1	0.91	0.12	48,48,48,48	0
56	MG	1E	302	1/1	0.91	0.26	30,30,30,30	0
56	MG	1a	1666	1/1	0.91	0.19	65,65,65,65	0
56	MG	1A	3257	1/1	0.91	0.18	55,55,55,55	0
56	MG	1F	305	1/1	0.91	0.18	28,28,28,28	0
56	MG	1A	3689	1/1	0.91	0.12	37,37,37,37	0
56	MG	1A	3124	1/1	0.91	0.17	40,40,40,40	0
56	MG	2A	3129	1/1	0.91	0.26	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3156	1/1	0.91	0.23	41,41,41,41	0
56	MG	2A	3017	1/1	0.91	0.36	48,48,48,48	0
56	MG	2A	3490	1/1	0.91	0.17	42,42,42,42	0
56	MG	2A	3492	1/1	0.91	0.13	45,45,45,45	0
56	MG	2A	3132	1/1	0.91	0.15	49,49,49,49	0
56	MG	2a	1629	1/1	0.91	0.09	78,78,78,78	0
56	MG	2A	3020	1/1	0.91	0.16	49,49,49,49	0
56	MG	1A	3871	1/1	0.91	0.12	43,43,43,43	0
56	MG	2A	3501	1/1	0.91	0.07	60,60,60,60	0
56	MG	1A	3341	1/1	0.91	0.09	35,35,35,35	0
56	MG	1A	3701	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3506	1/1	0.91	0.15	61,61,61,61	0
56	MG	1A	3128	1/1	0.91	0.21	43,43,43,43	0
56	MG	1A	3877	1/1	0.91	0.09	35,35,35,35	0
56	MG	2A	3026	1/1	0.91	0.17	41,41,41,41	0
56	MG	1A	3091	1/1	0.91	0.23	23,23,23,23	0
56	MG	1A	3267	1/1	0.91	0.24	52,52,52,52	0
56	MG	1A	3489	1/1	0.91	0.12	32,32,32,32	0
56	MG	1A	3268	1/1	0.91	0.21	40,40,40,40	0
56	MG	2A	3152	1/1	0.91	0.27	51,51,51,51	0
56	MG	2A	3032	1/1	0.91	0.29	63,63,63,63	0
56	MG	2A	3529	1/1	0.91	0.13	59,59,59,59	0
56	MG	1V	203	1/1	0.91	0.06	62,62,62,62	0
56	MG	1A	3225	1/1	0.91	0.48	38,38,38,38	0
56	MG	1A	3895	1/1	0.91	0.12	35,35,35,35	0
56	MG	2A	3544	1/1	0.91	0.08	61,61,61,61	0
56	MG	1A	3904	1/1	0.91	0.07	53,53,53,53	0
56	MG	1A	3227	1/1	0.91	0.09	39,39,39,39	0
56	MG	2A	3161	1/1	0.91	0.14	47,47,47,47	0
56	MG	13	102	1/1	0.91	0.16	53,53,53,53	0
56	MG	2A	3166	1/1	0.91	0.28	49,49,49,49	0
56	MG	1A	3908	1/1	0.91	0.09	41,41,41,41	0
56	MG	1A	3379	1/1	0.91	0.15	43,43,43,43	0
56	MG	1A	3497	1/1	0.91	0.31	45,45,45,45	0
56	MG	1A	3039	1/1	0.91	0.28	53,53,53,53	0
56	MG	2A	3344	1/1	0.91	0.22	61,61,61,61	0
56	MG	1A	3188	1/1	0.91	0.08	42,42,42,42	0
56	MG	1A	3594	1/1	0.91	0.10	48,48,48,48	0
56	MG	2A	3351	1/1	0.91	0.09	53,53,53,53	0
56	MG	2A	3576	1/1	0.91	0.08	70,70,70,70	0
56	MG	2A	3050	1/1	0.91	0.11	56,56,56,56	0
56	MG	1A	3596	1/1	0.91	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3354	1/1	0.91	0.08	59,59,59,59	0
56	MG	1a	1699	1/1	0.91	0.16	68,68,68,68	0
56	MG	1A	3118	1/1	0.91	0.33	39,39,39,39	0
56	MG	1A	3730	1/1	0.91	0.32	40,40,40,40	0
56	MG	1A	3393	1/1	0.91	0.10	31,31,31,31	0
56	MG	2A	3606	1/1	0.91	0.08	47,47,47,47	0
56	MG	2A	3363	1/1	0.91	0.09	44,44,44,44	0
56	MG	1A	3396	1/1	0.91	0.16	41,41,41,41	0
56	MG	2A	3624	1/1	0.91	0.09	48,48,48,48	0
56	MG	2A	3626	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3605	1/1	0.91	0.08	47,47,47,47	0
56	MG	2a	1679	1/1	0.91	0.37	62,62,62,62	0
56	MG	2A	3630	1/1	0.91	0.22	50,50,50,50	0
56	MG	1A	3233	1/1	0.91	0.26	50,50,50,50	0
56	MG	2A	3640	1/1	0.91	0.19	59,59,59,59	0
56	MG	2A	3186	1/1	0.91	0.31	59,59,59,59	0
56	MG	1A	3400	1/1	0.91	0.14	61,61,61,61	0
56	MG	2A	3375	1/1	0.91	0.20	50,50,50,50	0
56	MG	1a	1839	1/1	0.91	0.10	63,63,63,63	0
56	MG	1A	3167	1/1	0.91	0.20	50,50,50,50	0
56	MG	2A	3652	1/1	0.91	0.27	41,41,41,41	0
56	MG	2A	3653	1/1	0.91	0.29	52,52,52,52	0
56	MG	1A	3410	1/1	0.91	0.07	50,50,50,50	0
56	MG	1A	3085	1/1	0.91	0.27	42,42,42,42	0
56	MG	1A	3285	1/1	0.91	0.13	37,37,37,37	0
56	MG	1A	3943	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3198	1/1	0.91	0.32	59,59,59,59	0
56	MG	2A	3390	1/1	0.91	0.11	49,49,49,49	0
56	MG	1a	1628	1/1	0.91	0.38	63,63,63,63	0
56	MG	1A	3291	1/1	0.91	0.19	26,26,26,26	0
56	MG	1A	3946	1/1	0.91	0.21	29,29,29,29	0
56	MG	2A	3673	1/1	0.91	0.13	51,51,51,51	0
56	MG	1A	3619	1/1	0.91	0.18	32,32,32,32	0
56	MG	1A	3200	1/1	0.91	0.07	46,46,46,46	0
56	MG	1A	3120	1/1	0.91	0.08	55,55,55,55	0
56	MG	2A	3678	1/1	0.91	0.11	53,53,53,53	0
56	MG	1A	3769	1/1	0.91	0.05	67,67,67,67	0
56	MG	1A	3532	1/1	0.91	0.08	40,40,40,40	0
56	MG	2A	3409	1/1	0.91	0.12	56,56,56,56	0
56	MG	1A	3626	1/1	0.91	0.11	51,51,51,51	0
56	MG	2A	3210	1/1	0.91	0.20	42,42,42,42	0
56	MG	2A	3211	1/1	0.91	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1724	1/1	0.91	0.07	74,74,74,74	0
56	MG	1A	3435	1/1	0.91	0.14	35,35,35,35	0
56	MG	1A	3630	1/1	0.91	0.10	37,37,37,37	0
56	MG	2A	3214	1/1	0.91	0.37	49,49,49,49	0
56	MG	1A	3790	1/1	0.91	0.09	32,32,32,32	0
56	MG	1a	1749	1/1	0.91	0.09	59,59,59,59	0
56	MG	1A	3042	1/1	0.91	0.30	21,21,21,21	0
56	MG	2a	1757	1/1	0.91	0.10	69,69,69,69	0
56	MG	2A	3425	1/1	0.91	0.09	48,48,48,48	0
56	MG	1A	3147	1/1	0.91	0.45	36,36,36,36	0
56	MG	1A	3451	1/1	0.91	0.10	38,38,38,38	0
56	MG	1A	3796	1/1	0.91	0.21	37,37,37,37	0
56	MG	1A	3641	1/1	0.91	0.11	40,40,40,40	0
56	MG	2D	303	1/1	0.91	0.09	58,58,58,58	0
56	MG	2D	306	1/1	0.91	0.11	54,54,54,54	0
56	MG	1B	225	1/1	0.91	0.16	55,55,55,55	0
56	MG	1A	3645	1/1	0.91	0.16	37,37,37,37	0
56	MG	2A	3436	1/1	0.91	0.12	41,41,41,41	0
56	MG	2f	3001	1/1	0.91	0.14	67,67,67,67	0
56	MG	2F	301	1/1	0.91	0.11	45,45,45,45	0
56	MG	1A	3058	1/1	0.91	0.16	52,52,52,52	0
56	MG	1A	3215	1/1	0.91	0.19	48,48,48,48	0
56	MG	2A	3101	1/1	0.91	0.26	47,47,47,47	0
56	MG	1A	3466	1/1	0.91	0.23	29,29,29,29	0
56	MG	2I	3001	1/1	0.91	0.13	74,74,74,74	0
56	MG	1A	3153	1/1	0.91	0.23	49,49,49,49	0
56	MG	1A	3177	1/1	0.91	0.11	35,35,35,35	0
56	MG	1A	3470	1/1	0.91	0.06	37,37,37,37	0
56	MG	2A	3110	1/1	0.91	0.32	53,53,53,53	0
56	MG	1A	3556	1/1	0.91	0.27	39,39,39,39	0
56	MG	23	101	1/1	0.91	0.11	58,58,58,58	0
56	MG	28	102	1/1	0.91	0.14	49,49,49,49	0
56	MG	1A	3836	1/1	0.91	0.09	42,42,42,42	0
56	MG	1A	3838	1/1	0.91	0.11	45,45,45,45	0
56	MG	1A	3027	1/1	0.91	0.44	39,39,39,39	0
56	MG	1D	315	1/1	0.91	0.22	49,49,49,49	0
56	MG	1A	3843	1/1	0.91	0.11	29,29,29,29	0
56	MG	1A	3846	1/1	0.91	0.10	31,31,31,31	0
56	MG	1a	1662	1/1	0.91	0.09	70,70,70,70	0
56	MG	1A	3558	1/1	0.91	0.21	31,31,31,31	0
56	MG	1a	1650	1/1	0.92	0.29	51,51,51,51	0
56	MG	1A	3875	1/1	0.92	0.11	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1D	312	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3491	1/1	0.92	0.22	58,58,58,58	0
56	MG	2A	3276	1/1	0.92	0.11	47,47,47,47	0
56	MG	1A	3360	1/1	0.92	0.10	44,44,44,44	0
56	MG	1A	3205	1/1	0.92	0.07	30,30,30,30	0
56	MG	2A	3496	1/1	0.92	0.08	45,45,45,45	0
56	MG	1A	3539	1/1	0.92	0.21	53,53,53,53	0
56	MG	2a	1622	1/1	0.92	0.40	56,56,56,56	0
56	MG	1A	3540	1/1	0.92	0.16	42,42,42,42	0
56	MG	2A	3136	1/1	0.92	0.12	54,54,54,54	0
56	MG	1A	3542	1/1	0.92	0.09	49,49,49,49	0
56	MG	1A	3883	1/1	0.92	0.28	47,47,47,47	0
56	MG	2A	3508	1/1	0.92	0.15	50,50,50,50	0
56	MG	2A	3015	1/1	0.92	0.19	51,51,51,51	0
56	MG	2A	3514	1/1	0.92	0.07	63,63,63,63	0
56	MG	1A	3888	1/1	0.92	0.48	32,32,32,32	0
56	MG	2A	3019	1/1	0.92	0.07	51,51,51,51	0
56	MG	1E	303	1/1	0.92	0.43	33,33,33,33	0
56	MG	1E	304	1/1	0.92	0.08	50,50,50,50	0
56	MG	1a	1778	1/1	0.92	0.09	63,63,63,63	0
56	MG	2A	3149	1/1	0.92	0.15	44,44,44,44	0
56	MG	2A	3525	1/1	0.92	0.08	55,55,55,55	0
56	MG	1E	305	1/1	0.92	0.19	31,31,31,31	0
56	MG	2A	3317	1/1	0.92	0.08	54,54,54,54	0
56	MG	2A	3321	1/1	0.92	0.13	48,48,48,48	0
56	MG	2A	3530	1/1	0.92	0.09	56,56,56,56	0
56	MG	2A	3153	1/1	0.92	0.16	51,51,51,51	0
56	MG	1A	3739	1/1	0.92	0.11	28,28,28,28	0
56	MG	1A	3033	1/1	0.92	0.18	45,45,45,45	0
56	MG	1F	306	1/1	0.92	0.24	31,31,31,31	0
56	MG	1A	3365	1/1	0.92	0.08	43,43,43,43	0
56	MG	1A	3902	1/1	0.92	0.22	35,35,35,35	0
56	MG	1a	1787	1/1	0.92	0.08	65,65,65,65	0
56	MG	1A	3178	1/1	0.92	0.19	37,37,37,37	0
56	MG	1A	3107	1/1	0.92	0.10	32,32,32,32	0
56	MG	2A	3163	1/1	0.92	0.38	48,48,48,48	0
56	MG	1A	3082	1/1	0.92	0.15	59,59,59,59	0
56	MG	2A	3342	1/1	0.92	0.24	61,61,61,61	0
56	MG	1A	3909	1/1	0.92	0.18	43,43,43,43	0
56	MG	1A	3378	1/1	0.92	0.10	40,40,40,40	0
56	MG	1a	1796	1/1	0.92	0.11	68,68,68,68	0
56	MG	1a	1798	1/1	0.92	0.07	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1N	202	1/1	0.92	0.07	46,46,46,46	0
56	MG	1A	3631	1/1	0.92	0.12	43,43,43,43	0
56	MG	1A	3478	1/1	0.92	0.07	41,41,41,41	0
56	MG	2A	3042	1/1	0.92	0.13	57,57,57,57	0
56	MG	2A	3356	1/1	0.92	0.16	55,55,55,55	0
56	MG	2A	3580	1/1	0.92	0.19	52,52,52,52	0
56	MG	1A	3633	1/1	0.92	0.14	31,31,31,31	0
56	MG	2A	3044	1/1	0.92	0.25	61,61,61,61	0
56	MG	2a	1667	1/1	0.92	0.17	66,66,66,66	0
56	MG	2A	3179	1/1	0.92	0.13	52,52,52,52	0
56	MG	1U	203	1/1	0.92	0.26	36,36,36,36	0
56	MG	1A	3919	1/1	0.92	0.18	41,41,41,41	0
56	MG	2A	3365	1/1	0.92	0.14	48,48,48,48	0
56	MG	1A	3019	1/1	0.92	0.36	27,27,27,27	0
56	MG	2A	3623	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	3639	1/1	0.92	0.22	45,45,45,45	0
56	MG	1A	3293	1/1	0.92	0.11	35,35,35,35	0
56	MG	1a	1810	1/1	0.92	0.22	74,74,74,74	0
56	MG	1A	3924	1/1	0.92	0.13	51,51,51,51	0
56	MG	10	102	1/1	0.92	0.15	43,43,43,43	0
56	MG	1A	3768	1/1	0.92	0.16	27,27,27,27	0
56	MG	2A	3382	1/1	0.92	0.22	56,56,56,56	0
56	MG	1A	3385	1/1	0.92	0.13	53,53,53,53	0
56	MG	2A	3192	1/1	0.92	0.08	50,50,50,50	0
56	MG	2A	3193	1/1	0.92	0.33	66,66,66,66	0
56	MG	1A	3386	1/1	0.92	0.12	32,32,32,32	0
56	MG	1A	3161	1/1	0.92	0.13	35,35,35,35	0
56	MG	2a	1688	1/1	0.92	0.07	58,58,58,58	0
56	MG	17	102	1/1	0.92	0.08	35,35,35,35	0
56	MG	2A	3391	1/1	0.92	0.09	48,48,48,48	0
56	MG	1a	1601	1/1	0.92	0.16	50,50,50,50	0
56	MG	1A	3929	1/1	0.92	0.29	31,31,31,31	0
56	MG	2A	3395	1/1	0.92	0.15	58,58,58,58	0
56	MG	1A	3389	1/1	0.92	0.10	44,44,44,44	0
56	MG	1A	3931	1/1	0.92	0.17	42,42,42,42	0
56	MG	1A	3295	1/1	0.92	0.17	50,50,50,50	0
56	MG	1A	3164	1/1	0.92	0.38	29,29,29,29	0
56	MG	1A	3791	1/1	0.92	0.11	60,60,60,60	0
56	MG	1A	3661	1/1	0.92	0.10	40,40,40,40	0
56	MG	1A	3939	1/1	0.92	0.18	32,32,32,32	0
56	MG	2A	3208	1/1	0.92	0.18	50,50,50,50	0
56	MG	1A	3941	1/1	0.92	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1711	1/1	0.92	0.49	77,77,77,77	0
56	MG	1a	1710	1/1	0.92	0.16	58,58,58,58	0
56	MG	1A	3186	1/1	0.92	0.12	34,34,34,34	0
56	MG	1A	3023	1/1	0.92	0.16	35,35,35,35	0
56	MG	1A	3666	1/1	0.92	0.14	37,37,37,37	0
56	MG	1A	3141	1/1	0.92	0.08	43,43,43,43	0
56	MG	1A	3676	1/1	0.92	0.17	34,34,34,34	0
56	MG	1A	3048	1/1	0.92	0.33	40,40,40,40	0
56	MG	1a	1622	1/1	0.92	0.22	65,65,65,65	0
56	MG	1a	1727	1/1	0.92	0.12	51,51,51,51	0
56	MG	1a	1623	1/1	0.92	0.09	65,65,65,65	0
56	MG	1A	3815	1/1	0.92	0.09	27,27,27,27	0
56	MG	2a	1730	1/1	0.92	0.09	66,66,66,66	0
56	MG	1a	1731	1/1	0.92	0.16	63,63,63,63	0
56	MG	1A	3403	1/1	0.92	0.10	35,35,35,35	0
56	MG	1B	203	1/1	0.92	0.18	55,55,55,55	0
56	MG	1a	1734	1/1	0.92	0.10	54,54,54,54	0
56	MG	1A	3261	1/1	0.92	0.22	52,52,52,52	0
56	MG	1A	3262	1/1	0.92	0.20	42,42,42,42	0
56	MG	1d	504	1/1	0.92	0.07	82,82,82,82	0
56	MG	1A	3685	1/1	0.92	0.15	42,42,42,42	0
56	MG	2D	305	1/1	0.92	0.13	46,46,46,46	0
56	MG	1A	3053	1/1	0.92	0.43	34,34,34,34	0
56	MG	1A	3414	1/1	0.92	0.11	63,63,63,63	0
56	MG	1A	3191	1/1	0.92	0.19	40,40,40,40	0
56	MG	2a	1772	1/1	0.92	0.15	62,62,62,62	0
56	MG	1A	3589	1/1	0.92	0.15	46,46,46,46	0
56	MG	1A	3420	1/1	0.92	0.06	43,43,43,43	0
56	MG	1A	3028	1/1	0.92	0.08	39,39,39,39	0
56	MG	1A	3030	1/1	0.92	0.10	28,28,28,28	0
56	MG	2a	1783	1/1	0.92	0.16	67,67,67,67	0
56	MG	1a	1750	1/1	0.92	0.11	63,63,63,63	0
56	MG	1A	3431	1/1	0.92	0.09	29,29,29,29	0
56	MG	1A	3597	1/1	0.92	0.15	34,34,34,34	0
56	MG	1a	1753	1/1	0.92	0.19	50,50,50,50	0
56	MG	1A	3333	1/1	0.92	0.09	45,45,45,45	0
56	MG	2R	8001	1/1	0.92	0.16	50,50,50,50	0
56	MG	1A	3337	1/1	0.92	0.11	36,36,36,36	0
56	MG	2A	3467	1/1	0.92	0.08	62,62,62,62	0
56	MG	1A	3860	1/1	0.92	0.16	35,35,35,35	0
56	MG	20	8001	1/1	0.92	0.12	60,60,60,60	0
56	MG	21	101	1/1	0.92	0.07	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3471	1/1	0.92	0.13	48,48,48,48	0
56	MG	1a	1643	1/1	0.92	0.07	65,65,65,65	0
56	MG	2A	3473	1/1	0.92	0.06	57,57,57,57	0
56	MG	1A	3096	1/1	0.92	0.16	33,33,33,33	0
56	MG	2A	3262	1/1	0.92	0.22	49,49,49,49	0
56	MG	1A	3528	1/1	0.92	0.20	45,45,45,45	0
56	MG	1A	3076	1/1	0.92	0.43	37,37,37,37	0
56	MG	2A	3481	1/1	0.92	0.11	59,59,59,59	0
57	UNX	1A	3906	1/1	0.92	0.32	38,38,38,38	0
56	MG	1A	3024	1/1	0.92	0.35	34,34,34,34	0
56	MG	1A	3534	1/1	0.92	0.07	36,36,36,36	0
56	MG	2A	3271	1/1	0.92	0.10	60,60,60,60	0
59	ARG	1B	229	12/12	0.92	0.14	41,46,51,52	0
56	MG	1D	310	1/1	0.92	0.10	36,36,36,36	0
56	MG	2A	3137	1/1	0.93	0.25	49,49,49,49	0
56	MG	2A	3609	1/1	0.93	0.06	58,58,58,58	0
56	MG	1a	1833	1/1	0.93	0.06	73,73,73,73	0
56	MG	2A	3414	1/1	0.93	0.10	53,53,53,53	0
56	MG	1A	3083	1/1	0.93	0.09	34,34,34,34	0
56	MG	1A	3137	1/1	0.93	0.13	32,32,32,32	0
56	MG	1A	3495	1/1	0.93	0.08	37,37,37,37	0
56	MG	1A	3252	1/1	0.93	0.40	41,41,41,41	0
56	MG	1A	3561	1/1	0.93	0.08	54,54,54,54	0
56	MG	2A	3631	1/1	0.93	0.07	57,57,57,57	0
56	MG	2A	3259	1/1	0.93	0.23	59,59,59,59	0
56	MG	2A	3639	1/1	0.93	0.09	57,57,57,57	0
56	MG	1A	3563	1/1	0.93	0.18	23,23,23,23	0
56	MG	1A	3254	1/1	0.93	0.10	52,52,52,52	0
56	MG	1a	1850	1/1	0.93	0.10	72,72,72,72	0
56	MG	2A	3150	1/1	0.93	0.28	46,46,46,46	0
56	MG	1A	3362	1/1	0.93	0.07	41,41,41,41	0
56	MG	15	101	1/1	0.93	0.20	32,32,32,32	0
56	MG	2A	3432	1/1	0.93	0.06	49,49,49,49	0
56	MG	1A	3571	1/1	0.93	0.08	45,45,45,45	0
56	MG	2A	3053	1/1	0.93	0.32	58,58,58,58	0
56	MG	1A	3097	1/1	0.93	0.32	34,34,34,34	0
56	MG	19	101	1/1	0.93	0.24	48,48,48,48	0
56	MG	1A	3649	1/1	0.93	0.11	36,36,36,36	0
56	MG	2A	3058	1/1	0.93	0.13	31,31,31,31	0
56	MG	1B	214	1/1	0.93	0.18	44,44,44,44	0
56	MG	2A	3664	1/1	0.93	0.08	55,55,55,55	0
56	MG	1A	3747	1/1	0.93	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3282	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3062	1/1	0.93	0.29	44,44,44,44	0
56	MG	2A	3063	1/1	0.93	0.08	53,53,53,53	0
56	MG	2A	3286	1/1	0.93	0.13	51,51,51,51	0
56	MG	1A	3195	1/1	0.93	0.13	41,41,41,41	0
56	MG	1a	1605	1/1	0.93	0.09	67,67,67,67	0
56	MG	1a	1676	1/1	0.93	0.28	54,54,54,54	0
56	MG	2A	3170	1/1	0.93	0.14	52,52,52,52	0
56	MG	1B	217	1/1	0.93	0.08	59,59,59,59	0
56	MG	2A	3464	1/1	0.93	0.14	65,65,65,65	0
56	MG	2A	3070	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3006	1/1	0.93	0.16	34,34,34,34	0
56	MG	1a	1608	1/1	0.93	0.12	78,78,78,78	0
56	MG	1B	220	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3075	1/1	0.93	0.11	42,42,42,42	0
56	MG	2A	3315	1/1	0.93	0.10	48,48,48,48	0
56	MG	1A	3752	1/1	0.93	0.07	50,50,50,50	0
56	MG	1A	3296	1/1	0.93	0.07	45,45,45,45	0
56	MG	2a	1691	1/1	0.93	0.18	60,60,60,60	0
56	MG	2A	3318	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3320	1/1	0.93	0.07	56,56,56,56	0
56	MG	2A	3478	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3060	1/1	0.93	0.18	33,33,33,33	0
56	MG	1A	3375	1/1	0.93	0.06	56,56,56,56	0
56	MG	1A	3885	1/1	0.93	0.22	30,30,30,30	0
56	MG	2a	1700	1/1	0.93	0.08	65,65,65,65	0
56	MG	2A	3324	1/1	0.93	0.22	51,51,51,51	0
56	MG	1A	3887	1/1	0.93	0.10	36,36,36,36	0
56	MG	1A	3376	1/1	0.93	0.10	29,29,29,29	0
56	MG	1A	3519	1/1	0.93	0.09	56,56,56,56	0
56	MG	2a	1707	1/1	0.93	0.15	68,68,68,68	0
56	MG	1A	3892	1/1	0.93	0.26	31,31,31,31	0
56	MG	1a	1784	1/1	0.93	0.12	60,60,60,60	0
56	MG	1x	102	1/1	0.93	0.20	64,64,64,64	0
56	MG	1A	3765	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3377	1/1	0.93	0.09	34,34,34,34	0
56	MG	2A	3338	1/1	0.93	0.22	40,40,40,40	0
56	MG	2A	3495	1/1	0.93	0.08	65,65,65,65	0
56	MG	1x	105	1/1	0.93	0.15	64,64,64,64	0
56	MG	1A	3670	1/1	0.93	0.15	46,46,46,46	0
56	MG	2A	3500	1/1	0.93	0.11	51,51,51,51	0
56	MG	2Q	202	1/1	0.93	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1x	107	1/1	0.93	0.16	56,56,56,56	0
56	MG	2A	3346	1/1	0.93	0.13	60,60,60,60	0
56	MG	1A	3773	1/1	0.93	0.08	44,44,44,44	0
56	MG	2V	202	1/1	0.93	0.15	53,53,53,53	0
56	MG	2a	1732	1/1	0.93	0.05	74,74,74,74	0
56	MG	2a	1734	1/1	0.93	0.08	69,69,69,69	0
56	MG	1a	1626	1/1	0.93	0.13	60,60,60,60	0
56	MG	2A	3095	1/1	0.93	0.22	47,47,47,47	0
56	MG	2a	1747	1/1	0.93	0.08	66,66,66,66	0
56	MG	1A	3457	1/1	0.93	0.08	28,28,28,28	0
56	MG	1A	3672	1/1	0.93	0.12	45,45,45,45	0
56	MG	1A	3226	1/1	0.93	0.37	36,36,36,36	0
56	MG	1A	3463	1/1	0.93	0.09	31,31,31,31	0
56	MG	2A	3003	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3465	1/1	0.93	0.06	50,50,50,50	0
56	MG	1A	3026	1/1	0.93	0.27	32,32,32,32	0
56	MG	1A	3380	1/1	0.93	0.19	44,44,44,44	0
56	MG	1A	3017	1/1	0.93	0.22	25,25,25,25	0
56	MG	1A	3533	1/1	0.93	0.07	51,51,51,51	0
56	MG	2a	1769	1/1	0.93	0.09	73,73,73,73	0
56	MG	2a	1770	1/1	0.93	0.06	68,68,68,68	0
56	MG	1A	3008	1/1	0.93	0.20	47,47,47,47	0
56	MG	1a	1805	1/1	0.93	0.13	70,70,70,70	0
56	MG	1A	3112	1/1	0.93	0.17	37,37,37,37	0
56	MG	2a	1777	1/1	0.93	0.12	66,66,66,66	0
56	MG	1A	3473	1/1	0.93	0.16	39,39,39,39	0
56	MG	2A	3532	1/1	0.93	0.10	50,50,50,50	0
56	MG	1F	303	1/1	0.93	0.29	38,38,38,38	0
56	MG	1A	3809	1/1	0.93	0.06	40,40,40,40	0
56	MG	1A	3321	1/1	0.93	0.16	26,26,26,26	0
56	MG	2A	3117	1/1	0.93	0.18	55,55,55,55	0
56	MG	1A	3207	1/1	0.93	0.21	35,35,35,35	0
56	MG	1A	3391	1/1	0.93	0.09	50,50,50,50	0
56	MG	1A	3185	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3820	1/1	0.93	0.11	33,33,33,33	0
56	MG	1A	3480	1/1	0.93	0.07	35,35,35,35	0
56	MG	1A	3209	1/1	0.93	0.37	40,40,40,40	0
56	MG	1A	3824	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3211	1/1	0.93	0.64	30,30,30,30	0
56	MG	2A	3568	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3392	1/1	0.93	0.12	52,52,52,52	0
56	MG	1a	1821	1/1	0.93	0.07	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3832	1/1	0.93	0.11	45,45,45,45	0
56	MG	2A	3030	1/1	0.93	0.20	51,51,51,51	0
56	MG	1A	3330	1/1	0.93	0.20	33,33,33,33	0
56	MG	1A	3213	1/1	0.93	0.39	37,37,37,37	0
56	MG	2A	3236	1/1	0.93	0.17	50,50,50,50	0
56	MG	1R	201	1/1	0.93	0.19	35,35,35,35	0
56	MG	2A	3400	1/1	0.93	0.17	54,54,54,54	0
56	MG	1R	203	1/1	0.93	0.10	39,39,39,39	0
56	MG	1A	3020	1/1	0.93	0.28	36,36,36,36	0
56	MG	1A	3093	1/1	0.93	0.18	50,50,50,50	0
56	MG	1A	3133	1/1	0.93	0.17	35,35,35,35	0
56	MG	1A	3564	1/1	0.94	0.09	35,35,35,35	0
56	MG	1A	3566	1/1	0.94	0.10	41,41,41,41	0
56	MG	1A	3813	1/1	0.94	0.07	35,35,35,35	0
56	MG	1A	3669	1/1	0.94	0.06	64,64,64,64	0
56	MG	2A	3281	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	3310	1/1	0.94	0.08	30,30,30,30	0
56	MG	1A	3063	1/1	0.94	0.09	37,37,37,37	0
56	MG	1B	210	1/1	0.94	0.06	57,57,57,57	0
56	MG	1A	3136	1/1	0.94	0.07	33,33,33,33	0
56	MG	1A	3095	1/1	0.94	0.26	44,44,44,44	0
56	MG	2a	1617	1/1	0.94	0.16	51,51,51,51	0
56	MG	1A	3575	1/1	0.94	0.12	55,55,55,55	0
56	MG	2A	3293	1/1	0.94	0.07	63,63,63,63	0
56	MG	1A	3823	1/1	0.94	0.09	59,59,59,59	0
56	MG	1A	3318	1/1	0.94	0.08	25,25,25,25	0
56	MG	2A	3304	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3319	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3831	1/1	0.94	0.07	58,58,58,58	0
56	MG	1A	3682	1/1	0.94	0.08	41,41,41,41	0
56	MG	1A	3833	1/1	0.94	0.06	59,59,59,59	0
56	MG	1A	3038	1/1	0.94	0.20	39,39,39,39	0
56	MG	2A	3145	1/1	0.94	0.35	53,53,53,53	0
56	MG	1A	3322	1/1	0.94	0.06	68,68,68,68	0
56	MG	1A	3837	1/1	0.94	0.08	46,46,46,46	0
56	MG	1A	3687	1/1	0.94	0.15	46,46,46,46	0
56	MG	1B	230	1/1	0.94	0.08	55,55,55,55	0
56	MG	1A	3839	1/1	0.94	0.18	41,41,41,41	0
56	MG	1a	1775	1/1	0.94	0.14	66,66,66,66	0
56	MG	1A	3688	1/1	0.94	0.16	40,40,40,40	0
56	MG	1A	3582	1/1	0.94	0.30	39,39,39,39	0
56	MG	1A	3845	1/1	0.94	0.07	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3402	1/1	0.94	0.07	36,36,36,36	0
56	MG	1A	3847	1/1	0.94	0.07	46,46,46,46	0
56	MG	1A	3003	1/1	0.94	0.14	40,40,40,40	0
56	MG	1A	3324	1/1	0.94	0.08	34,34,34,34	0
56	MG	2A	3333	1/1	0.94	0.13	58,58,58,58	0
56	MG	1A	3700	1/1	0.94	0.07	35,35,35,35	0
56	MG	2a	1645	1/1	0.94	0.15	68,68,68,68	0
56	MG	1A	3046	1/1	0.94	0.23	37,37,37,37	0
56	MG	2A	3534	1/1	0.94	0.19	50,50,50,50	0
56	MG	1A	3859	1/1	0.94	0.06	35,35,35,35	0
56	MG	1A	3702	1/1	0.94	0.10	37,37,37,37	0
56	MG	2A	3034	1/1	0.94	0.21	49,49,49,49	0
56	MG	1a	1788	1/1	0.94	0.07	67,67,67,67	0
56	MG	1A	3864	1/1	0.94	0.10	42,42,42,42	0
56	MG	1a	1790	1/1	0.94	0.08	59,59,59,59	0
56	MG	1D	318	1/1	0.94	0.18	51,51,51,51	0
56	MG	1A	3100	1/1	0.94	0.15	28,28,28,28	0
56	MG	1A	3704	1/1	0.94	0.12	36,36,36,36	0
56	MG	2A	3350	1/1	0.94	0.13	65,65,65,65	0
56	MG	1A	3327	1/1	0.94	0.06	46,46,46,46	0
56	MG	2A	3566	1/1	0.94	0.11	62,62,62,62	0
56	MG	1A	3194	1/1	0.94	0.09	40,40,40,40	0
56	MG	2A	3569	1/1	0.94	0.13	66,66,66,66	0
56	MG	1A	3514	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3874	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3572	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3178	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3265	1/1	0.94	0.16	32,32,32,32	0
56	MG	1A	3169	1/1	0.94	0.32	37,37,37,37	0
56	MG	1A	3145	1/1	0.94	0.26	38,38,38,38	0
56	MG	2A	3359	1/1	0.94	0.09	47,47,47,47	0
56	MG	2A	3182	1/1	0.94	0.28	57,57,57,57	0
56	MG	2A	3362	1/1	0.94	0.10	46,46,46,46	0
56	MG	2A	3048	1/1	0.94	0.36	51,51,51,51	0
56	MG	2A	3049	1/1	0.94	0.09	62,62,62,62	0
56	MG	2A	3599	1/1	0.94	0.07	59,59,59,59	0
56	MG	1A	3429	1/1	0.94	0.12	34,34,34,34	0
56	MG	2A	3366	1/1	0.94	0.08	44,44,44,44	0
56	MG	2A	3604	1/1	0.94	0.10	49,49,49,49	0
56	MG	2A	3367	1/1	0.94	0.09	59,59,59,59	0
56	MG	1F	307	1/1	0.94	0.19	36,36,36,36	0
56	MG	1A	3199	1/1	0.94	0.26	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3525	1/1	0.94	0.12	31,31,31,31	0
56	MG	2A	3189	1/1	0.94	0.09	49,49,49,49	0
56	MG	1G	3001	1/1	0.94	0.07	69,69,69,69	0
56	MG	1A	3231	1/1	0.94	0.11	36,36,36,36	0
56	MG	1A	3271	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3886	1/1	0.94	0.11	38,38,38,38	0
56	MG	1A	3726	1/1	0.94	0.05	51,51,51,51	0
56	MG	1A	3342	1/1	0.94	0.14	33,33,33,33	0
56	MG	1a	1815	1/1	0.94	0.11	57,57,57,57	0
56	MG	2A	3197	1/1	0.94	0.25	50,50,50,50	0
56	MG	1A	3728	1/1	0.94	0.06	38,38,38,38	0
56	MG	1A	3071	1/1	0.94	0.19	32,32,32,32	0
56	MG	1A	3611	1/1	0.94	0.09	50,50,50,50	0
56	MG	1A	3894	1/1	0.94	0.07	53,53,53,53	0
56	MG	1A	3530	1/1	0.94	0.18	43,43,43,43	0
56	MG	1A	3897	1/1	0.94	0.22	34,34,34,34	0
56	MG	1A	3531	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3357	1/1	0.94	0.13	29,29,29,29	0
56	MG	2A	3656	1/1	0.94	0.12	50,50,50,50	0
56	MG	1U	205	1/1	0.94	0.13	40,40,40,40	0
56	MG	2a	1705	1/1	0.94	0.06	62,62,62,62	0
56	MG	1A	3359	1/1	0.94	0.08	34,34,34,34	0
56	MG	1A	3618	1/1	0.94	0.18	30,30,30,30	0
56	MG	1A	3458	1/1	0.94	0.11	69,69,69,69	0
56	MG	2A	3403	1/1	0.94	0.13	60,60,60,60	0
56	MG	1A	3172	1/1	0.94	0.21	37,37,37,37	0
56	MG	1A	3173	1/1	0.94	0.13	40,40,40,40	0
56	MG	2A	3406	1/1	0.94	0.10	56,56,56,56	0
56	MG	10	104	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	3464	1/1	0.94	0.10	26,26,26,26	0
56	MG	1A	3915	1/1	0.94	0.15	29,29,29,29	0
56	MG	2a	1718	1/1	0.94	0.06	62,62,62,62	0
56	MG	2A	3675	1/1	0.94	0.07	59,59,59,59	0
56	MG	1a	1701	1/1	0.94	0.07	53,53,53,53	0
56	MG	11	101	1/1	0.94	0.07	34,34,34,34	0
56	MG	11	103	1/1	0.94	0.14	41,41,41,41	0
56	MG	2A	3417	1/1	0.94	0.08	62,62,62,62	0
56	MG	2a	1727	1/1	0.94	0.09	64,64,64,64	0
56	MG	1A	3750	1/1	0.94	0.06	44,44,44,44	0
56	MG	1A	3239	1/1	0.94	0.09	41,41,41,41	0
56	MG	2a	1733	1/1	0.94	0.10	75,75,75,75	0
56	MG	1A	3001	1/1	0.94	0.25	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1738	1/1	0.94	0.07	58,58,58,58	0
56	MG	2a	1742	1/1	0.94	0.12	70,70,70,70	0
56	MG	1A	3279	1/1	0.94	0.07	49,49,49,49	0
56	MG	1A	3051	1/1	0.94	0.30	32,32,32,32	0
56	MG	1a	1715	1/1	0.94	0.17	59,59,59,59	0
56	MG	19	103	1/1	0.94	0.07	51,51,51,51	0
56	MG	1a	1720	1/1	0.94	0.18	52,52,52,52	0
56	MG	2A	3229	1/1	0.94	0.28	45,45,45,45	0
56	MG	1A	3283	1/1	0.94	0.12	32,32,32,32	0
56	MG	1A	3549	1/1	0.94	0.17	32,32,32,32	0
56	MG	1a	1861	1/1	0.94	0.07	72,72,72,72	0
56	MG	1A	3471	1/1	0.94	0.07	33,33,33,33	0
56	MG	2A	3435	1/1	0.94	0.06	54,54,54,54	0
56	MG	1A	3638	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3150	1/1	0.94	0.39	32,32,32,32	0
56	MG	2a	1767	1/1	0.94	0.14	63,63,63,63	0
56	MG	1A	3286	1/1	0.94	0.10	27,27,27,27	0
56	MG	2A	3238	1/1	0.94	0.21	55,55,55,55	0
56	MG	2a	1771	1/1	0.94	0.05	79,79,79,79	0
56	MG	1a	1730	1/1	0.94	0.05	55,55,55,55	0
56	MG	2D	307	1/1	0.94	0.24	46,46,46,46	0
56	MG	2A	3103	1/1	0.94	0.06	63,63,63,63	0
56	MG	2E	304	1/1	0.94	0.17	47,47,47,47	0
56	MG	2A	3443	1/1	0.94	0.13	53,53,53,53	0
56	MG	2a	1780	1/1	0.94	0.06	70,70,70,70	0
56	MG	2A	3241	1/1	0.94	0.14	45,45,45,45	0
56	MG	2A	3242	1/1	0.94	0.09	55,55,55,55	0
56	MG	2A	3451	1/1	0.94	0.06	53,53,53,53	0
56	MG	2A	3104	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3287	1/1	0.94	0.21	41,41,41,41	0
56	MG	1A	3777	1/1	0.94	0.13	39,39,39,39	0
56	MG	1A	3644	1/1	0.94	0.17	38,38,38,38	0
56	MG	2A	3109	1/1	0.94	0.20	54,54,54,54	0
56	MG	1A	3245	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3646	1/1	0.94	0.09	37,37,37,37	0
56	MG	1A	3152	1/1	0.94	0.36	36,36,36,36	0
56	MG	2T	3001	1/1	0.94	0.15	54,54,54,54	0
56	MG	1A	3029	1/1	0.94	0.06	30,30,30,30	0
56	MG	2U	201	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3656	1/1	0.94	0.08	41,41,41,41	0
56	MG	1A	3109	1/1	0.94	0.30	40,40,40,40	0
56	MG	2V	203	1/1	0.94	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3129	1/1	0.94	0.22	30,30,30,30	0
56	MG	1A	3111	1/1	0.94	0.15	30,30,30,30	0
56	MG	1A	3945	1/1	0.94	0.33	38,38,38,38	0
56	MG	2A	3265	1/1	0.94	0.07	60,60,60,60	0
56	MG	1A	3062	1/1	0.94	0.22	41,41,41,41	0
56	MG	1a	1747	1/1	0.94	0.10	56,56,56,56	0
56	MG	1a	1748	1/1	0.94	0.07	74,74,74,74	0
56	MG	1A	3159	1/1	0.94	0.37	38,38,38,38	0
56	MG	1A	3664	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3807	1/1	0.94	0.09	60,60,60,60	0
56	MG	2A	3595	1/1	0.95	0.07	66,66,66,66	0
56	MG	2A	3596	1/1	0.95	0.06	56,56,56,56	0
56	MG	1A	3568	1/1	0.95	0.08	44,44,44,44	0
56	MG	1A	3219	1/1	0.95	0.08	34,34,34,34	0
56	MG	1F	301	1/1	0.95	0.05	44,44,44,44	0
56	MG	2A	3267	1/1	0.95	0.07	49,49,49,49	0
56	MG	1F	302	1/1	0.95	0.14	31,31,31,31	0
56	MG	1a	1836	1/1	0.95	0.07	61,61,61,61	0
56	MG	1A	3708	1/1	0.95	0.14	35,35,35,35	0
56	MG	2A	3617	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3918	1/1	0.95	0.06	27,27,27,27	0
56	MG	1A	3709	1/1	0.95	0.08	37,37,37,37	0
56	MG	1A	3266	1/1	0.95	0.34	31,31,31,31	0
56	MG	1A	3299	1/1	0.95	0.08	47,47,47,47	0
56	MG	2A	3278	1/1	0.95	0.16	61,61,61,61	0
56	MG	2A	3056	1/1	0.95	0.26	41,41,41,41	0
56	MG	1A	3151	1/1	0.95	0.13	31,31,31,31	0
56	MG	2A	3634	1/1	0.95	0.08	48,48,48,48	0
56	MG	1A	3524	1/1	0.95	0.07	55,55,55,55	0
56	MG	2A	3165	1/1	0.95	0.28	47,47,47,47	0
56	MG	2A	3059	1/1	0.95	0.16	46,46,46,46	0
56	MG	2A	3284	1/1	0.95	0.07	44,44,44,44	0
56	MG	1A	3343	1/1	0.95	0.09	25,25,25,25	0
56	MG	2A	3646	1/1	0.95	0.06	66,66,66,66	0
56	MG	1A	3090	1/1	0.95	0.20	29,29,29,29	0
56	MG	1G	3003	1/1	0.95	0.17	60,60,60,60	0
56	MG	2A	3291	1/1	0.95	0.07	52,52,52,52	0
56	MG	1A	3643	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3305	1/1	0.95	0.21	47,47,47,47	0
56	MG	2A	3066	1/1	0.95	0.17	59,59,59,59	0
56	MG	2A	3300	1/1	0.95	0.24	42,42,42,42	0
56	MG	2A	3446	1/1	0.95	0.06	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3447	1/1	0.95	0.16	42,42,42,42	0
56	MG	1A	3047	1/1	0.95	0.37	44,44,44,44	0
56	MG	2A	3302	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3099	1/1	0.95	0.74	34,34,34,34	0
56	MG	2A	3453	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3408	1/1	0.95	0.13	42,42,42,42	0
56	MG	2A	3306	1/1	0.95	0.08	59,59,59,59	0
56	MG	1O	8001	1/1	0.95	0.06	44,44,44,44	0
56	MG	1A	3652	1/1	0.95	0.16	40,40,40,40	0
56	MG	1A	3933	1/1	0.95	0.23	49,49,49,49	0
56	MG	2A	3073	1/1	0.95	0.12	50,50,50,50	0
56	MG	1A	3184	1/1	0.95	0.05	37,37,37,37	0
56	MG	1A	3092	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3733	1/1	0.95	0.07	29,29,29,29	0
56	MG	1d	505	1/1	0.95	0.12	77,77,77,77	0
56	MG	1U	201	1/1	0.95	0.21	37,37,37,37	0
56	MG	2A	3468	1/1	0.95	0.05	69,69,69,69	0
56	MG	2A	3469	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3735	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3251	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3113	1/1	0.95	0.26	35,35,35,35	0
56	MG	1A	3253	1/1	0.95	0.09	40,40,40,40	0
56	MG	1A	3418	1/1	0.95	0.07	52,52,52,52	0
56	MG	2A	3084	1/1	0.95	0.16	42,42,42,42	0
56	MG	1i	3001	1/1	0.95	0.17	68,68,68,68	0
56	MG	1Y	502	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3848	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	3320	1/1	0.95	0.09	26,26,26,26	0
56	MG	1A	3663	1/1	0.95	0.08	48,48,48,48	0
56	MG	10	103	1/1	0.95	0.06	42,42,42,42	0
56	MG	1A	3423	1/1	0.95	0.06	57,57,57,57	0
56	MG	1A	3372	1/1	0.95	0.06	28,28,28,28	0
56	MG	2D	304	1/1	0.95	0.63	44,44,44,44	0
56	MG	2A	3487	1/1	0.95	0.07	56,56,56,56	0
56	MG	1a	1673	1/1	0.95	0.28	53,53,53,53	0
56	MG	2A	3339	1/1	0.95	0.05	65,65,65,65	0
56	MG	1A	3857	1/1	0.95	0.11	44,44,44,44	0
56	MG	2E	301	1/1	0.95	0.27	45,45,45,45	0
56	MG	2E	302	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3858	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3114	1/1	0.95	0.16	34,34,34,34	0
56	MG	1A	3428	1/1	0.95	0.10	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1B	207	1/1	0.95	0.24	45,45,45,45	0
56	MG	1a	1780	1/1	0.95	0.06	71,71,71,71	0
56	MG	1A	3861	1/1	0.95	0.06	50,50,50,50	0
56	MG	17	101	1/1	0.95	0.06	36,36,36,36	0
56	MG	1A	3546	1/1	0.95	0.06	41,41,41,41	0
56	MG	1x	112	1/1	0.95	0.07	65,65,65,65	0
56	MG	2O	201	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	3603	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	3126	1/1	0.95	0.15	32,32,32,32	0
56	MG	2A	3106	1/1	0.95	0.18	49,49,49,49	0
56	MG	1A	3755	1/1	0.95	0.07	45,45,45,45	0
56	MG	1a	1686	1/1	0.95	0.18	67,67,67,67	0
56	MG	2a	1744	1/1	0.95	0.10	62,62,62,62	0
56	MG	2A	3511	1/1	0.95	0.07	64,64,64,64	0
56	MG	1A	3673	1/1	0.95	0.17	44,44,44,44	0
56	MG	2A	3360	1/1	0.95	0.17	62,62,62,62	0
56	MG	2V	201	1/1	0.95	0.06	64,64,64,64	0
56	MG	1A	3674	1/1	0.95	0.06	39,39,39,39	0
56	MG	1A	3762	1/1	0.95	0.07	45,45,45,45	0
56	MG	1a	1690	1/1	0.95	0.15	55,55,55,55	0
56	MG	2A	3221	1/1	0.95	0.21	51,51,51,51	0
56	MG	1A	3675	1/1	0.95	0.10	36,36,36,36	0
56	MG	1A	3101	1/1	0.95	0.24	32,32,32,32	0
56	MG	1A	3432	1/1	0.95	0.12	34,34,34,34	0
56	MG	1A	3767	1/1	0.95	0.17	43,43,43,43	0
56	MG	1A	3880	1/1	0.95	0.06	35,35,35,35	0
56	MG	1a	1610	1/1	0.95	0.07	71,71,71,71	0
56	MG	1a	1800	1/1	0.95	0.05	66,66,66,66	0
56	MG	1a	1611	1/1	0.95	0.20	49,49,49,49	0
56	MG	1A	3608	1/1	0.95	0.09	36,36,36,36	0
56	MG	2A	3380	1/1	0.95	0.07	59,59,59,59	0
56	MG	1A	3434	1/1	0.95	0.07	38,38,38,38	0
56	MG	2A	3541	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3770	1/1	0.95	0.05	50,50,50,50	0
56	MG	1A	3045	1/1	0.95	0.28	40,40,40,40	0
56	MG	2a	1781	1/1	0.95	0.48	50,50,50,50	0
56	MG	1A	3776	1/1	0.95	0.08	40,40,40,40	0
56	MG	2A	3385	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3212	1/1	0.95	0.38	30,30,30,30	0
56	MG	1a	1707	1/1	0.95	0.11	47,47,47,47	0
56	MG	1A	3501	1/1	0.95	0.06	43,43,43,43	0
56	MG	2A	3561	1/1	0.95	0.07	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1709	1/1	0.95	0.10	56,56,56,56	0
56	MG	1a	1811	1/1	0.95	0.07	73,73,73,73	0
56	MG	1A	3502	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3891	1/1	0.95	0.15	38,38,38,38	0
56	MG	2a	1623	1/1	0.95	0.33	49,49,49,49	0
56	MG	1A	3049	1/1	0.95	0.11	28,28,28,28	0
56	MG	1A	3131	1/1	0.95	0.20	35,35,35,35	0
56	MG	2A	3247	1/1	0.95	0.11	52,52,52,52	0
56	MG	1A	3328	1/1	0.95	0.19	49,49,49,49	0
56	MG	1A	3691	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3288	1/1	0.95	0.07	25,25,25,25	0
56	MG	1A	3900	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3079	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3696	1/1	0.95	0.09	40,40,40,40	0
56	MG	1A	3217	1/1	0.95	0.42	33,33,33,33	0
56	MG	1A	3513	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3627	1/1	0.95	0.08	40,40,40,40	0
56	MG	1A	3461	1/1	0.95	0.08	30,30,30,30	0
56	MG	1A	3196	1/1	0.95	0.06	41,41,41,41	0
56	MG	2A	3586	1/1	0.95	0.08	68,68,68,68	0
60	ZN	24	501	1/1	0.95	0.25	94,94,94,94	0
56	MG	2A	3594	1/1	0.95	0.07	82,82,82,82	0
56	MG	1A	3065	1/1	0.96	0.14	37,37,37,37	0
56	MG	1A	3068	1/1	0.96	0.15	40,40,40,40	0
56	MG	1A	3509	1/1	0.96	0.10	39,39,39,39	0
56	MG	2A	3155	1/1	0.96	0.07	46,46,46,46	0
56	MG	2A	3592	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3315	1/1	0.96	0.10	48,48,48,48	0
56	MG	1A	3016	1/1	0.96	0.35	30,30,30,30	0
56	MG	1A	3787	1/1	0.96	0.06	31,31,31,31	0
56	MG	1a	1834	1/1	0.96	0.07	57,57,57,57	0
56	MG	1A	3788	1/1	0.96	0.08	55,55,55,55	0
56	MG	2A	3601	1/1	0.96	0.10	54,54,54,54	0
56	MG	1a	1838	1/1	0.96	0.05	69,69,69,69	0
56	MG	2A	3603	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3423	1/1	0.96	0.05	56,56,56,56	0
56	MG	1A	3278	1/1	0.96	0.08	28,28,28,28	0
56	MG	2A	3608	1/1	0.96	0.09	62,62,62,62	0
56	MG	1A	3896	1/1	0.96	0.13	31,31,31,31	0
56	MG	1A	3697	1/1	0.96	0.17	37,37,37,37	0
56	MG	2A	3615	1/1	0.96	0.06	63,63,63,63	0
56	MG	1A	3898	1/1	0.96	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3899	1/1	0.96	0.14	41,41,41,41	0
56	MG	1a	1741	1/1	0.96	0.07	63,63,63,63	0
56	MG	1a	1846	1/1	0.96	0.05	48,48,48,48	0
56	MG	2A	3433	1/1	0.96	0.09	52,52,52,52	0
56	MG	2A	3287	1/1	0.96	0.06	60,60,60,60	0
56	MG	2A	3629	1/1	0.96	0.05	57,57,57,57	0
56	MG	2A	3288	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3699	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3102	1/1	0.96	0.11	31,31,31,31	0
56	MG	1A	3903	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3407	1/1	0.96	0.08	47,47,47,47	0
56	MG	2A	3294	1/1	0.96	0.07	50,50,50,50	0
56	MG	2A	3296	1/1	0.96	0.14	42,42,42,42	0
56	MG	2A	3643	1/1	0.96	0.07	54,54,54,54	0
56	MG	1A	3516	1/1	0.96	0.06	38,38,38,38	0
56	MG	2A	3645	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3517	1/1	0.96	0.10	33,33,33,33	0
56	MG	2A	3648	1/1	0.96	0.07	64,64,64,64	0
56	MG	1A	3518	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3570	1/1	0.96	0.20	42,42,42,42	0
56	MG	1A	3706	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3810	1/1	0.96	0.22	28,28,28,28	0
56	MG	1A	3054	1/1	0.96	0.06	30,30,30,30	0
56	MG	1A	3637	1/1	0.96	0.08	33,33,33,33	0
56	MG	2A	3655	1/1	0.96	0.06	46,46,46,46	0
56	MG	1A	3814	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3572	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3573	1/1	0.96	0.10	35,35,35,35	0
56	MG	2A	3660	1/1	0.96	0.30	47,47,47,47	0
56	MG	2A	3313	1/1	0.96	0.06	44,44,44,44	0
56	MG	1A	3817	1/1	0.96	0.09	32,32,32,32	0
56	MG	2A	3461	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3105	1/1	0.96	0.31	42,42,42,42	0
56	MG	1A	3923	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3521	1/1	0.96	0.05	44,44,44,44	0
56	MG	2A	3671	1/1	0.96	0.09	44,44,44,44	0
56	MG	2a	1685	1/1	0.96	0.05	68,68,68,68	0
56	MG	1A	3642	1/1	0.96	0.09	32,32,32,32	0
56	MG	2A	3319	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3135	1/1	0.96	0.15	33,33,33,33	0
56	MG	1A	3237	1/1	0.96	0.16	38,38,38,38	0
56	MG	1A	3238	1/1	0.96	0.04	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3055	1/1	0.96	0.08	37,37,37,37	0
56	MG	1R	204	1/1	0.96	0.10	39,39,39,39	0
56	MG	1T	201	1/1	0.96	0.12	52,52,52,52	0
56	MG	2A	3681	1/1	0.96	0.09	54,54,54,54	0
56	MG	1A	3648	1/1	0.96	0.09	37,37,37,37	0
56	MG	2A	3474	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3417	1/1	0.96	0.08	34,34,34,34	0
56	MG	1U	202	1/1	0.96	0.25	42,42,42,42	0
56	MG	1A	3374	1/1	0.96	0.06	31,31,31,31	0
56	MG	2A	3200	1/1	0.96	0.29	52,52,52,52	0
56	MG	1a	1772	1/1	0.96	0.08	68,68,68,68	0
56	MG	1A	3094	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3157	1/1	0.96	0.04	33,33,33,33	0
56	MG	1A	3004	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3732	1/1	0.96	0.07	46,46,46,46	0
56	MG	1W	3001	1/1	0.96	0.24	38,38,38,38	0
56	MG	1W	3002	1/1	0.96	0.24	41,41,41,41	0
56	MG	1A	3018	1/1	0.96	0.13	33,33,33,33	0
56	MG	1A	3841	1/1	0.96	0.07	45,45,45,45	0
56	MG	2D	301	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3734	1/1	0.96	0.06	49,49,49,49	0
56	MG	1A	3110	1/1	0.96	0.08	35,35,35,35	0
56	MG	1A	3660	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3738	1/1	0.96	0.35	36,36,36,36	0
56	MG	1A	3297	1/1	0.96	0.17	37,37,37,37	0
56	MG	2A	3004	1/1	0.96	0.13	52,52,52,52	0
56	MG	1A	3592	1/1	0.96	0.06	43,43,43,43	0
56	MG	1A	3382	1/1	0.96	0.08	30,30,30,30	0
56	MG	2a	1726	1/1	0.96	0.08	70,70,70,70	0
56	MG	1A	3850	1/1	0.96	0.07	44,44,44,44	0
56	MG	2E	303	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3011	1/1	0.96	0.14	37,37,37,37	0
56	MG	1A	3852	1/1	0.96	0.10	47,47,47,47	0
56	MG	1a	1791	1/1	0.96	0.13	74,74,74,74	0
56	MG	2a	1737	1/1	0.96	0.05	74,74,74,74	0
56	MG	2A	3505	1/1	0.96	0.07	59,59,59,59	0
56	MG	2a	1740	1/1	0.96	0.06	73,73,73,73	0
56	MG	1B	204	1/1	0.96	0.08	56,56,56,56	0
56	MG	2A	3012	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	3744	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3433	1/1	0.96	0.11	48,48,48,48	0
56	MG	2A	3512	1/1	0.96	0.09	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1750	1/1	0.96	0.05	76,76,76,76	0
56	MG	2N	8001	1/1	0.96	0.04	55,55,55,55	0
56	MG	1A	3163	1/1	0.96	0.07	33,33,33,33	0
56	MG	2a	1753	1/1	0.96	0.07	58,58,58,58	0
56	MG	2A	3515	1/1	0.96	0.06	62,62,62,62	0
56	MG	2a	1755	1/1	0.96	0.07	72,72,72,72	0
56	MG	2P	3401	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3667	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3018	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3668	1/1	0.96	0.18	51,51,51,51	0
56	MG	2A	3122	1/1	0.96	0.25	44,44,44,44	0
56	MG	2T	3002	1/1	0.96	0.05	58,58,58,58	0
56	MG	2T	3003	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	3335	1/1	0.96	0.07	44,44,44,44	0
56	MG	2a	1768	1/1	0.96	0.13	69,69,69,69	0
56	MG	1A	3493	1/1	0.96	0.08	29,29,29,29	0
56	MG	2A	3524	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3144	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3866	1/1	0.96	0.14	36,36,36,36	0
56	MG	2A	3377	1/1	0.96	0.08	49,49,49,49	0
56	MG	2a	1775	1/1	0.96	0.07	65,65,65,65	0
56	MG	2A	3378	1/1	0.96	0.09	50,50,50,50	0
56	MG	1A	3602	1/1	0.96	0.10	48,48,48,48	0
56	MG	1A	3439	1/1	0.96	0.09	31,31,31,31	0
56	MG	1A	3757	1/1	0.96	0.07	38,38,38,38	0
56	MG	28	101	1/1	0.96	0.11	62,62,62,62	0
56	MG	1A	3443	1/1	0.96	0.06	35,35,35,35	0
56	MG	1B	221	1/1	0.96	0.13	51,51,51,51	0
56	MG	1A	3547	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3077	1/1	0.96	0.18	41,41,41,41	0
56	MG	2A	3245	1/1	0.96	0.06	56,56,56,56	0
56	MG	1A	3677	1/1	0.96	0.11	40,40,40,40	0
56	MG	2A	3388	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3499	1/1	0.96	0.22	43,43,43,43	0
56	MG	1A	3446	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3766	1/1	0.96	0.21	42,42,42,42	0
56	MG	2A	3138	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3879	1/1	0.96	0.05	66,66,66,66	0
56	MG	2A	3252	1/1	0.96	0.08	41,41,41,41	0
56	MG	1a	1618	1/1	0.96	0.06	73,73,73,73	0
56	MG	2A	3255	1/1	0.96	0.09	69,69,69,69	0
56	MG	1A	3450	1/1	0.96	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3567	1/1	0.96	0.07	69,69,69,69	0
56	MG	1D	303	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3306	1/1	0.96	0.07	40,40,40,40	0
56	MG	1A	3307	1/1	0.96	0.09	34,34,34,34	0
56	MG	2A	3261	1/1	0.96	0.06	52,52,52,52	0
56	MG	1a	1722	1/1	0.96	0.15	67,67,67,67	0
56	MG	1A	3505	1/1	0.96	0.10	50,50,50,50	0
56	MG	1A	3127	1/1	0.96	0.27	28,28,28,28	0
56	MG	2A	3407	1/1	0.96	0.07	59,59,59,59	0
56	MG	2A	3408	1/1	0.96	0.06	66,66,66,66	0
56	MG	1A	3617	1/1	0.96	0.04	60,60,60,60	0
61	SF4	1d	501	8/8	0.96	0.06	72,75,79,82	0
56	MG	1a	1726	1/1	0.96	0.06	60,60,60,60	0
56	MG	2A	3638	1/1	0.97	0.06	58,58,58,58	0
56	MG	1A	3453	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3232	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3456	1/1	0.97	0.06	36,36,36,36	0
56	MG	2A	3642	1/1	0.97	0.15	51,51,51,51	0
56	MG	1A	3276	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3073	1/1	0.97	0.20	32,32,32,32	0
56	MG	1A	3719	1/1	0.97	0.10	42,42,42,42	0
56	MG	1a	1825	1/1	0.97	0.06	66,66,66,66	0
56	MG	2A	3647	1/1	0.97	0.06	60,60,60,60	0
56	MG	2A	3232	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3459	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3723	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	3647	1/1	0.97	0.08	28,28,28,28	0
56	MG	1a	1829	1/1	0.97	0.09	55,55,55,55	0
56	MG	1A	3578	1/1	0.97	0.11	36,36,36,36	0
56	MG	1A	3394	1/1	0.97	0.07	33,33,33,33	0
56	MG	2A	3480	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3825	1/1	0.97	0.07	46,46,46,46	0
56	MG	2A	3657	1/1	0.97	0.22	49,49,49,49	0
56	MG	1A	3650	1/1	0.97	0.05	40,40,40,40	0
56	MG	1A	3829	1/1	0.97	0.07	40,40,40,40	0
56	MG	1A	3395	1/1	0.97	0.07	43,43,43,43	0
56	MG	2A	3485	1/1	0.97	0.09	53,53,53,53	0
56	MG	1A	3653	1/1	0.97	0.05	47,47,47,47	0
56	MG	1A	3002	1/1	0.97	0.04	44,44,44,44	0
56	MG	1A	3347	1/1	0.97	0.07	30,30,30,30	0
56	MG	1A	3835	1/1	0.97	0.07	59,59,59,59	0
56	MG	1A	3350	1/1	0.97	0.10	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3670	1/1	0.97	0.10	50,50,50,50	0
56	MG	1A	3355	1/1	0.97	0.07	31,31,31,31	0
56	MG	2A	3369	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3736	1/1	0.97	0.07	37,37,37,37	0
56	MG	2A	3371	1/1	0.97	0.04	50,50,50,50	0
56	MG	1A	3356	1/1	0.97	0.06	26,26,26,26	0
56	MG	2A	3373	1/1	0.97	0.05	45,45,45,45	0
56	MG	2A	3497	1/1	0.97	0.10	51,51,51,51	0
56	MG	2A	3151	1/1	0.97	0.18	41,41,41,41	0
56	MG	1a	1848	1/1	0.97	0.07	69,69,69,69	0
56	MG	1A	3313	1/1	0.97	0.06	35,35,35,35	0
56	MG	1Q	202	1/1	0.97	0.08	35,35,35,35	0
56	MG	2a	1686	1/1	0.97	0.04	69,69,69,69	0
56	MG	2A	3503	1/1	0.97	0.05	62,62,62,62	0
56	MG	2A	3257	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3132	1/1	0.97	0.16	39,39,39,39	0
56	MG	1Q	204	1/1	0.97	0.10	44,44,44,44	0
56	MG	1A	3588	1/1	0.97	0.08	33,33,33,33	0
56	MG	1A	3844	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3280	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3937	1/1	0.97	0.24	32,32,32,32	0
56	MG	2A	3513	1/1	0.97	0.11	52,52,52,52	0
56	MG	1A	3938	1/1	0.97	0.17	33,33,33,33	0
56	MG	2A	3064	1/1	0.97	0.11	46,46,46,46	0
56	MG	2A	3516	1/1	0.97	0.08	57,57,57,57	0
56	MG	1A	3590	1/1	0.97	0.07	47,47,47,47	0
56	MG	2A	3164	1/1	0.97	0.10	46,46,46,46	0
56	MG	2B	3017	1/1	0.97	0.06	66,66,66,66	0
56	MG	2A	3269	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	3940	1/1	0.97	0.06	42,42,42,42	0
56	MG	2a	1706	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3281	1/1	0.97	0.08	35,35,35,35	0
56	MG	1A	3067	1/1	0.97	0.09	35,35,35,35	0
56	MG	1A	3007	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3475	1/1	0.97	0.03	32,32,32,32	0
56	MG	1A	3364	1/1	0.97	0.05	39,39,39,39	0
56	MG	1A	3415	1/1	0.97	0.05	55,55,55,55	0
56	MG	2A	3277	1/1	0.97	0.15	67,67,67,67	0
56	MG	1A	3148	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	3087	1/1	0.97	0.25	38,38,38,38	0
56	MG	1A	3536	1/1	0.97	0.15	35,35,35,35	0
56	MG	1A	3481	1/1	0.97	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3756	1/1	0.97	0.06	39,39,39,39	0
56	MG	2A	3536	1/1	0.97	0.09	57,57,57,57	0
56	MG	1A	3368	1/1	0.97	0.05	58,58,58,58	0
56	MG	2a	1722	1/1	0.97	0.05	66,66,66,66	0
56	MG	2A	3540	1/1	0.97	0.06	47,47,47,47	0
56	MG	1A	3483	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	3541	1/1	0.97	0.08	35,35,35,35	0
56	MG	2A	3547	1/1	0.97	0.07	55,55,55,55	0
56	MG	2a	1729	1/1	0.97	0.12	64,64,64,64	0
56	MG	1A	3370	1/1	0.97	0.06	35,35,35,35	0
56	MG	2A	3550	1/1	0.97	0.05	43,43,43,43	0
56	MG	1a	1677	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3242	1/1	0.97	0.07	29,29,29,29	0
56	MG	2a	1735	1/1	0.97	0.12	74,74,74,74	0
56	MG	2a	1736	1/1	0.97	0.07	66,66,66,66	0
56	MG	1A	3162	1/1	0.97	0.06	36,36,36,36	0
56	MG	13	101	1/1	0.97	0.12	38,38,38,38	0
56	MG	2A	3415	1/1	0.97	0.08	52,52,52,52	0
56	MG	2a	1741	1/1	0.97	0.12	68,68,68,68	0
56	MG	1A	3206	1/1	0.97	0.06	35,35,35,35	0
56	MG	2A	3562	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3683	1/1	0.97	0.05	46,46,46,46	0
56	MG	15	103	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3125	1/1	0.97	0.04	29,29,29,29	0
56	MG	2A	3298	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3013	1/1	0.97	0.18	29,29,29,29	0
56	MG	1A	3686	1/1	0.97	0.19	49,49,49,49	0
56	MG	1A	3430	1/1	0.97	0.06	32,32,32,32	0
56	MG	2A	3424	1/1	0.97	0.06	63,63,63,63	0
56	MG	2X	101	1/1	0.97	0.09	61,61,61,61	0
56	MG	1A	3492	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3303	1/1	0.97	0.07	44,44,44,44	0
56	MG	2a	1758	1/1	0.97	0.10	66,66,66,66	0
56	MG	1A	3775	1/1	0.97	0.05	36,36,36,36	0
56	MG	2a	1760	1/1	0.97	0.05	65,65,65,65	0
56	MG	1A	3014	1/1	0.97	0.16	41,41,41,41	0
56	MG	2a	1762	1/1	0.97	0.04	79,79,79,79	0
56	MG	2A	3429	1/1	0.97	0.06	58,58,58,58	0
56	MG	1A	3248	1/1	0.97	0.05	37,37,37,37	0
56	MG	2A	3307	1/1	0.97	0.04	48,48,48,48	0
56	MG	1A	3553	1/1	0.97	0.07	58,58,58,58	0
56	MG	1A	3620	1/1	0.97	0.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3210	1/1	0.97	0.06	33,33,33,33	0
56	MG	2A	3583	1/1	0.97	0.07	68,68,68,68	0
56	MG	2a	1607	1/1	0.97	0.07	70,70,70,70	0
56	MG	1A	3884	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3193	1/1	0.97	0.16	33,33,33,33	0
56	MG	2A	3587	1/1	0.97	0.05	70,70,70,70	0
56	MG	1A	3786	1/1	0.97	0.08	38,38,38,38	0
56	MG	2A	3438	1/1	0.97	0.05	56,56,56,56	0
56	MG	1D	301	1/1	0.97	0.10	35,35,35,35	0
56	MG	2a	1779	1/1	0.97	0.08	67,67,67,67	0
56	MG	1A	3031	1/1	0.97	0.28	32,32,32,32	0
56	MG	2A	3598	1/1	0.97	0.04	54,54,54,54	0
56	MG	1A	3625	1/1	0.97	0.10	36,36,36,36	0
56	MG	1A	3889	1/1	0.97	0.24	35,35,35,35	0
56	MG	1a	1702	1/1	0.97	0.10	51,51,51,51	0
56	MG	1A	3436	1/1	0.97	0.07	33,33,33,33	0
56	MG	1a	1704	1/1	0.97	0.04	63,63,63,63	0
56	MG	1A	3037	1/1	0.97	0.34	38,38,38,38	0
56	MG	1A	3302	1/1	0.97	0.05	36,36,36,36	0
56	MG	2A	3607	1/1	0.97	0.06	66,66,66,66	0
56	MG	2A	3449	1/1	0.97	0.11	42,42,42,42	0
56	MG	2A	3016	1/1	0.97	0.13	50,50,50,50	0
56	MG	2A	3611	1/1	0.97	0.04	57,57,57,57	0
56	MG	1A	3442	1/1	0.97	0.05	61,61,61,61	0
56	MG	1A	3503	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3384	1/1	0.97	0.07	30,30,30,30	0
56	MG	2A	3619	1/1	0.97	0.05	55,55,55,55	0
56	MG	1A	3444	1/1	0.97	0.07	31,31,31,31	0
56	MG	2A	3456	1/1	0.97	0.10	63,63,63,63	0
56	MG	1A	3798	1/1	0.97	0.07	37,37,37,37	0
56	MG	2A	3625	1/1	0.97	0.05	65,65,65,65	0
56	MG	1A	3303	1/1	0.97	0.10	32,32,32,32	0
56	MG	2A	3627	1/1	0.97	0.04	46,46,46,46	0
56	MG	1A	3304	1/1	0.97	0.08	47,47,47,47	0
56	MG	1a	1717	1/1	0.97	0.09	67,67,67,67	0
56	MG	1A	3448	1/1	0.97	0.15	30,30,30,30	0
56	MG	1A	3338	1/1	0.97	0.12	31,31,31,31	0
56	MG	1A	3214	1/1	0.97	0.14	30,30,30,30	0
60	ZN	14	501	1/1	0.97	0.19	89,89,89,89	0
56	MG	2A	3635	1/1	0.97	0.05	48,48,48,48	0
56	MG	1D	320	1/1	0.97	0.06	46,46,46,46	0
61	SF4	2d	501	8/8	0.97	0.04	70,73,77,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3637	1/1	0.97	0.08	60,60,60,60	0
56	MG	1a	1735	1/1	0.98	0.04	62,62,62,62	0
56	MG	1A	3698	1/1	0.98	0.04	30,30,30,30	0
56	MG	2A	3591	1/1	0.98	0.11	68,68,68,68	0
56	MG	1A	3901	1/1	0.98	0.16	51,51,51,51	0
56	MG	1A	3192	1/1	0.98	0.09	32,32,32,32	0
56	MG	1A	3103	1/1	0.98	0.09	48,48,48,48	0
56	MG	2a	1692	1/1	0.98	0.04	62,62,62,62	0
56	MG	1A	3409	1/1	0.98	0.05	38,38,38,38	0
56	MG	2A	3376	1/1	0.98	0.04	50,50,50,50	0
56	MG	1a	1822	1/1	0.98	0.04	60,60,60,60	0
56	MG	1A	3651	1/1	0.98	0.11	74,74,74,74	0
56	MG	1A	3604	1/1	0.98	0.05	54,54,54,54	0
56	MG	10	106	1/1	0.98	0.06	46,46,46,46	0
56	MG	1A	3240	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3485	1/1	0.98	0.09	47,47,47,47	0
56	MG	11	102	1/1	0.98	0.03	41,41,41,41	0
56	MG	1A	3655	1/1	0.98	0.07	49,49,49,49	0
56	MG	1A	3447	1/1	0.98	0.09	34,34,34,34	0
56	MG	1D	305	1/1	0.98	0.10	34,34,34,34	0
56	MG	13	103	1/1	0.98	0.11	42,42,42,42	0
56	MG	2A	3613	1/1	0.98	0.06	56,56,56,56	0
56	MG	1A	3344	1/1	0.98	0.05	31,31,31,31	0
56	MG	1A	3916	1/1	0.98	0.13	42,42,42,42	0
56	MG	2a	1710	1/1	0.98	0.03	73,73,73,73	0
56	MG	2A	3616	1/1	0.98	0.13	73,73,73,73	0
56	MG	1A	3449	1/1	0.98	0.06	53,53,53,53	0
56	MG	2Y	201	1/1	0.98	0.13	60,60,60,60	0
56	MG	2A	3290	1/1	0.98	0.04	55,55,55,55	0
56	MG	2A	3620	1/1	0.98	0.04	44,44,44,44	0
56	MG	1A	3610	1/1	0.98	0.09	45,45,45,45	0
56	MG	2A	3622	1/1	0.98	0.04	67,67,67,67	0
56	MG	1A	3772	1/1	0.98	0.08	45,45,45,45	0
56	MG	18	101	1/1	0.98	0.08	49,49,49,49	0
56	MG	1A	3139	1/1	0.98	0.07	33,33,33,33	0
56	MG	1A	3774	1/1	0.98	0.06	45,45,45,45	0
56	MG	2A	3297	1/1	0.98	0.11	43,43,43,43	0
56	MG	1A	3140	1/1	0.98	0.05	31,31,31,31	0
56	MG	1A	3452	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3349	1/1	0.98	0.05	26,26,26,26	0
56	MG	2A	3401	1/1	0.98	0.06	56,56,56,56	0
56	MG	2a	1728	1/1	0.98	0.09	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1847	1/1	0.98	0.06	72,72,72,72	0
56	MG	1A	3853	1/1	0.98	0.05	43,43,43,43	0
56	MG	1A	3615	1/1	0.98	0.07	59,59,59,59	0
56	MG	1A	3454	1/1	0.98	0.06	36,36,36,36	0
56	MG	1A	3284	1/1	0.98	0.07	39,39,39,39	0
56	MG	2A	3507	1/1	0.98	0.11	72,72,72,72	0
56	MG	1A	3352	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3215	1/1	0.98	0.07	47,47,47,47	0
56	MG	1a	1853	1/1	0.98	0.05	66,66,66,66	0
56	MG	1A	3722	1/1	0.98	0.11	36,36,36,36	0
56	MG	2A	3412	1/1	0.98	0.04	47,47,47,47	0
56	MG	1A	3074	1/1	0.98	0.11	32,32,32,32	0
56	MG	1A	3066	1/1	0.98	0.18	13,13,13,13	0
56	MG	1a	1857	1/1	0.98	0.04	64,64,64,64	0
56	MG	1A	3498	1/1	0.98	0.07	56,56,56,56	0
56	MG	2a	1746	1/1	0.98	0.04	71,71,71,71	0
56	MG	1E	306	1/1	0.98	0.07	47,47,47,47	0
56	MG	2a	1748	1/1	0.98	0.05	60,60,60,60	0
56	MG	2a	1749	1/1	0.98	0.07	59,59,59,59	0
56	MG	1A	3537	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3422	1/1	0.98	0.08	40,40,40,40	0
56	MG	1A	3869	1/1	0.98	0.07	46,46,46,46	0
56	MG	1A	3081	1/1	0.98	0.46	39,39,39,39	0
56	MG	2A	3523	1/1	0.98	0.04	57,57,57,57	0
56	MG	2A	3141	1/1	0.98	0.08	57,57,57,57	0
56	MG	1A	3358	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3731	1/1	0.98	0.09	32,32,32,32	0
56	MG	1A	3425	1/1	0.98	0.09	44,44,44,44	0
56	MG	1A	3009	1/1	0.98	0.14	27,27,27,27	0
56	MG	1A	3289	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3806	1/1	0.98	0.14	60,60,60,60	0
56	MG	1A	3309	1/1	0.98	0.05	36,36,36,36	0
56	MG	1A	3290	1/1	0.98	0.05	34,34,34,34	0
56	MG	1A	3311	1/1	0.98	0.04	28,28,28,28	0
56	MG	1A	3634	1/1	0.98	0.07	34,34,34,34	0
56	MG	2A	3537	1/1	0.98	0.06	60,60,60,60	0
56	MG	2A	3669	1/1	0.98	0.05	47,47,47,47	0
56	MG	1A	3812	1/1	0.98	0.06	37,37,37,37	0
56	MG	1a	1705	1/1	0.98	0.10	51,51,51,51	0
56	MG	1A	3635	1/1	0.98	0.05	35,35,35,35	0
56	MG	2A	3542	1/1	0.98	0.04	56,56,56,56	0
56	MG	1A	3332	1/1	0.98	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3545	1/1	0.98	0.07	57,57,57,57	0
56	MG	1N	203	1/1	0.98	0.10	59,59,59,59	0
56	MG	1A	3052	1/1	0.98	0.08	28,28,28,28	0
56	MG	2A	3549	1/1	0.98	0.10	53,53,53,53	0
56	MG	2A	3244	1/1	0.98	0.04	58,58,58,58	0
56	MG	2A	3343	1/1	0.98	0.07	58,58,58,58	0
56	MG	2A	3553	1/1	0.98	0.14	63,63,63,63	0
56	MG	2A	3554	1/1	0.98	0.10	63,63,63,63	0
56	MG	1P	202	1/1	0.98	0.04	55,55,55,55	0
56	MG	2A	3556	1/1	0.98	0.11	47,47,47,47	0
56	MG	1A	3742	1/1	0.98	0.11	33,33,33,33	0
56	MG	2A	3347	1/1	0.98	0.07	42,42,42,42	0
56	MG	1A	3235	1/1	0.98	0.09	32,32,32,32	0
56	MG	1A	3367	1/1	0.98	0.08	33,33,33,33	0
56	MG	1a	1797	1/1	0.98	0.10	76,76,76,76	0
56	MG	1A	3819	1/1	0.98	0.12	53,53,53,53	0
56	MG	1A	3202	1/1	0.98	0.12	29,29,29,29	0
56	MG	2A	3450	1/1	0.98	0.06	50,50,50,50	0
56	MG	1A	3050	1/1	0.98	0.14	36,36,36,36	0
56	MG	2B	3014	1/1	0.98	0.03	64,64,64,64	0
56	MG	2A	3253	1/1	0.98	0.05	53,53,53,53	0
56	MG	1a	1719	1/1	0.98	0.09	71,71,71,71	0
56	MG	1A	3595	1/1	0.98	0.13	49,49,49,49	0
56	MG	1B	211	1/1	0.98	0.05	41,41,41,41	0
56	MG	1A	3438	1/1	0.98	0.07	46,46,46,46	0
56	MG	1A	3339	1/1	0.98	0.06	43,43,43,43	0
56	MG	1A	3441	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3574	1/1	0.98	0.07	60,60,60,60	0
56	MG	1A	3694	1/1	0.98	0.05	39,39,39,39	0
56	MG	1A	3828	1/1	0.98	0.08	43,43,43,43	0
56	MG	1B	218	1/1	0.98	0.04	39,39,39,39	0
56	MG	1A	3599	1/1	0.98	0.04	35,35,35,35	0
56	MG	1V	202	1/1	0.98	0.04	46,46,46,46	0
56	MG	1A	3754	1/1	0.98	0.08	41,41,41,41	0
56	MG	1A	3264	1/1	0.98	0.06	34,34,34,34	0
60	ZN	29	501	1/1	0.98	0.03	67,67,67,67	0
60	ZN	2n	102	1/1	0.98	0.06	84,84,84,84	0
56	MG	1B	222	1/1	0.98	0.07	49,49,49,49	0
56	MG	2E	306	1/1	0.98	0.05	46,46,46,46	0
56	MG	1W	3003	1/1	0.98	0.17	33,33,33,33	0
56	MG	1a	1844	1/1	0.99	0.04	68,68,68,68	0
56	MG	1A	3761	1/1	0.99	0.04	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3348	1/1	0.99	0.03	32,32,32,32	0
56	MG	1A	3197	1/1	0.99	0.06	29,29,29,29	0
56	MG	1D	314	1/1	0.99	0.05	33,33,33,33	0
56	MG	2A	3310	1/1	0.99	0.07	48,48,48,48	0
56	MG	1A	3577	1/1	0.99	0.06	28,28,28,28	0
56	MG	1A	3336	1/1	0.99	0.07	41,41,41,41	0
56	MG	2A	3560	1/1	0.99	0.04	54,54,54,54	0
56	MG	1a	1714	1/1	0.99	0.04	53,53,53,53	0
56	MG	1A	3427	1/1	0.99	0.05	53,53,53,53	0
56	MG	1a	1716	1/1	0.99	0.05	49,49,49,49	0
56	MG	1A	3695	1/1	0.99	0.05	38,38,38,38	0
56	MG	1A	3405	1/1	0.99	0.05	26,26,26,26	0
56	MG	1A	3406	1/1	0.99	0.03	34,34,34,34	0
56	MG	2a	1725	1/1	0.99	0.04	63,63,63,63	0
56	MG	1A	3387	1/1	0.99	0.07	34,34,34,34	0
56	MG	1a	1721	1/1	0.99	0.04	55,55,55,55	0
56	MG	1A	3771	1/1	0.99	0.10	33,33,33,33	0
56	MG	1A	3351	1/1	0.99	0.06	29,29,29,29	0
56	MG	2A	3402	1/1	0.99	0.04	52,52,52,52	0
56	MG	2a	1731	1/1	0.99	0.04	69,69,69,69	0
56	MG	1A	3298	1/1	0.99	0.09	28,28,28,28	0
56	MG	1A	3390	1/1	0.99	0.07	35,35,35,35	0
56	MG	1A	3353	1/1	0.99	0.04	43,43,43,43	0
56	MG	2A	3327	1/1	0.99	0.04	58,58,58,58	0
56	MG	1A	3827	1/1	0.99	0.04	47,47,47,47	0
56	MG	2A	3329	1/1	0.99	0.03	50,50,50,50	0
56	MG	2A	3680	1/1	0.99	0.04	65,65,65,65	0
56	MG	2a	1739	1/1	0.99	0.04	57,57,57,57	0
56	MG	2A	3330	1/1	0.99	0.04	48,48,48,48	0
56	MG	1A	3354	1/1	0.99	0.10	31,31,31,31	0
56	MG	1A	3292	1/1	0.99	0.04	45,45,45,45	0
56	MG	1A	3830	1/1	0.99	0.10	33,33,33,33	0
56	MG	2A	3582	1/1	0.99	0.10	60,60,60,60	0
56	MG	1A	3312	1/1	0.99	0.06	27,27,27,27	0
56	MG	1A	3562	1/1	0.99	0.07	45,45,45,45	0
56	MG	2A	3585	1/1	0.99	0.13	59,59,59,59	0
56	MG	1A	3780	1/1	0.99	0.04	44,44,44,44	0
56	MG	1A	3346	1/1	0.99	0.07	43,43,43,43	0
56	MG	2A	3588	1/1	0.99	0.03	47,47,47,47	0
56	MG	2A	3590	1/1	0.99	0.04	47,47,47,47	0
56	MG	2A	3498	1/1	0.99	0.04	42,42,42,42	0
56	MG	1A	3512	1/1	0.99	0.07	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3593	1/1	0.99	0.03	48,48,48,48	0
56	MG	1A	3783	1/1	0.99	0.04	51,51,51,51	0
56	MG	1A	3785	1/1	0.99	0.04	36,36,36,36	0
56	MG	2A	3341	1/1	0.99	0.10	55,55,55,55	0
56	MG	2A	3597	1/1	0.99	0.07	52,52,52,52	0
56	MG	1a	1738	1/1	0.99	0.05	57,57,57,57	0
56	MG	1A	3381	1/1	0.99	0.08	38,38,38,38	0
56	MG	1A	3621	1/1	0.99	0.06	53,53,53,53	0
56	MG	2A	3345	1/1	0.99	0.11	64,64,64,64	0
56	MG	1A	3840	1/1	0.99	0.04	39,39,39,39	0
56	MG	2A	3268	1/1	0.99	0.03	45,45,45,45	0
56	MG	2a	1765	1/1	0.99	0.09	66,66,66,66	0
56	MG	1A	3680	1/1	0.99	0.03	30,30,30,30	0
56	MG	2A	3605	1/1	0.99	0.03	49,49,49,49	0
56	MG	2A	3510	1/1	0.99	0.13	67,67,67,67	0
56	MG	1A	3789	1/1	0.99	0.06	41,41,41,41	0
56	MG	1B	212	1/1	0.99	0.03	40,40,40,40	0
56	MG	1A	3440	1/1	0.99	0.08	23,23,23,23	0
56	MG	2A	3610	1/1	0.99	0.06	62,62,62,62	0
56	MG	2a	1773	1/1	0.99	0.06	63,63,63,63	0
56	MG	1A	3748	1/1	0.99	0.03	49,49,49,49	0
56	MG	2A	3612	1/1	0.99	0.04	51,51,51,51	0
56	MG	1P	201	1/1	0.99	0.06	34,34,34,34	0
56	MG	1A	3397	1/1	0.99	0.05	34,34,34,34	0
56	MG	1A	3419	1/1	0.99	0.02	42,42,42,42	0
56	MG	1A	3794	1/1	0.99	0.06	44,44,44,44	0
56	MG	1A	3715	1/1	0.99	0.10	69,69,69,69	0
56	MG	2A	3618	1/1	0.99	0.06	42,42,42,42	0
56	MG	1A	3398	1/1	0.99	0.05	33,33,33,33	0
56	MG	1A	3468	1/1	0.99	0.03	47,47,47,47	0
56	MG	1R	202	1/1	0.99	0.05	38,38,38,38	0
56	MG	1A	3718	1/1	0.99	0.06	72,72,72,72	0
56	MG	1A	3799	1/1	0.99	0.04	32,32,32,32	0
56	MG	1A	3912	1/1	0.99	0.06	54,54,54,54	0
56	MG	1A	3913	1/1	0.99	0.04	32,32,32,32	0
56	MG	2A	3527	1/1	0.99	0.11	60,60,60,60	0
56	MG	1A	3800	1/1	0.99	0.07	51,51,51,51	0
56	MG	1A	3801	1/1	0.99	0.03	51,51,51,51	0
56	MG	1A	3421	1/1	0.99	0.05	55,55,55,55	0
56	MG	1A	3856	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3803	1/1	0.99	0.07	53,53,53,53	0
56	MG	2A	3632	1/1	0.99	0.04	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3805	1/1	0.99	0.06	31,31,31,31	0
56	MG	1A	3628	1/1	0.99	0.09	43,43,43,43	0
56	MG	2A	3535	1/1	0.99	0.08	52,52,52,52	0
56	MG	2a	1694	1/1	0.99	0.04	63,63,63,63	0
56	MG	1A	3369	1/1	0.99	0.05	43,43,43,43	0
56	MG	1A	3808	1/1	0.99	0.11	55,55,55,55	0
56	MG	2A	3538	1/1	0.99	0.10	56,56,56,56	0
56	MG	2A	3295	1/1	0.99	0.06	52,52,52,52	0
56	MG	1a	1835	1/1	0.99	0.05	64,64,64,64	0
56	MG	1A	3862	1/1	0.99	0.06	31,31,31,31	0
56	MG	1a	1837	1/1	0.99	0.07	57,57,57,57	0
56	MG	2A	3543	1/1	0.99	0.06	45,45,45,45	0
60	ZN	1Y	501	1/1	0.99	0.03	63,63,63,63	0
56	MG	1A	3758	1/1	0.99	0.03	31,31,31,31	0
60	ZN	1n	102	1/1	0.99	0.04	76,76,76,76	0
60	ZN	2Y	202	1/1	0.99	0.03	77,77,77,77	0
56	MG	1X	101	1/1	0.99	0.07	39,39,39,39	0
60	ZN	26	101	1/1	0.99	0.03	67,67,67,67	0
56	MG	2A	3546	1/1	0.99	0.03	56,56,56,56	0
56	MG	1A	3865	1/1	0.99	0.06	44,44,44,44	0
56	MG	1A	3044	1/1	0.99	0.03	26,26,26,26	0
56	MG	1A	3867	1/1	0.99	0.12	52,52,52,52	0
56	MG	1A	3724	1/1	0.99	0.15	44,44,44,44	0
56	MG	2A	3552	1/1	1.00	0.02	47,47,47,47	0
56	MG	1A	3462	1/1	1.00	0.04	30,30,30,30	0
56	MG	1A	3411	1/1	1.00	0.04	62,62,62,62	0
56	MG	1A	3565	1/1	1.00	0.05	31,31,31,31	0
56	MG	1A	3784	1/1	1.00	0.03	39,39,39,39	0
56	MG	2A	3589	1/1	1.00	0.04	47,47,47,47	0
56	MG	1A	3863	1/1	1.00	0.05	29,29,29,29	0
56	MG	1A	3720	1/1	1.00	0.03	34,34,34,34	0
56	MG	1E	301	1/1	1.00	0.06	34,34,34,34	0
60	ZN	15	102	1/1	1.00	0.01	54,54,54,54	0
60	ZN	16	101	1/1	1.00	0.03	49,49,49,49	0
60	ZN	19	102	1/1	1.00	0.03	52,52,52,52	0
56	MG	1A	3804	1/1	1.00	0.04	37,37,37,37	0
56	MG	1A	3476	1/1	1.00	0.02	38,38,38,38	0
56	MG	2A	3325	1/1	1.00	0.02	50,50,50,50	0
60	ZN	25	101	1/1	1.00	0.03	65,65,65,65	0
56	MG	1A	3334	1/1	1.00	0.07	33,33,33,33	0
56	MG	2A	3444	1/1	1.00	0.02	46,46,46,46	0
56	MG	1A	3543	1/1	1.00	0.03	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3633	1/1	1.00	0.02	48,48,48,48	0
56	MG	2A	3460	1/1	1.00	0.02	46,46,46,46	0
56	MG	1A	3404	1/1	1.00	0.03	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.