



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 16, 2026 – 11:14 PM UTC

PDB ID : 8VTV / pdb_00008vtv
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with macrolone MCX-91, mRNA, aminoacylated A-site Phe-tRNA^{phe}, aminoacylated P-site fMet-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.55Å resolution
Authors : Aleksandrova, E.V.; Ma, C.-X.; Klepacki, D.; Alizadeh, F.; Vazquez-Laslop, N.; Liang, J.-H.; Polikanov, Y.S.; Mankin, A.S.
Deposited on : 2024-01-27
Resolution : 2.55 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

<https://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
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

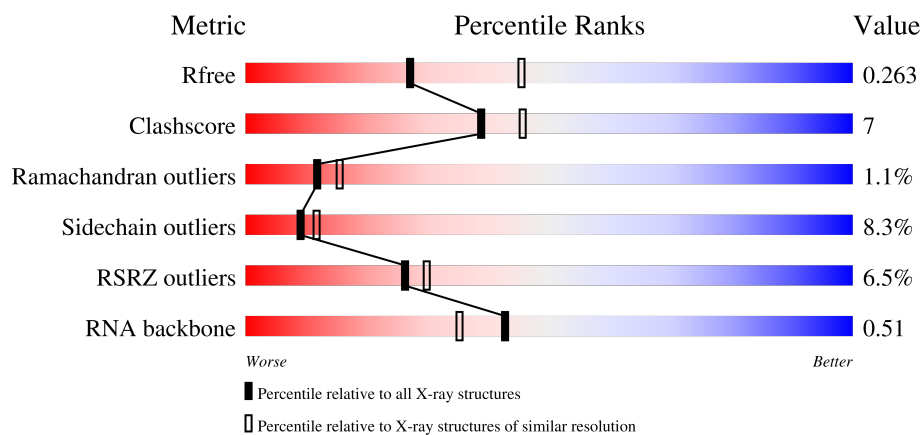
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

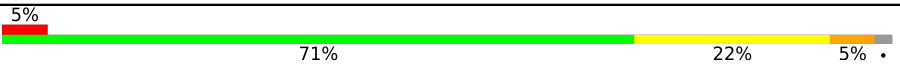
The reported resolution of this entry is 2.55 Å.

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}	164625	1004 (2.54-2.54)
Clashscore	180529	1055 (2.54-2.54)
Ramachandran outliers	177936	1048 (2.54-2.54)
Sidechain outliers	177891	1048 (2.54-2.54)
RSRZ outliers	164620	1004 (2.54-2.54)
RNA backbone	3690	1040 (2.80-2.28)

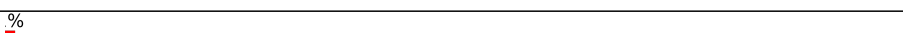
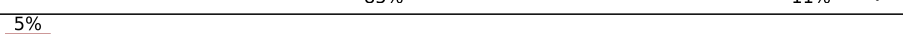
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	2A	2915	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48.1

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Mol	Chain	Length	Quality of chain
2	1B	121	 78%20%..
2	2B	121	 61%32%6%. .
3	1D	276	 %85%12%. .
3	2D	276	 %82%16%. .
4	1E	206	 85%13%..
4	2E	206	 %76%20%..
5	1F	210	 74%21%..
5	2F	210	 %68%26%..
6	1G	182	 5%73%24%..
6	2G	182	 9%58%36%..
7	1H	180	 2%76%17%..
7	2H	180	 18%70%24%..
8	1I	148	 5%66%28%..
8	2I	148	 61%45%38%14%..
9	1N	140	 %85%11%. .
9	2N	140	 5%76%21%. .
10	1O	122	 84%13%. .
10	2O	122	 87%12%. .
11	1P	150	 %77%19%...
11	2P	150	 6%71%27%..
12	1Q	141	 86%10%. .
12	2Q	141	 6%81%19%
13	1R	118	 85%13%. .
13	2R	118	 2%85%14%. .
14	1S	112	 88%11%. .

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Mol	Chain	Length	Quality of chain
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	

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Mol	Chain	Length	Quality of chain
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	

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Mol	Chain	Length	Quality of chain
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	

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Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 300368 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	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
			873	550	174	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
			771	495	140	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a RNA chain called Aminoacylated Phe-tRNA_{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	286	517	74	2			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	279	501	72	2			

- Molecule 55 is a RNA chain called Aminoacylated fMet-tRNA_{met}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			

- Molecule 56 is a RNA chain called Deacylated tRNA_{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
56	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1108	Total	Mg	0	0
			1108	1108		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	13	Total	Mg	0	0
			13	13		
57	1E	14	Total	Mg	0	0
			14	14		
57	1F	13	Total	Mg	0	0
			13	13		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	5	Total 5	Mg 5	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	7	Total 7	Mg 7	0	0
57	1O	5	Total 5	Mg 5	0	0
57	1P	6	Total 6	Mg 6	0	0
57	1Q	6	Total 6	Mg 6	0	0
57	1R	5	Total 5	Mg 5	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	2	Total 2	Mg 2	0	0
57	1U	7	Total 7	Mg 7	0	0
57	1V	8	Total 8	Mg 8	0	0
57	1W	6	Total 6	Mg 6	0	0
57	1X	8	Total 8	Mg 8	0	0
57	1Y	2	Total 2	Mg 2	0	0
57	1Z	3	Total 3	Mg 3	0	0
57	10	9	Total 9	Mg 9	0	0
57	11	4	Total 4	Mg 4	0	0
57	12	2	Total 2	Mg 2	0	0
57	13	4	Total 4	Mg 4	0	0
57	14	1	Total 1	Mg 1	0	0
57	15	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	16	3	Total 3	Mg 3	0	0
57	17	4	Total 4	Mg 4	0	0
57	18	3	Total 3	Mg 3	0	0
57	19	2	Total 2	Mg 2	0	0
57	1a	217	Total 217	Mg 217	0	0
57	1b	1	Total 1	Mg 1	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1e	2	Total 2	Mg 2	0	0
57	1f	2	Total 2	Mg 2	0	0
57	1h	1	Total 1	Mg 1	0	0
57	1l	2	Total 2	Mg 2	0	0
57	1m	2	Total 2	Mg 2	0	0
57	1n	2	Total 2	Mg 2	0	0
57	1q	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1v	1	Total 1	Mg 1	0	0
57	1w	8	Total 8	Mg 8	0	0
57	1x	14	Total 14	Mg 14	0	0
57	1y	1	Total 1	Mg 1	0	0
57	2A	861	Total 861	Mg 861	0	0
57	2B	19	Total 19	Mg 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2D	6	Total 6	Mg 6	0	0
57	2E	7	Total 7	Mg 7	0	0
57	2F	8	Total 8	Mg 8	0	0
57	2G	1	Total 1	Mg 1	0	0
57	2O	2	Total 2	Mg 2	0	0
57	2P	2	Total 2	Mg 2	0	0
57	2Q	2	Total 2	Mg 2	0	0
57	2R	2	Total 2	Mg 2	0	0
57	2S	1	Total 1	Mg 1	0	0
57	2T	4	Total 4	Mg 4	0	0
57	2U	2	Total 2	Mg 2	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	2	Total 2	Mg 2	0	0
57	2X	2	Total 2	Mg 2	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	2	Total 2	Mg 2	0	0
57	21	3	Total 3	Mg 3	0	0
57	23	2	Total 2	Mg 2	0	0
57	25	7	Total 7	Mg 7	0	0
57	26	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	27	2	Total Mg 2 2	0	0
57	28	3	Total Mg 3 3	0	0
57	29	1	Total Mg 1 1	0	0
57	2a	238	Total Mg 238 238	0	0
57	2d	2	Total Mg 2 2	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	2	Total Mg 2 2	0	0
57	2g	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2l	3	Total Mg 3 3	0	0
57	2p	1	Total Mg 1 1	0	0
57	2q	2	Total Mg 2 2	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	2	Total Mg 2 2	0	0
57	2w	7	Total Mg 7 7	0	0
57	2x	6	Total Mg 6 6	0	0
57	2y	4	Total Mg 4 4	0	0

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

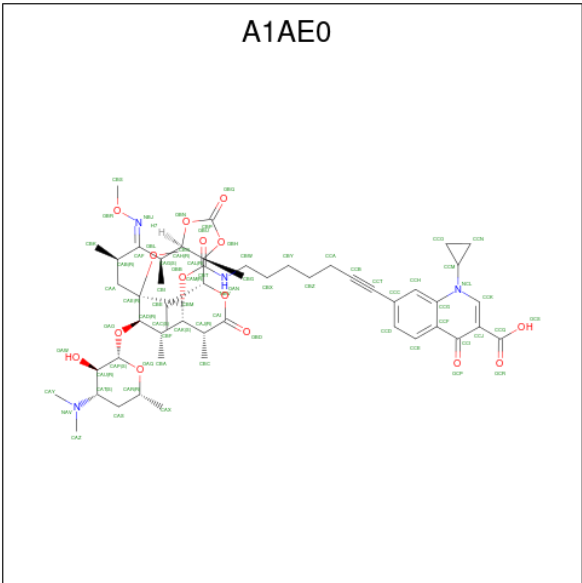
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total K 1 1	0	0

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

- Molecule 59 is 1-cyclopropyl-7-{7-[(3aR,4R,7R,8S,9S,10R,11R,13R,14E,15S,15aR)-10-[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy}-4-ethyl-11-methoxy-14-(methoxyimino)-3a,7,9,11,13,15-hexamethyl-2,6-dioxododecahydro-2H,4H-[1,3]dioxolo[4,5-c]oxacyclotetradecin-8-yl]oxy}carbonyl)amino]hept-1-yn-1-yl}-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (non-preferred name) (CCD ID: A1AE0) (formula: C₅₃H₇₆N₄O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	1A	1	Total	C	N	O	0	0
			72	53	4	15		
59	2A	1	Total	C	N	O	0	0
			72	53	4	15		

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

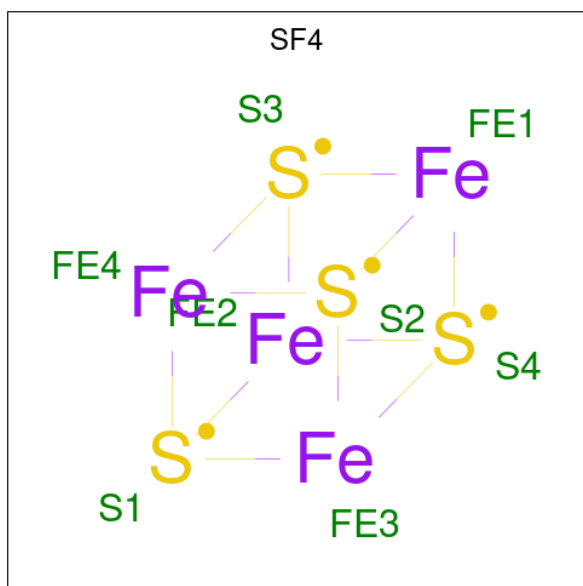
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		

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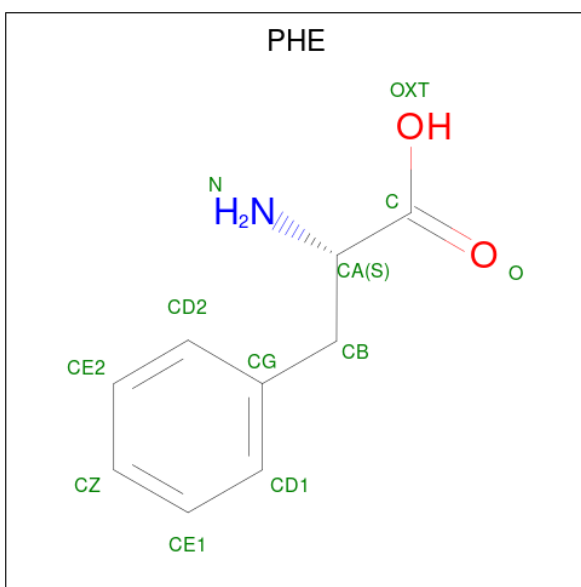
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		
60	29	1	Total	Zn	0	0
			1	1		
60	2n	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



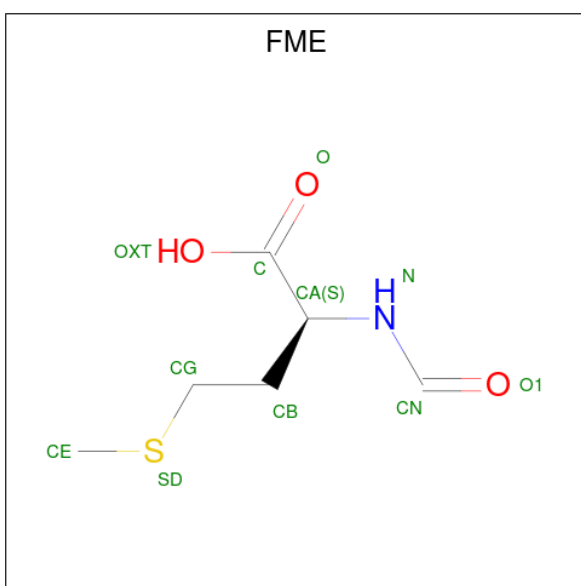
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	1d	1	Total	Fe	S	0	0
			8	4	4		
61	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: $\text{C}_9\text{H}_{11}\text{NO}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
62	1w	1	Total	C	N	O	0	0
			11	9	1	1		
62	2w	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 63 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
63	1x	1	Total	C	N	O	S	0	0
			10	6	1	2	1		
63	2x	1	Total	C	N	O	S	0	0
			10	6	1	2	1		

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	1A	2019	Total O 2019 2019	0	0
64	1B	62	Total O 62 62	0	0
64	1D	27	Total O 27 27	0	0
64	1E	25	Total O 25 25	0	0
64	1F	18	Total O 18 18	0	0
64	1G	2	Total O 2 2	0	0
64	1H	2	Total O 2 2	0	0
64	1N	5	Total O 5 5	0	0
64	1O	6	Total O 6 6	0	0
64	1P	21	Total O 21 21	0	0
64	1Q	9	Total O 9 9	0	0
64	1R	11	Total O 11 11	0	0
64	1S	3	Total O 3 3	0	0
64	1T	7	Total O 7 7	0	0
64	1U	11	Total O 11 11	0	0
64	1V	7	Total O 7 7	0	0
64	1W	8	Total O 8 8	0	0
64	1X	4	Total O 4 4	0	0
64	1Y	3	Total O 3 3	0	0
64	1Z	1	Total O 1 1	0	0
64	10	11	Total O 11 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	11	12	Total 12	O 12	0	0
64	12	4	Total 4	O 4	0	0
64	13	5	Total 5	O 5	0	0
64	14	1	Total 1	O 1	0	0
64	15	6	Total 6	O 6	0	0
64	16	3	Total 3	O 3	0	0
64	17	7	Total 7	O 7	0	0
64	18	12	Total 12	O 12	0	0
64	1a	391	Total 391	O 391	0	0
64	1b	1	Total 1	O 1	0	0
64	1d	1	Total 1	O 1	0	0
64	1e	1	Total 1	O 1	0	0
64	1f	1	Total 1	O 1	0	0
64	1g	1	Total 1	O 1	0	0
64	1j	1	Total 1	O 1	0	0
64	1l	5	Total 5	O 5	0	0
64	1m	1	Total 1	O 1	0	0
64	1n	1	Total 1	O 1	0	0
64	1o	1	Total 1	O 1	0	0
64	1p	1	Total 1	O 1	0	0
64	1q	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	1t	1	Total 1	O 1	0	0
64	1u	1	Total 1	O 1	0	0
64	1v	5	Total 5	O 5	0	0
64	1w	13	Total 13	O 13	0	0
64	1x	12	Total 12	O 12	0	0
64	1y	1	Total 1	O 1	0	0
64	2A	1149	Total 1149	O 1149	0	0
64	2B	20	Total 20	O 20	0	0
64	2D	20	Total 20	O 20	0	0
64	2E	14	Total 14	O 14	0	0
64	2F	12	Total 12	O 12	0	0
64	2I	1	Total 1	O 1	0	0
64	2O	1	Total 1	O 1	0	0
64	2P	12	Total 12	O 12	0	0
64	2Q	1	Total 1	O 1	0	0
64	2R	4	Total 4	O 4	0	0
64	2T	5	Total 5	O 5	0	0
64	2U	3	Total 3	O 3	0	0
64	2W	3	Total 3	O 3	0	0
64	2X	1	Total 1	O 1	0	0
64	2Y	1	Total 1	O 1	0	0

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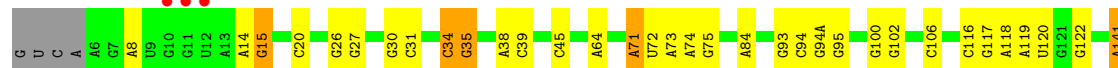
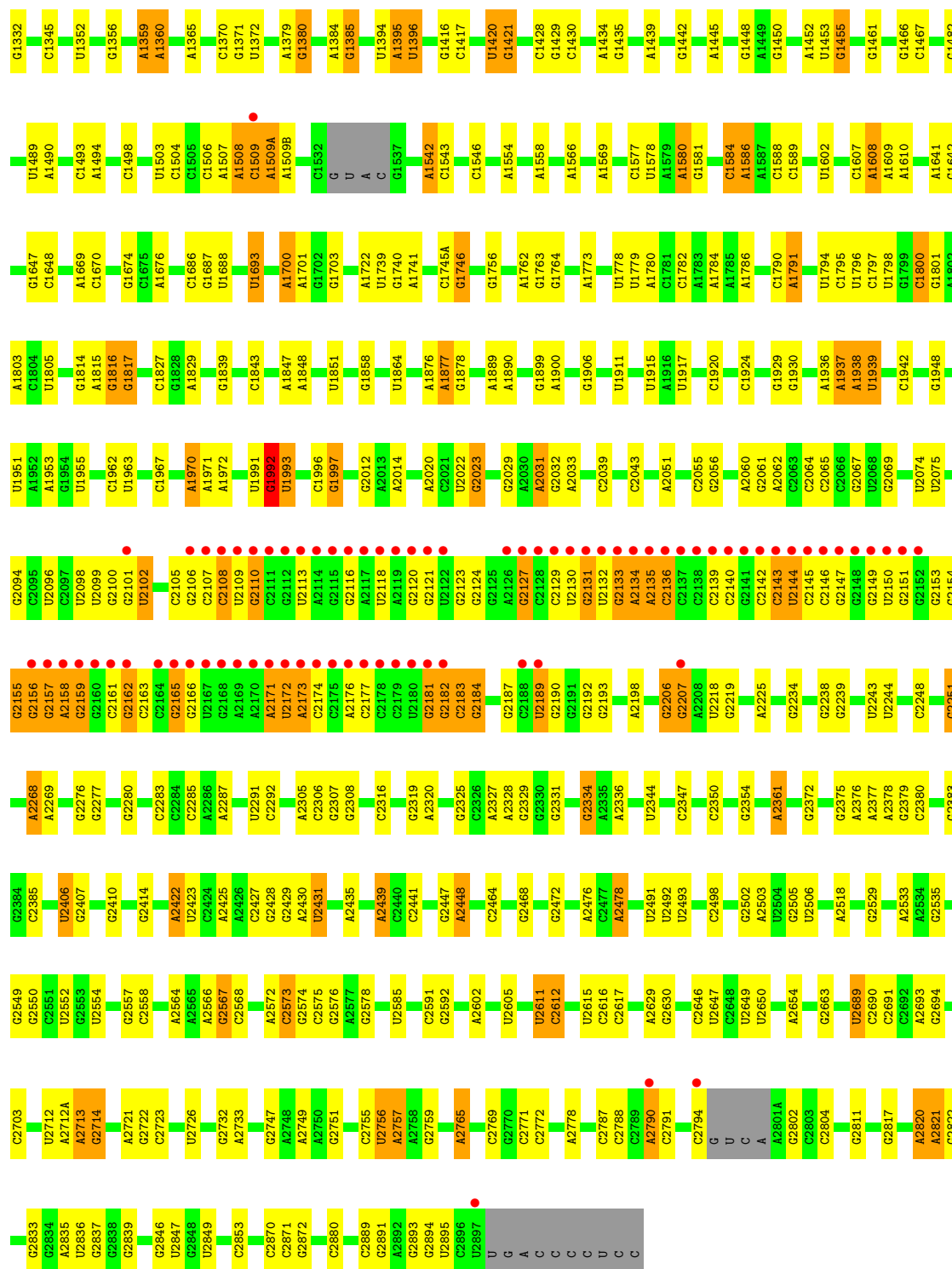
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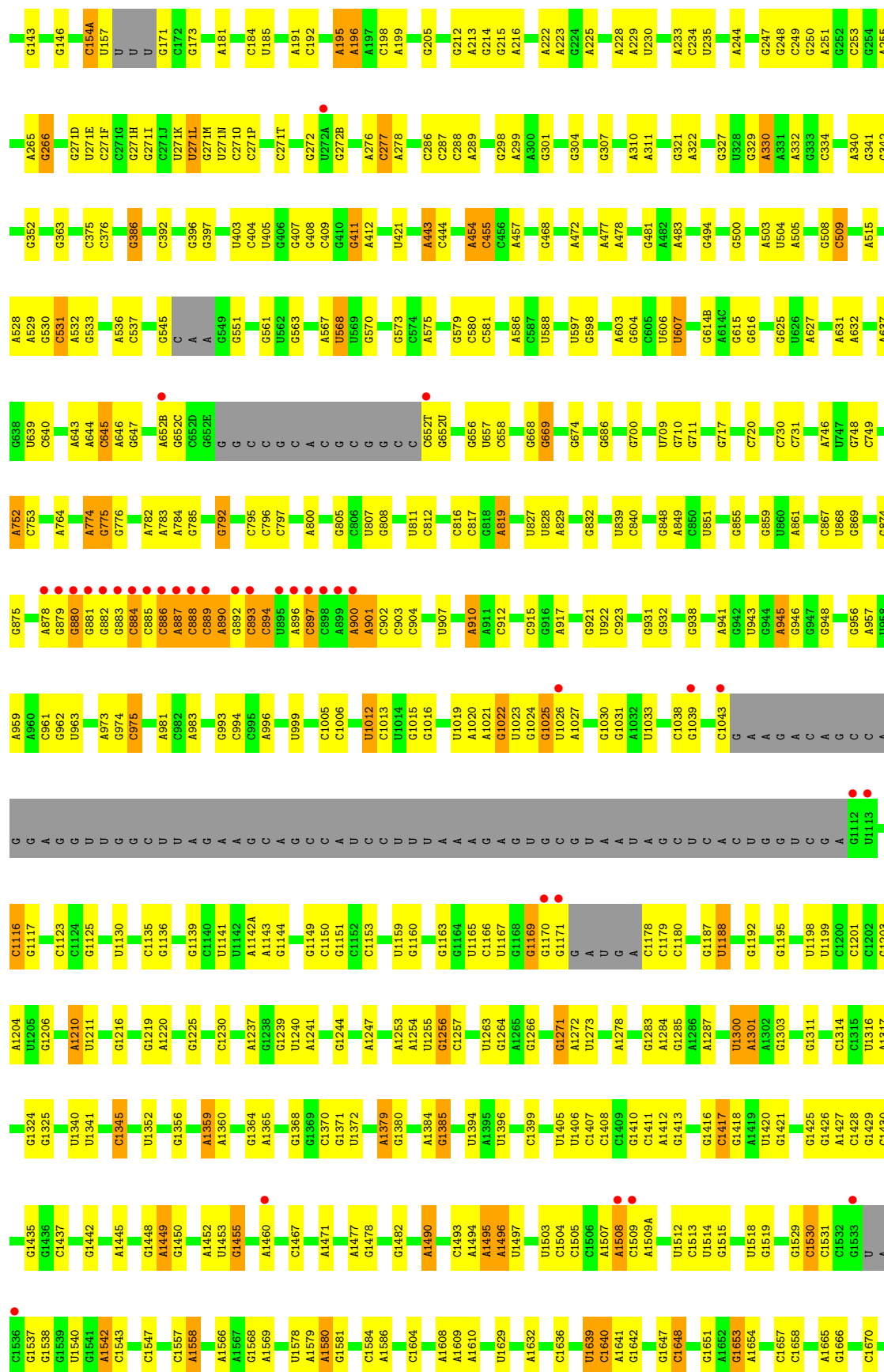
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	20	1	Total 1	O 1	0	0
64	21	11	Total 11	O 11	0	0
64	22	1	Total 1	O 1	0	0
64	23	3	Total 3	O 3	0	0
64	25	2	Total 2	O 2	0	0
64	27	4	Total 4	O 4	0	0
64	28	3	Total 3	O 3	0	0
64	29	1	Total 1	O 1	0	0
64	2a	288	Total 288	O 288	0	0
64	2c	1	Total 1	O 1	0	0
64	2d	3	Total 3	O 3	0	0
64	2e	2	Total 2	O 2	0	0
64	2j	1	Total 1	O 1	0	0
64	2l	6	Total 6	O 6	0	0
64	2n	1	Total 1	O 1	0	0
64	2p	2	Total 2	O 2	0	0
64	2q	1	Total 1	O 1	0	0
64	2r	1	Total 1	O 1	0	0
64	2t	2	Total 2	O 2	0	0
64	2v	2	Total 2	O 2	0	0
64	2w	3	Total 3	O 3	0	0

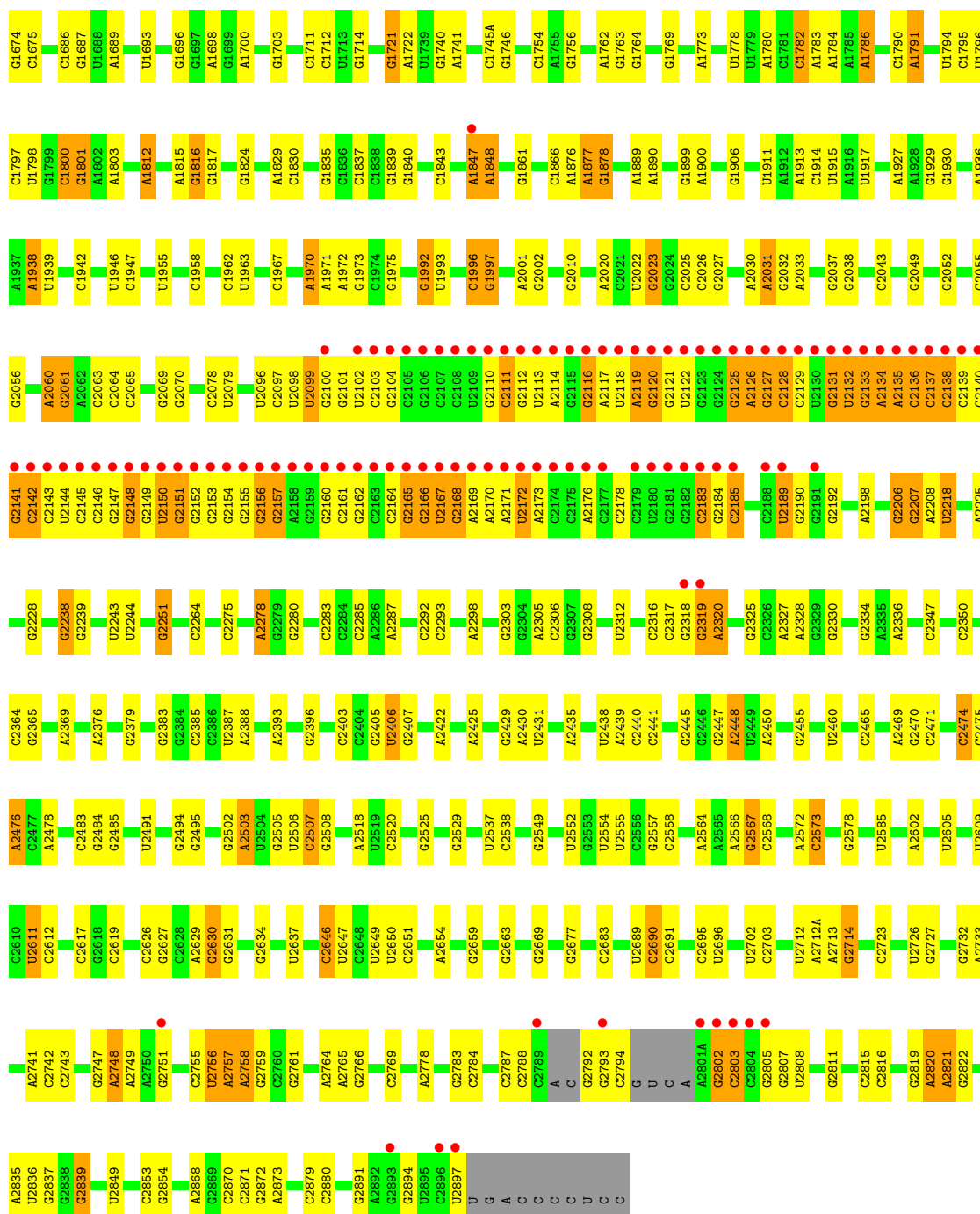
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	2x	9	Total	O	0	0
			9	9		
64	2y	5	Total	O	0	0
			5	5		







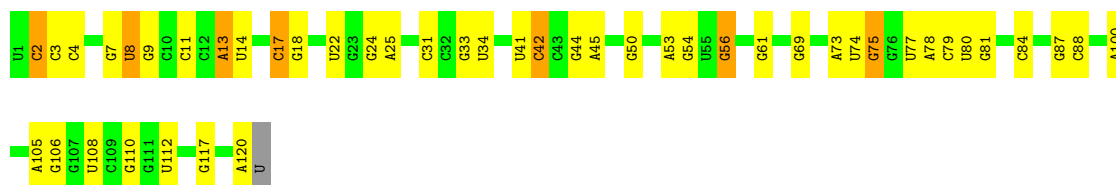
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 78% 20% ..

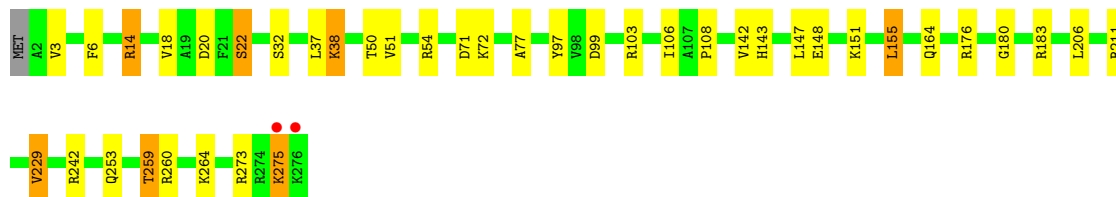
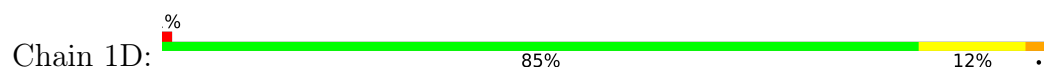


• Molecule 2: 5S Ribosomal RNA

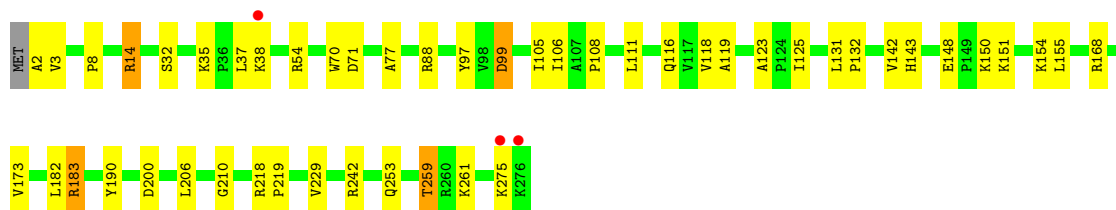
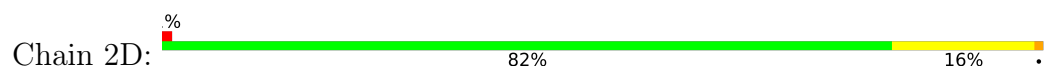
Chain 2B: 61% 32% 6% .



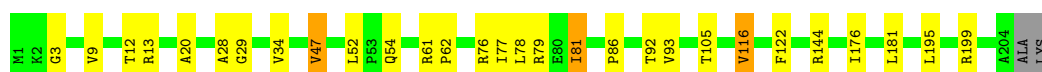
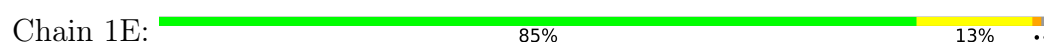
- Molecule 3: 50S ribosomal protein L2



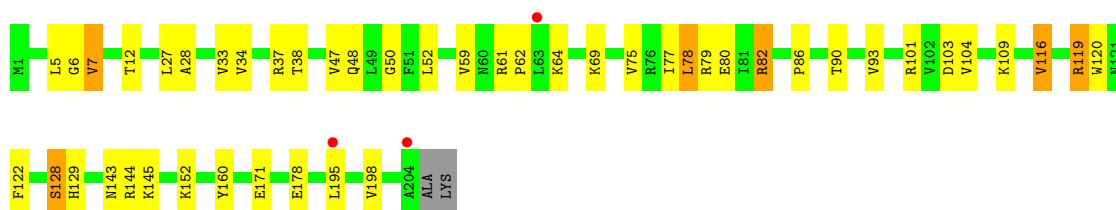
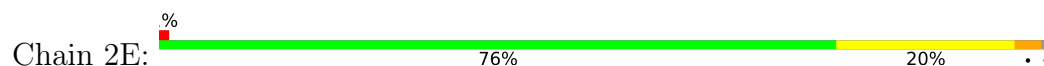
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3

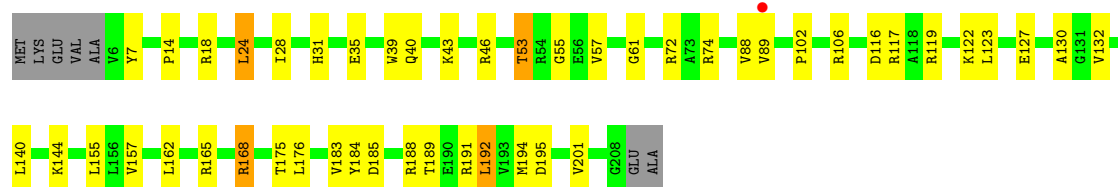


- Molecule 4: 50S ribosomal protein L3

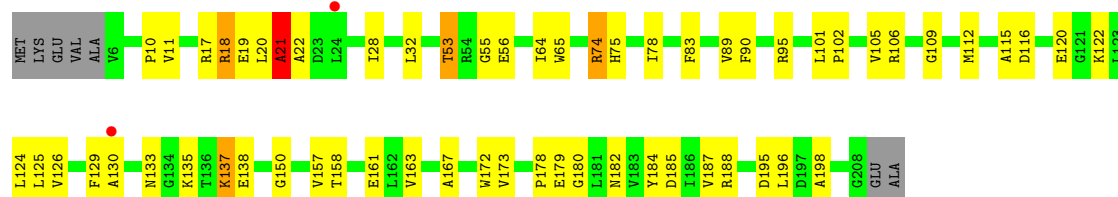


- Molecule 5: 50S ribosomal protein L4

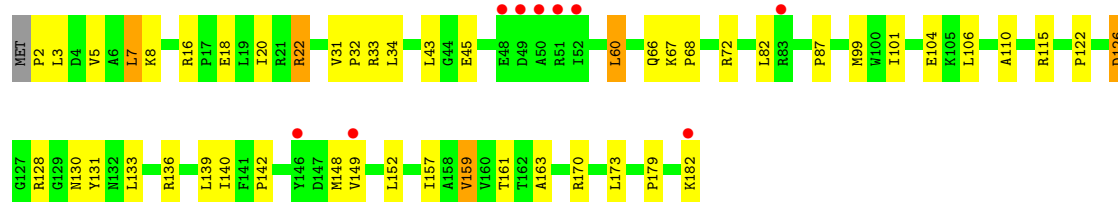
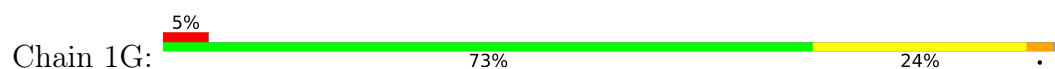




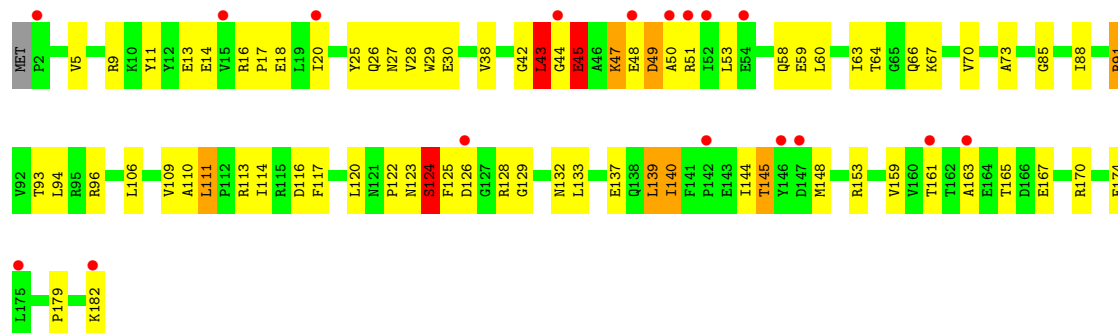
• Molecule 5: 50S ribosomal protein L4



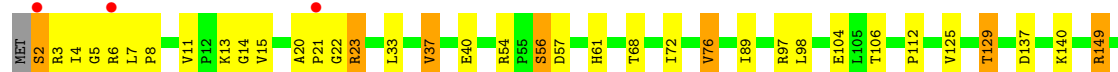
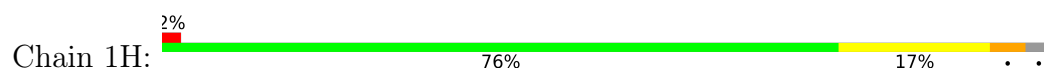
• Molecule 6: 50S ribosomal protein L5

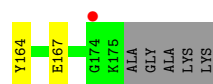


• Molecule 6: 50S ribosomal protein L5

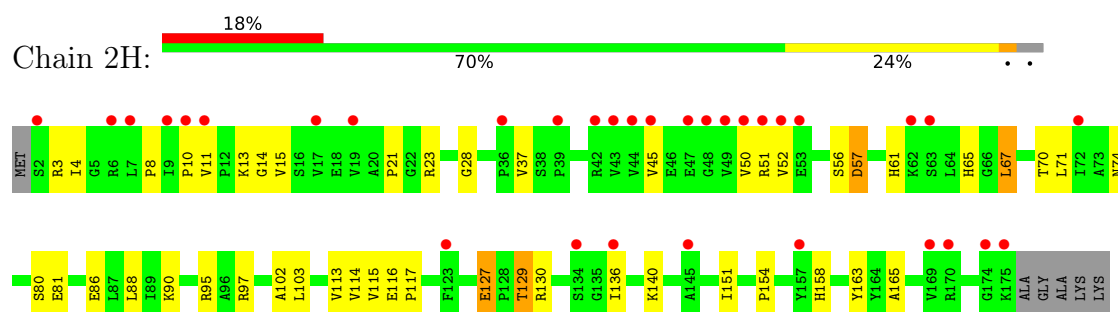


• Molecule 7: 50S ribosomal protein L6

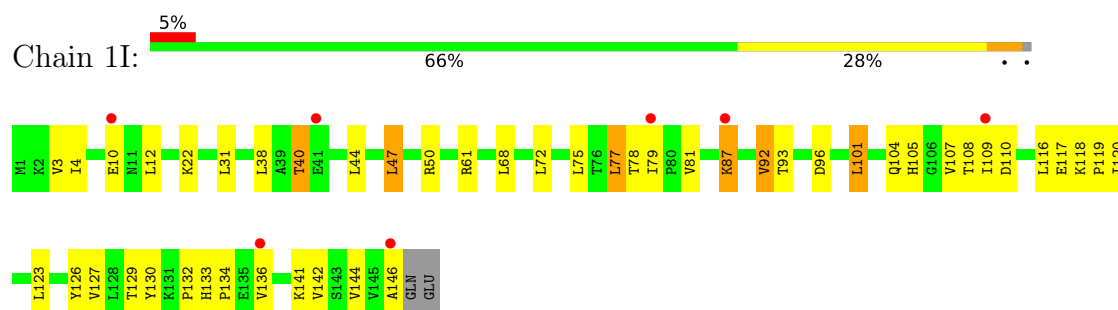




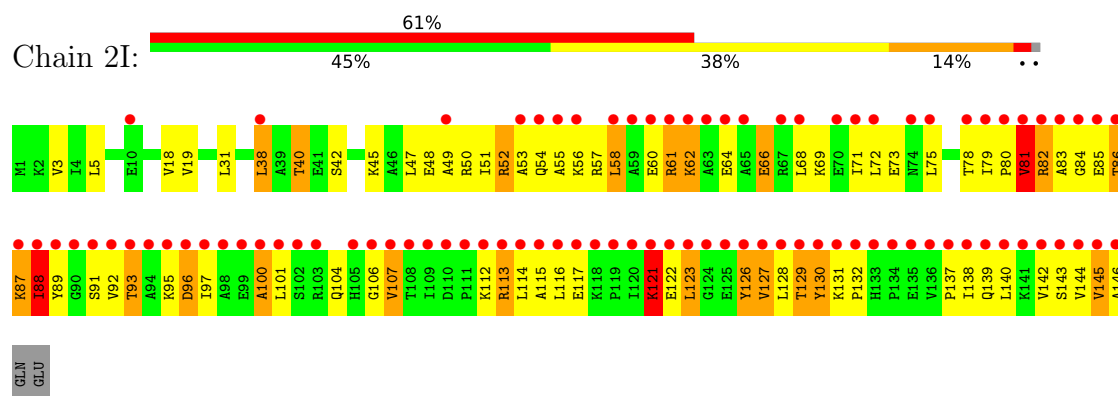
- Molecule 7: 50S ribosomal protein L6



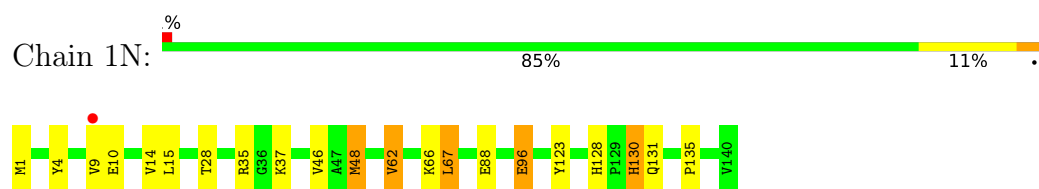
- Molecule 8: 50S ribosomal protein L9



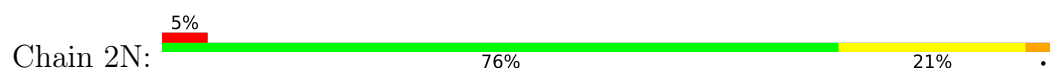
- Molecule 8: 50S ribosomal protein L9

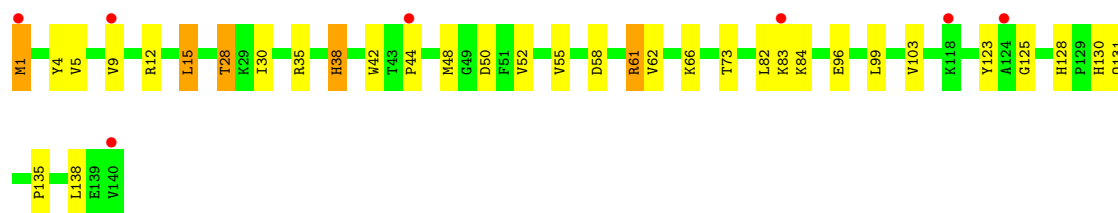


- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13





- Molecule 10: 50S ribosomal protein L14

Chain 10: 84% 13% .



- Molecule 10: 50S ribosomal protein L14

Chain 20: 87% 12% .



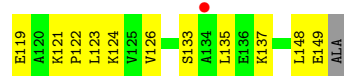
- Molecule 11: 50S ribosomal protein L15

Chain 1P: 77% 19% ...



- Molecule 11: 50S ribosomal protein L15

Chain 2P: 71% 27% ..



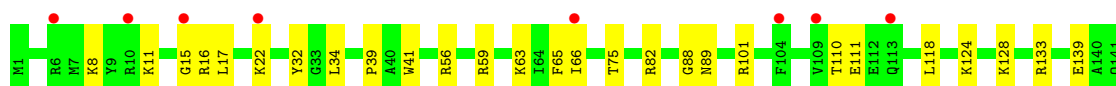
- Molecule 12: 50S ribosomal protein L16

Chain 1Q: 86% 10% .

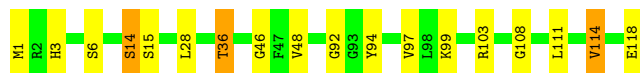
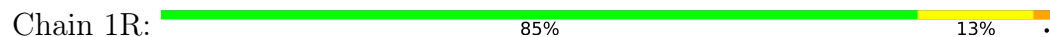


- Molecule 12: 50S ribosomal protein L16

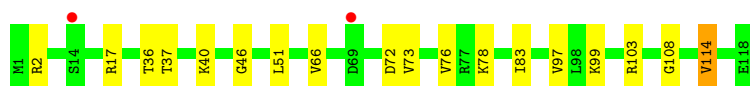
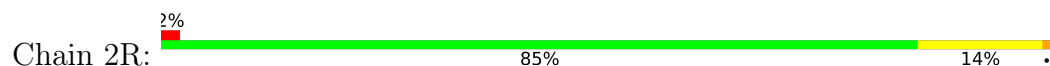
Chain 2Q: 81% 19%



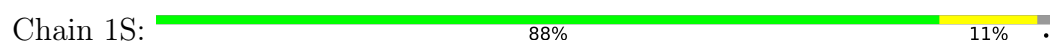
- Molecule 13: 50S ribosomal protein L17



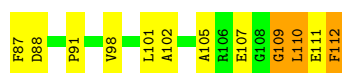
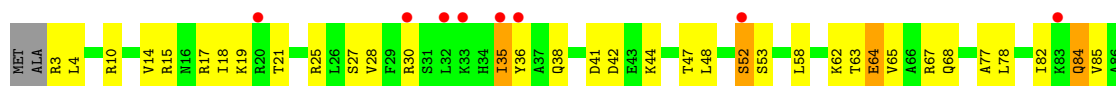
- Molecule 13: 50S ribosomal protein L17



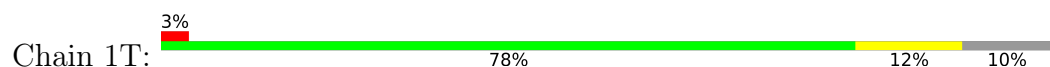
- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19

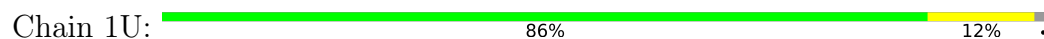


- Molecule 15: 50S ribosomal protein L19

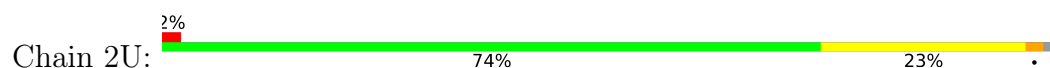




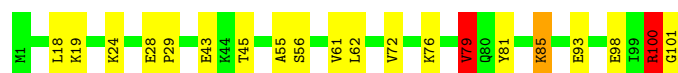
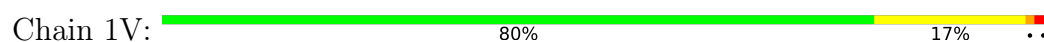
- Molecule 16: 50S ribosomal protein L20



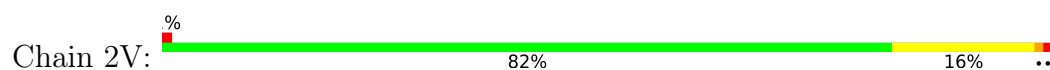
- Molecule 16: 50S ribosomal protein L20



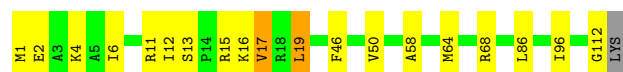
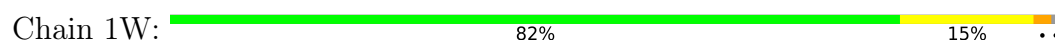
- Molecule 17: 50S ribosomal protein L21



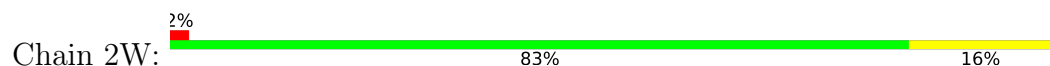
- Molecule 17: 50S ribosomal protein L21



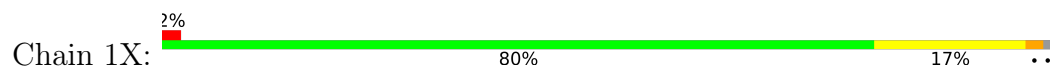
- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22

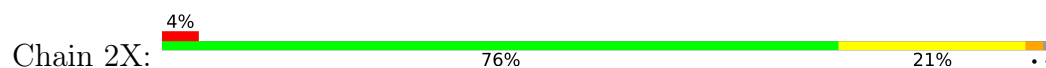


- Molecule 19: 50S ribosomal protein L23

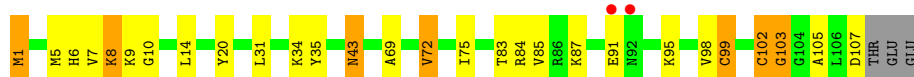




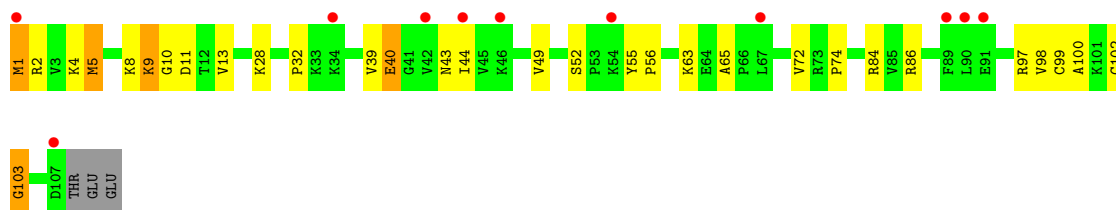
- Molecule 19: 50S ribosomal protein L23



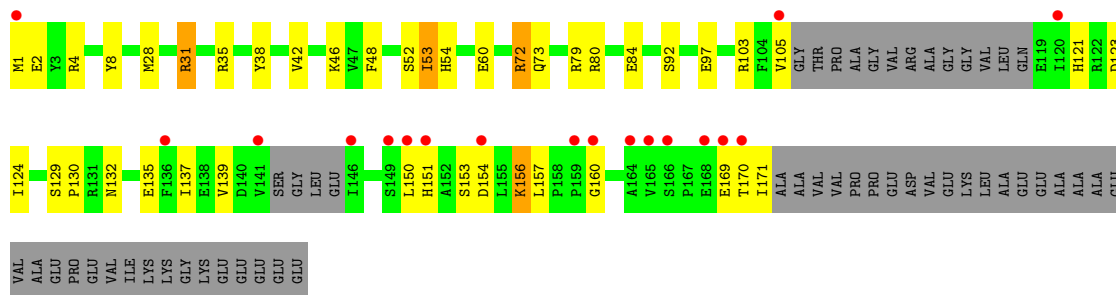
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

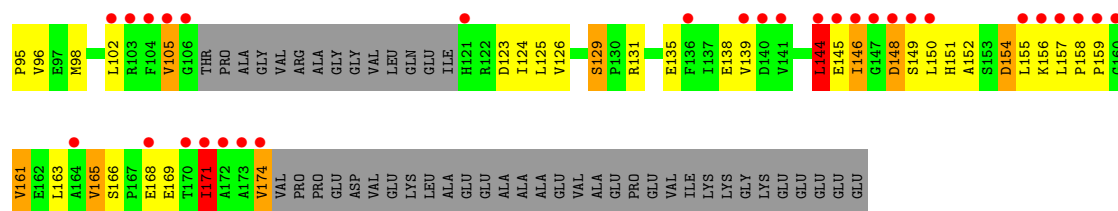


- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25





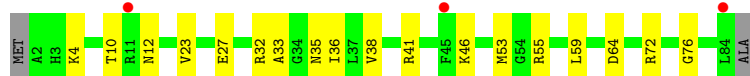
- Molecule 22: 50S ribosomal protein L27

Chain 10: 88% 8% ..



- Molecule 22: 50S ribosomal protein L27

Chain 20: 4% 76% 21% .



- Molecule 23: 50S ribosomal protein L28

Chain 11: % 86% 13% .



- Molecule 23: 50S ribosomal protein L28

Chain 21: 5% 71% 27% ..



- Molecule 24: 50S ribosomal protein L29

Chain 12: 3% 85% 11% ..

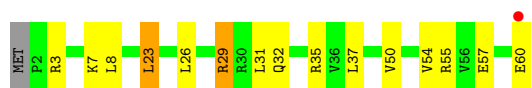
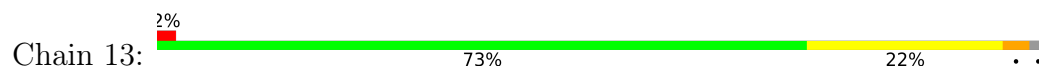


- Molecule 24: 50S ribosomal protein L29

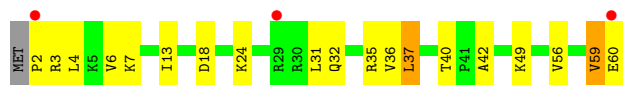
Chain 22: % 78% 19% .



- Molecule 25: 50S ribosomal protein L30



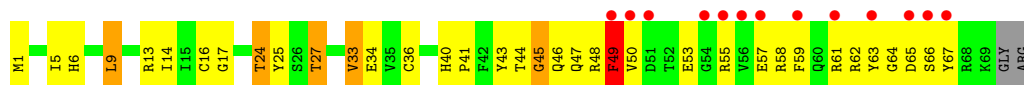
- Molecule 25: 50S ribosomal protein L30



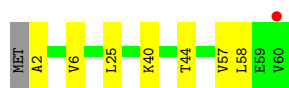
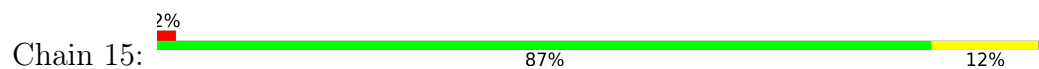
- Molecule 26: 50S ribosomal protein L31



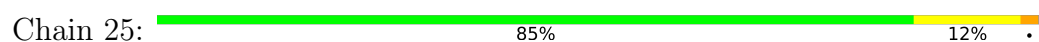
- Molecule 26: 50S ribosomal protein L31



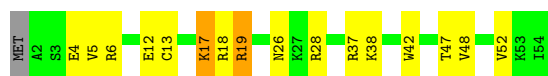
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



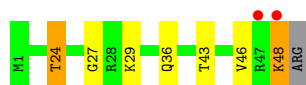
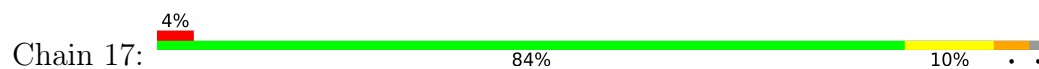
- Molecule 28: 50S ribosomal protein L33



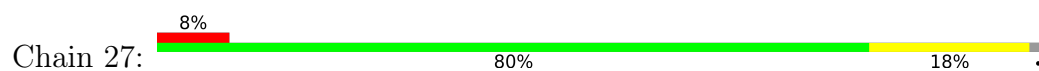
- Molecule 28: 50S ribosomal protein L33



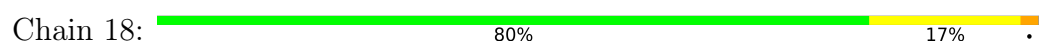
- Molecule 29: 50S ribosomal protein L34



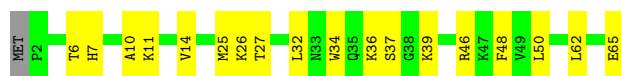
- Molecule 29: 50S ribosomal protein L34



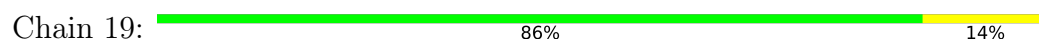
- Molecule 30: 50S ribosomal protein L35



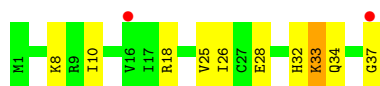
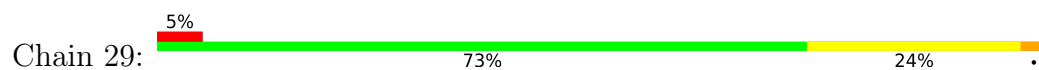
- Molecule 30: 50S ribosomal protein L35



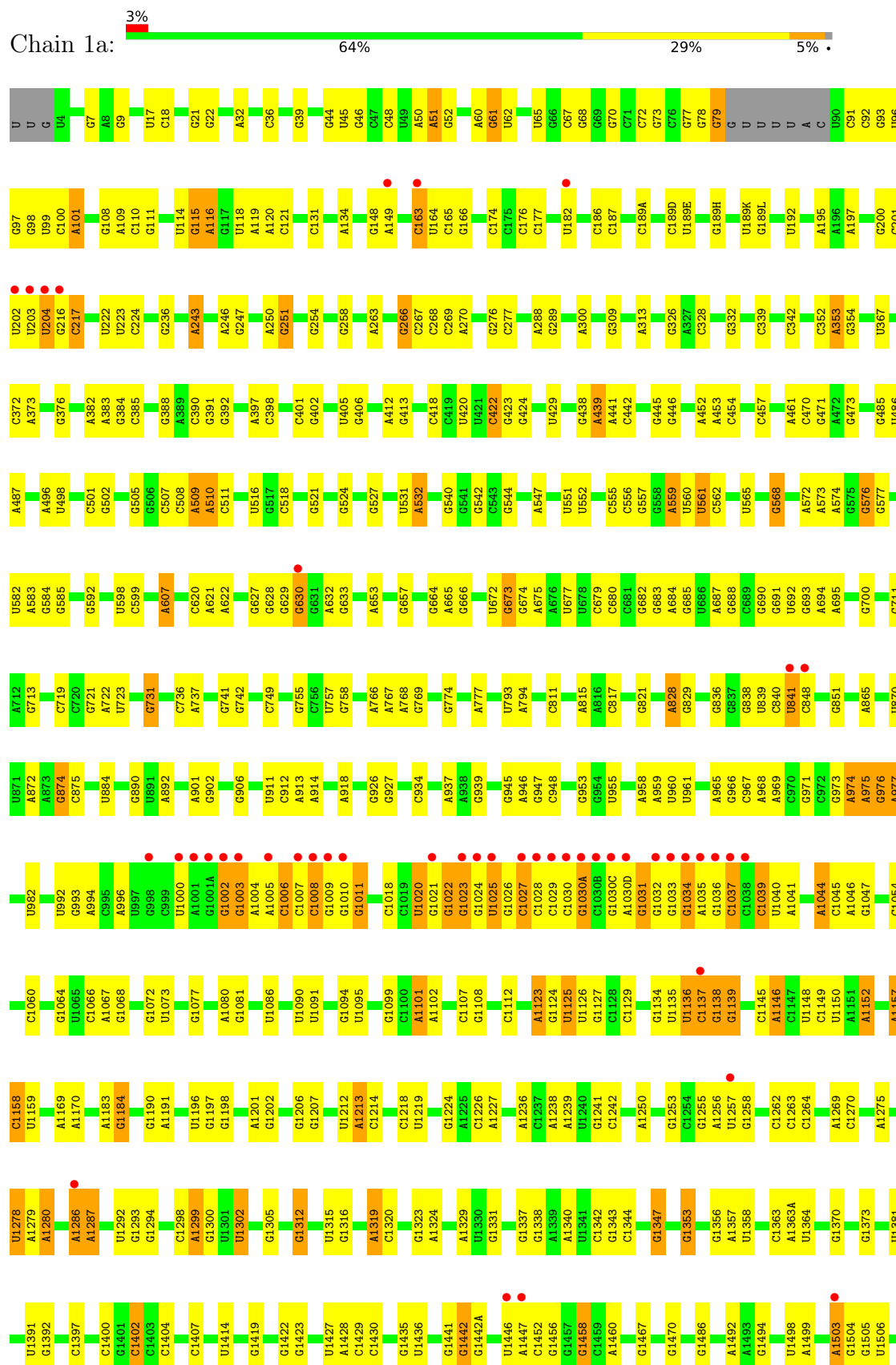
- Molecule 31: 50S ribosomal protein L36

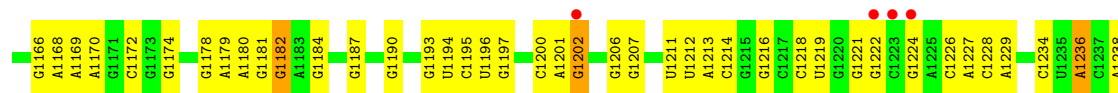


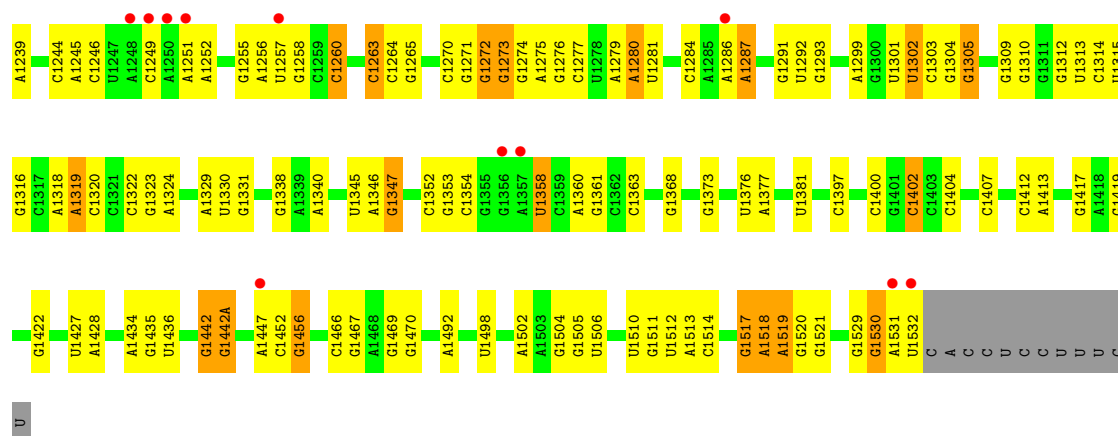
- Molecule 31: 50S ribosomal protein L36



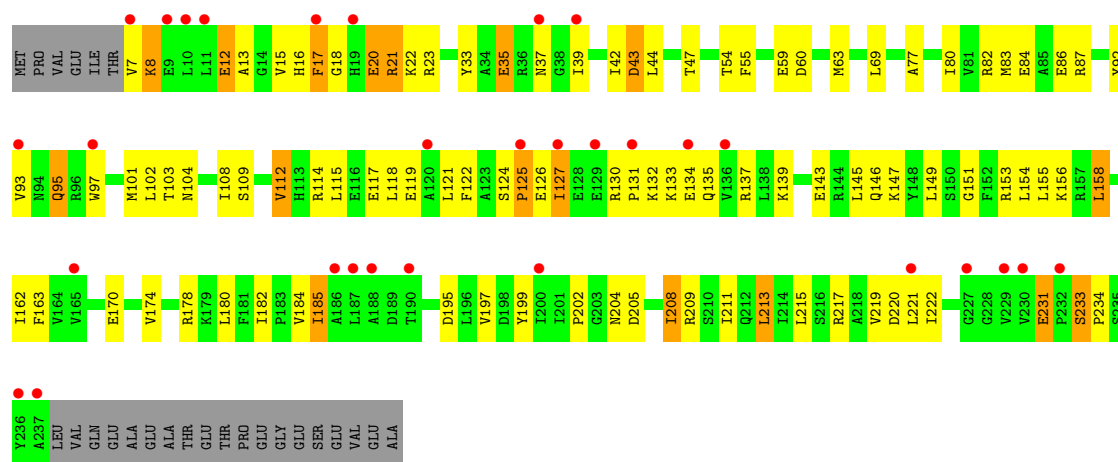
- Molecule 32: 16S Ribosomal RNA



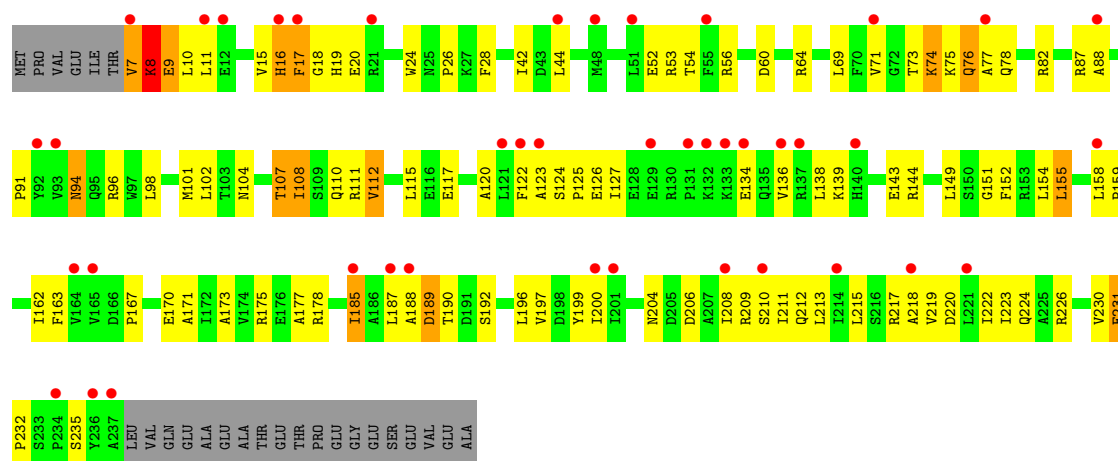




• Molecule 33: 30S ribosomal protein S2



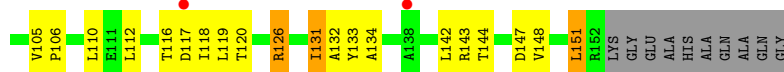
• Molecule 33: 30S ribosomal protein S2



• Molecule 34: 30S ribosomal protein S3



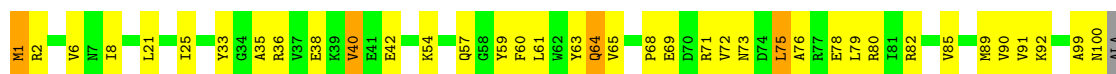
- Molecule 36: 30S ribosomal protein S5



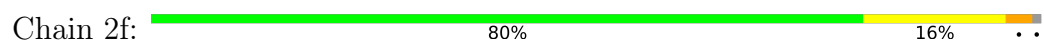
- Molecule 36: 30S ribosomal protein S5



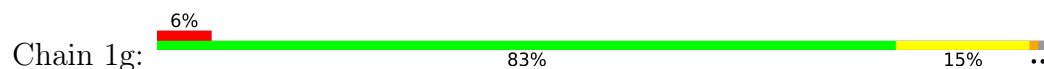
- Molecule 37: 30S ribosomal protein S6



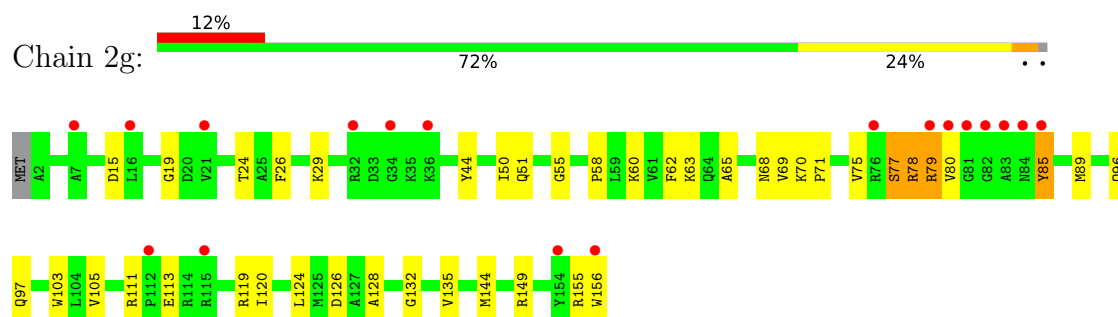
- Molecule 37: 30S ribosomal protein S6



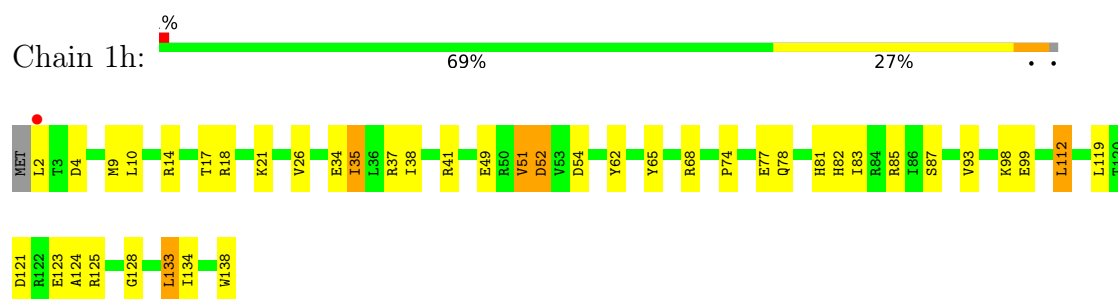
- Molecule 38: 30S ribosomal protein S7



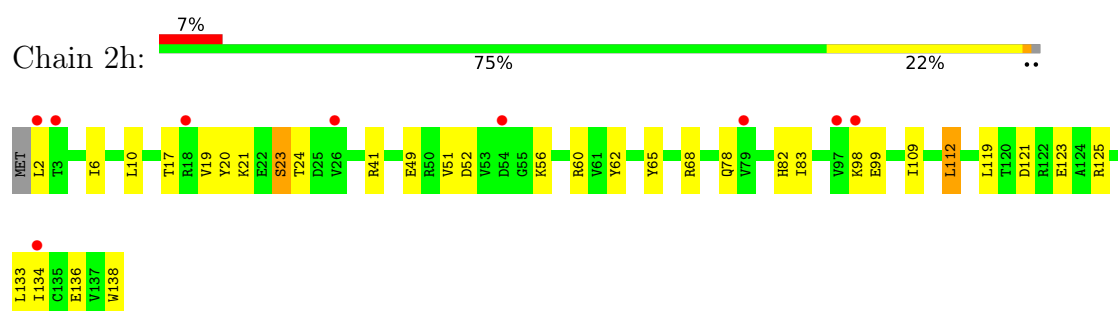
- Molecule 38: 30S ribosomal protein S7



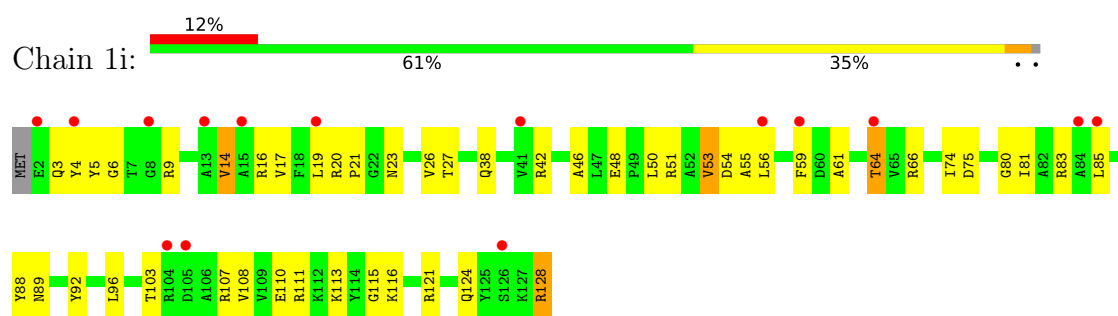
- Molecule 39: 30S ribosomal protein S8



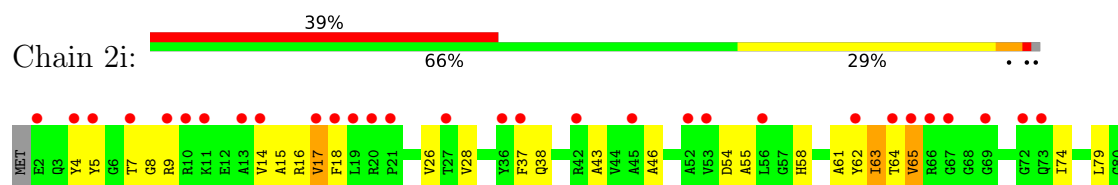
- Molecule 39: 30S ribosomal protein S8

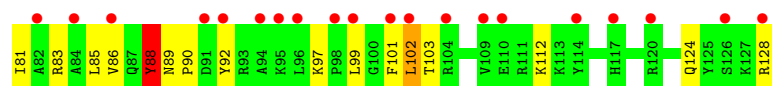


- Molecule 40: 30S ribosomal protein S9

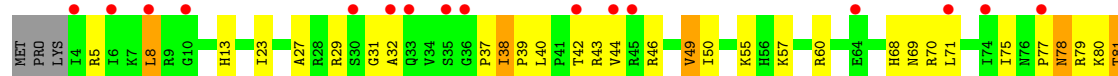


- Molecule 40: 30S ribosomal protein S9

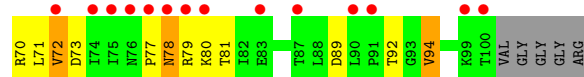
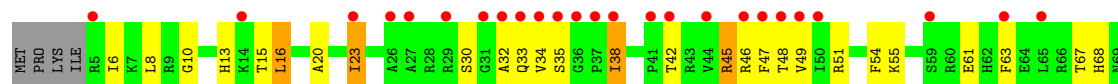




- Molecule 41: 30S ribosomal protein S10



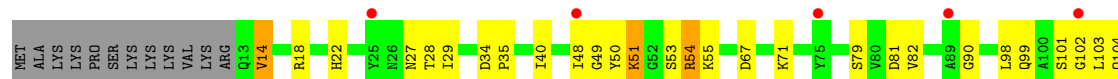
- Molecule 41: 30S ribosomal protein S10



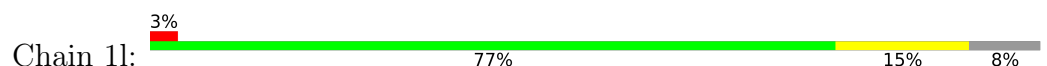
- Molecule 42: 30S ribosomal protein S11

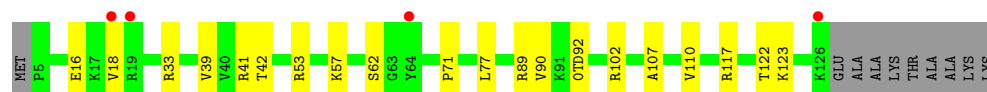


- Molecule 42: 30S ribosomal protein S11

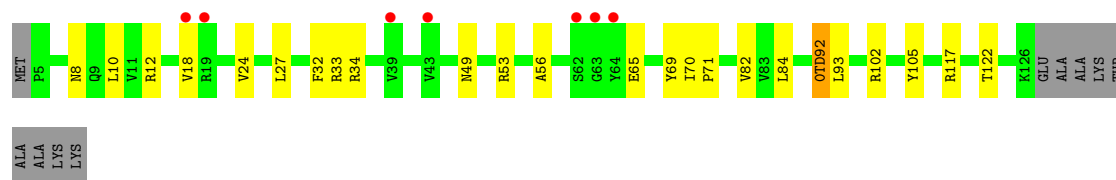
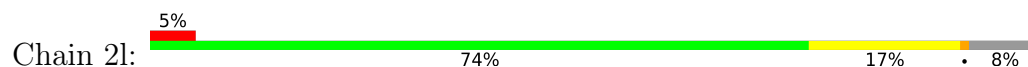


- Molecule 43: 30S ribosomal protein S12

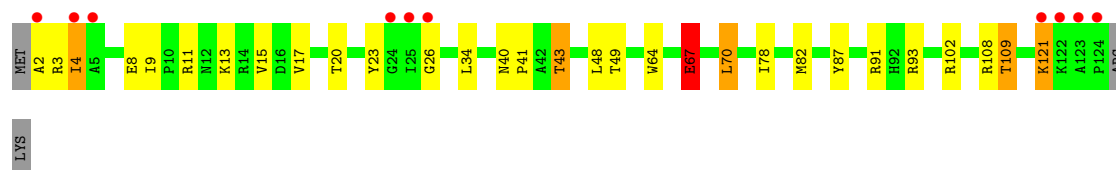
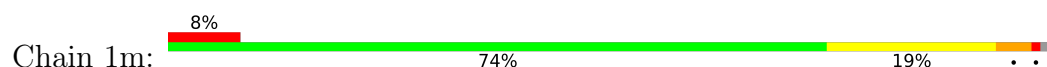




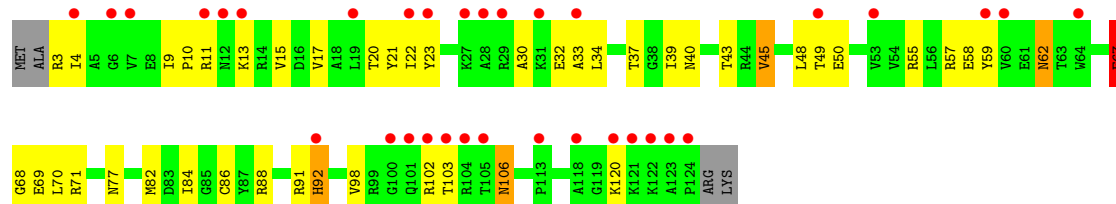
- Molecule 43: 30S ribosomal protein S12



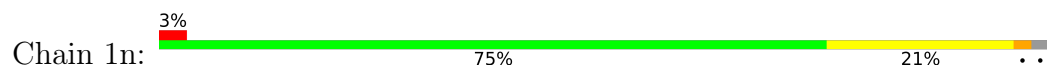
- Molecule 44: 30S ribosomal protein S13



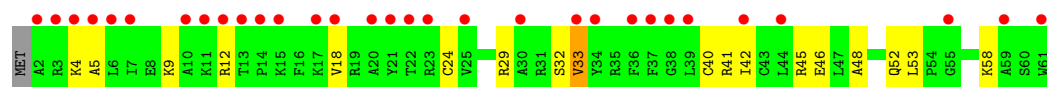
- Molecule 44: 30S ribosomal protein S13



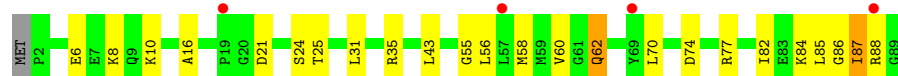
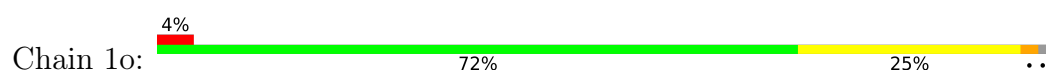
- Molecule 45: 30S ribosomal protein S14 type Z



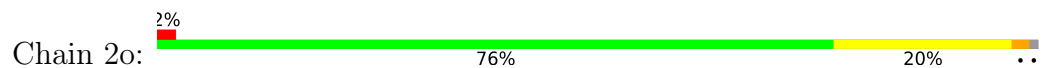
- Molecule 45: 30S ribosomal protein S14 type Z



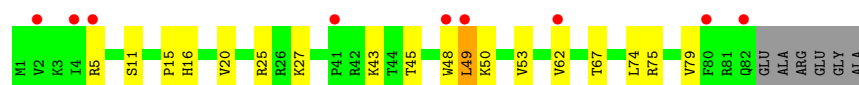
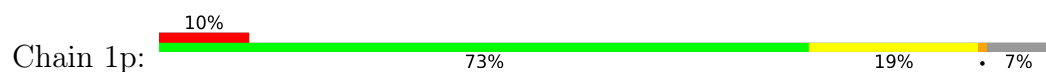
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



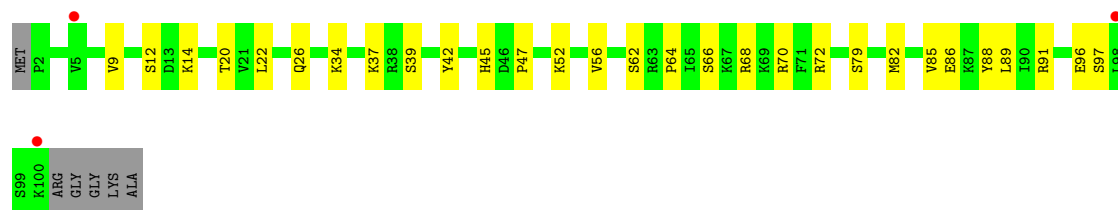
- Molecule 47: 30S ribosomal protein S16



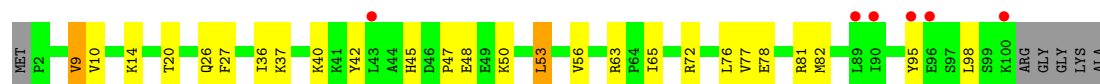
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17

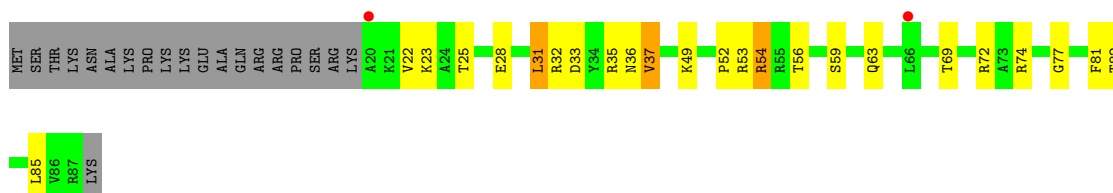


- Molecule 49: 30S ribosomal protein S18

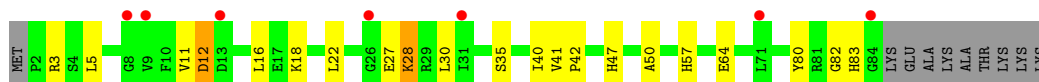




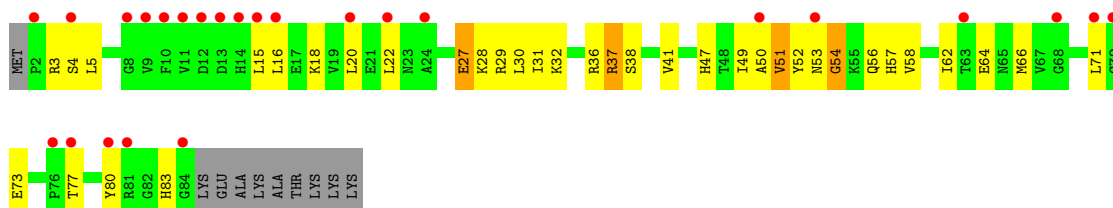
- Molecule 49: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S19



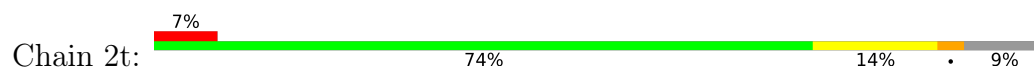
- Molecule 50: 30S ribosomal protein S19



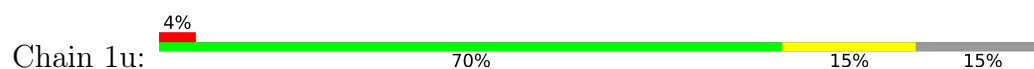
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

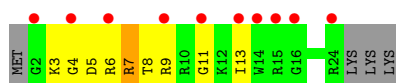
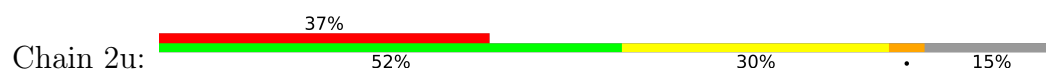


- Molecule 52: 30S ribosomal protein Thx





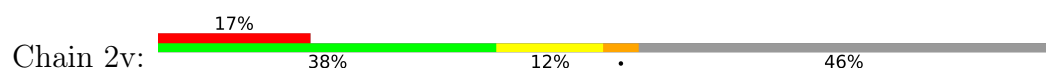
- Molecule 52: 30S ribosomal protein Thx



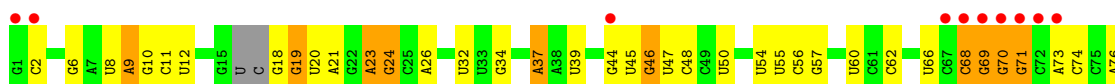
- Molecule 53: MF-mRNA



- Molecule 53: MF-mRNA



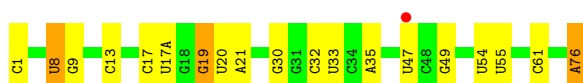
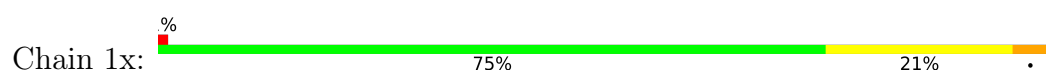
- Molecule 54: Aminoacylated Phe-tRNAphe



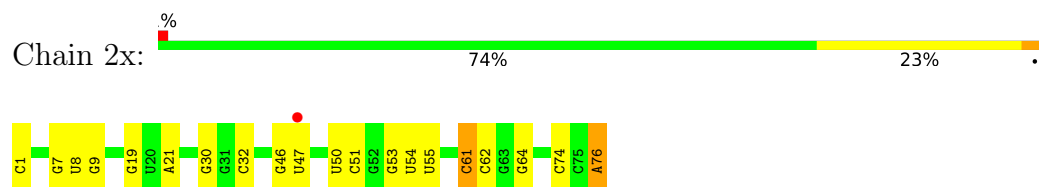
- Molecule 54: Aminoacylated Phe-tRNAphe



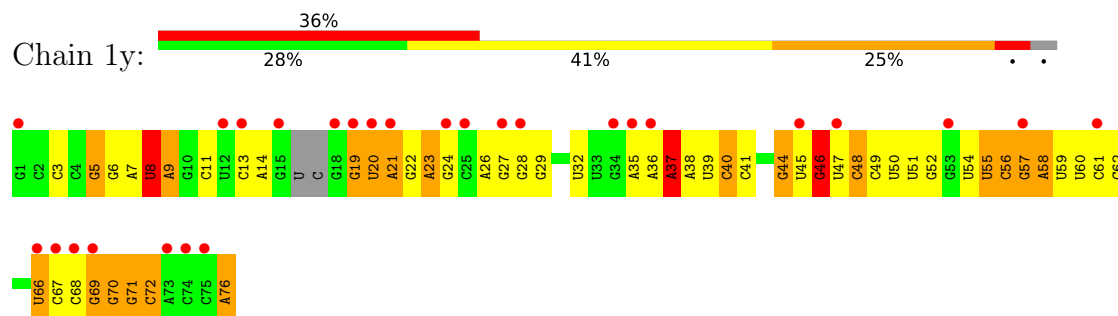
- Molecule 55: Aminoacylated fMet-tRNAmet



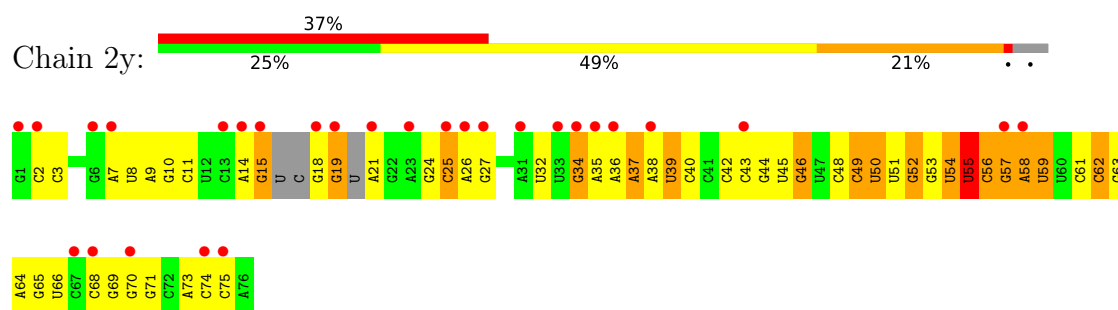
- Molecule 55: Aminoacylated fMet-tRNA^{Met}



- Molecule 56: Deacylated tRNA^{Phe}



- Molecule 56: Deacylated tRNA^{Phe}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.85Å 451.31Å 630.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.66 – 2.55 122.66 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (122.66-2.55) 99.4 (122.66-2.55)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.220 , 0.262 0.222 , 0.263	Depositor DCC
R_{free} test set	96493 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	300368	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, MIA, 8AN, K, 0TD, M2G, MA6, OMU, PSU, 2MA, SF4, OMC, 5MC, 4OC, 2MG, MG, UR3, A1AE0, FME, 4SU, ZN, 5MU, OMG

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	0.26	0/69011	0.46	2/107720 (0.0%)
1	2A	0.21	0/67295	0.40	2/105042 (0.0%)
2	1B	0.21	0/2882	0.39	0/4494
2	2B	0.19	0/2879	0.36	0/4487
3	1D	0.26	0/2186	0.52	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.26	0/1592	0.52	1/2149 (0.0%)
4	2E	0.20	0/1592	0.43	0/2149
5	1F	0.26	0/1619	0.50	0/2193
5	2F	0.20	0/1615	0.48	2/2188 (0.1%)
6	1G	0.21	0/1448	0.43	0/1957
6	2G	0.18	0/1453	0.43	1/1963 (0.1%)
7	1H	0.22	0/1356	0.42	0/1834
7	2H	0.18	0/1356	0.35	0/1834
8	1I	0.18	0/1112	0.42	0/1514
8	2I	0.33	0/1079	0.69	1/1475 (0.1%)
9	1N	0.24	0/1144	0.49	1/1543 (0.1%)
9	2N	0.19	0/1144	0.40	0/1543
10	1O	0.25	0/943	0.47	0/1269
10	2O	0.19	0/943	0.41	0/1269
11	1P	0.26	0/1152	0.57	0/1533
11	2P	0.21	0/1152	0.48	0/1533
12	1Q	0.25	0/1143	0.46	0/1527
12	2Q	0.19	0/1143	0.41	0/1527
13	1R	0.29	0/982	0.51	0/1312
13	2R	0.21	0/982	0.46	0/1312
14	1S	0.23	0/883	0.49	0/1176
14	2S	0.21	0/880	0.46	0/1172
15	1T	0.24	0/1105	0.44	0/1477
15	2T	0.21	0/1097	0.49	1/1468 (0.1%)
16	1U	0.27	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.39	0/1301
17	1V	0.24	0/782	0.48	0/1049
17	2V	0.20	0/782	0.42	0/1049
18	1W	0.27	0/897	0.46	0/1205
18	2W	0.22	0/897	0.41	0/1205
19	1X	0.26	0/764	0.51	0/1025
19	2X	0.21	0/764	0.48	0/1025
20	1Y	0.22	0/819	0.48	0/1095
20	2Y	0.20	0/819	0.39	0/1095
21	1Z	0.22	0/1267	0.46	0/1717
21	2Z	0.24	0/1299	0.50	1/1763 (0.1%)
22	10	0.27	0/662	0.49	0/881
22	20	0.20	0/662	0.45	0/881
23	11	0.23	0/762	0.42	0/1014
23	21	0.21	0/762	0.40	0/1014
24	12	0.24	0/590	0.43	0/781
24	22	0.18	0/590	0.39	0/781
25	13	0.25	0/474	0.47	0/635
25	23	0.19	0/469	0.44	0/630
26	14	0.23	0/565	0.56	0/761
26	24	0.24	0/545	0.47	0/737
27	15	0.25	0/469	0.50	0/635
27	25	0.20	0/469	0.42	0/635
28	16	0.24	0/460	0.42	0/613
28	26	0.22	0/456	0.46	0/608
29	17	0.30	0/426	0.53	0/561
29	27	0.25	0/426	0.51	0/561
30	18	0.26	0/525	0.47	0/691
30	28	0.20	0/525	0.41	0/691
31	19	0.26	0/310	0.49	0/407
31	29	0.19	0/310	0.45	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.19	0/35886	0.37	4/56005 (0.0%)
33	1b	0.20	0/1881	0.46	0/2542
33	2b	0.21	0/1860	0.46	0/2518
34	1c	0.20	0/1572	0.46	2/2126 (0.1%)
34	2c	0.20	0/1566	0.41	0/2119
35	1d	0.18	0/1685	0.42	0/2262
35	2d	0.20	0/1704	0.45	0/2284
36	1e	0.20	0/1145	0.45	0/1543
36	2e	0.21	0/1149	0.46	0/1548
37	1f	0.18	0/823	0.39	0/1115
37	2f	0.20	0/829	0.40	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1250	0.39	0/1679
38	2g	0.18	0/1254	0.41	0/1683
39	1h	0.19	0/1108	0.42	0/1494
39	2h	0.18	0/1108	0.44	0/1494
40	1i	0.20	0/1002	0.51	0/1346
40	2i	0.21	0/997	0.46	0/1343
41	1j	0.22	0/722	0.45	0/982
41	2j	0.22	0/727	0.47	0/988
42	1k	0.19	0/844	0.42	0/1145
42	2k	0.17	0/848	0.38	0/1149
43	1l	0.21	0/937	0.41	0/1260
43	2l	0.19	0/937	0.40	0/1260
44	1m	0.20	0/969	0.47	0/1302
44	2m	0.19	0/961	0.45	0/1291
45	1n	0.20	0/501	0.43	0/664
45	2n	0.22	0/501	0.47	0/664
46	1o	0.19	0/739	0.38	0/985
46	2o	0.18	0/739	0.38	0/985
47	1p	0.22	0/697	0.45	0/939
47	2p	0.19	0/693	0.43	0/935
48	1q	0.20	0/836	0.39	0/1117
48	2q	0.18	0/836	0.40	0/1117
49	1r	0.19	0/560	0.41	0/746
49	2r	0.18	0/560	0.39	0/746
50	1s	0.18	0/667	0.47	0/900
50	2s	0.25	0/661	0.56	0/893
51	1t	0.19	0/730	0.47	0/965
51	2t	0.22	0/729	0.47	0/965
52	1u	0.18	0/203	0.42	0/266
52	2u	0.20	0/203	0.43	0/266
53	1v	0.20	0/310	0.35	0/480
53	2v	0.20	0/310	0.36	0/480
54	1w	0.29	1/1581 (0.1%)	0.43	0/2458
54	2w	0.30	2/1531 (0.1%)	0.41	0/2379
55	1x	0.26	1/1723 (0.1%)	0.40	0/2684
55	2x	0.26	1/1723 (0.1%)	0.40	0/2684
56	1y	0.32	2/1606 (0.1%)	0.40	0/2497
56	2y	0.32	2/1583 (0.1%)	0.44	0/2459
All	All	0.22	9/316636 (0.0%)	0.42	18/474041 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
33	2b	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1y	46	G7M	O3'-P	5.75	1.62	1.56
56	2y	8	4SU	O3'-P	5.68	1.61	1.56
55	2x	8	4SU	O3'-P	5.42	1.61	1.56
56	1y	8	4SU	O3'-P	5.38	1.61	1.56
54	2w	8	4SU	O3'-P	5.27	1.61	1.56

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2I	66	GLU	N-CA-C	-7.62	105.15	114.75
32	2a	1272	G	N1-C2-N2	-6.99	95.23	116.20
4	1E	34	VAL	N-CA-C	-6.88	106.08	112.96
1	1A	1992	G	C2'-C3'-O3'	6.78	119.66	109.50
1	2A	1992	G	C2'-C3'-O3'	6.38	119.07	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	2b	8	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	427	0
1	2A	60322	0	30426	496	0
2	1B	2577	0	1305	13	0
2	2B	2575	0	1303	30	0
3	1D	2136	0	2218	28	0
3	2D	2136	0	2218	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1E	1559	0	1618	17	0
4	2E	1559	0	1618	26	0
5	1F	1584	0	1625	24	0
5	2F	1580	0	1619	37	0
6	1G	1423	0	1436	31	0
6	2G	1428	0	1438	48	0
7	1H	1330	0	1407	22	0
7	2H	1330	0	1407	25	0
8	1I	1097	0	1140	29	0
8	2I	1064	0	1082	76	0
9	1N	1117	0	1184	10	0
9	2N	1117	0	1184	19	0
10	1O	933	0	996	11	0
10	2O	933	0	996	11	0
11	1P	1135	0	1212	20	0
11	2P	1135	0	1212	28	0
12	1Q	1122	0	1179	11	0
12	2Q	1122	0	1179	15	0
13	1R	968	0	1033	11	0
13	2R	968	0	1033	13	0
14	1S	873	0	927	8	0
14	2S	870	0	923	32	0
15	1T	1091	0	1151	7	0
15	2T	1083	0	1136	26	0
16	1U	959	0	1019	7	0
16	2U	959	0	1019	20	0
17	1V	771	0	830	12	0
17	2V	771	0	830	12	0
18	1W	886	0	940	11	0
18	2W	886	0	940	8	0
19	1X	750	0	814	10	0
19	2X	750	0	814	17	0
20	1Y	806	0	881	17	0
20	2Y	806	0	881	18	0
21	1Z	1240	0	1240	26	0
21	2Z	1271	0	1273	47	0
22	10	653	0	674	6	0
22	20	653	0	674	12	0
23	11	755	0	826	7	0
23	21	755	0	826	16	0
24	12	588	0	643	5	0
24	22	588	0	643	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	13	469	0	518	7	0
25	23	464	0	514	11	0
26	14	552	0	533	27	0
26	24	532	0	503	26	0
27	15	455	0	465	3	0
27	25	455	0	465	4	0
28	16	453	0	473	12	0
28	26	449	0	469	12	0
29	17	418	0	467	5	0
29	27	418	0	467	6	0
30	18	517	0	582	7	0
30	28	517	0	582	9	0
31	19	307	0	335	3	0
31	29	307	0	335	6	0
32	1a	32246	0	16295	284	0
32	2a	32327	0	16338	354	0
33	1b	1846	0	1867	68	0
33	2b	1825	0	1828	77	0
34	1c	1548	0	1535	38	0
34	2c	1542	0	1517	48	0
35	1d	1655	0	1672	36	0
35	2d	1674	0	1714	52	0
36	1e	1129	0	1185	30	0
36	2e	1133	0	1191	37	0
37	1f	810	0	804	23	0
37	2f	816	0	808	15	0
38	1g	1231	0	1238	11	0
38	2g	1235	0	1249	24	0
39	1h	1088	0	1126	24	0
39	2h	1088	0	1126	16	0
40	1i	983	0	986	25	0
40	2i	978	0	966	31	0
41	1j	709	0	650	21	0
41	2j	714	0	672	25	0
42	1k	829	0	825	12	0
42	2k	833	0	836	18	0
43	1l	932	0	981	8	0
43	2l	932	0	981	13	0
44	1m	958	0	1002	21	0
44	2m	950	0	988	25	0
45	1n	492	0	529	6	0
45	2n	492	0	529	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1o	728	0	760	15	0
46	2o	728	0	760	13	0
47	1p	681	0	697	10	0
47	2p	677	0	686	15	0
48	1q	823	0	891	15	0
48	2q	823	0	891	14	0
49	1r	555	0	618	9	0
49	2r	555	0	618	22	0
50	1s	652	0	662	13	0
50	2s	646	0	644	28	0
51	1t	728	0	798	16	0
51	2t	727	0	796	12	0
52	1u	199	0	208	3	0
52	2u	199	0	208	6	0
53	1v	277	0	140	1	0
53	2v	277	0	140	1	0
54	1w	1592	0	817	16	0
54	2w	1544	0	786	24	0
55	1x	1646	0	838	10	0
55	2x	1646	0	838	8	0
56	1y	1585	0	803	33	0
56	2y	1565	0	794	30	0
57	10	9	0	0	0	0
57	11	4	0	0	0	0
57	12	2	0	0	0	0
57	13	4	0	0	0	0
57	14	1	0	0	0	0
57	15	8	0	0	0	0
57	16	3	0	0	0	0
57	17	4	0	0	0	0
57	18	3	0	0	0	0
57	19	2	0	0	0	0
57	1A	1108	0	0	0	0
57	1B	36	0	0	0	0
57	1D	13	0	0	0	0
57	1E	14	0	0	0	0
57	1F	13	0	0	0	0
57	1G	5	0	0	0	0
57	1I	1	0	0	0	0
57	1N	7	0	0	0	0
57	1O	5	0	0	0	0
57	1P	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1Q	6	0	0	0	0
57	1R	5	0	0	0	0
57	1S	3	0	0	0	0
57	1T	2	0	0	0	0
57	1U	7	0	0	0	0
57	1V	8	0	0	0	0
57	1W	6	0	0	0	0
57	1X	8	0	0	0	0
57	1Y	2	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	217	0	0	0	0
57	1b	1	0	0	0	0
57	1d	1	0	0	0	0
57	1e	2	0	0	0	0
57	1f	2	0	0	0	0
57	1h	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	2	0	0	0	0
57	1n	2	0	0	0	0
57	1q	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	8	0	0	0	0
57	1x	14	0	0	0	0
57	1y	1	0	0	0	0
57	20	2	0	0	0	0
57	21	3	0	0	0	0
57	23	2	0	0	0	0
57	25	7	0	0	0	0
57	26	1	0	0	0	0
57	27	2	0	0	0	0
57	28	3	0	0	0	0
57	29	1	0	0	0	0
57	2A	861	0	0	0	0
57	2B	19	0	0	0	0
57	2D	6	0	0	0	0
57	2E	7	0	0	0	0
57	2F	8	0	0	0	0
57	2G	1	0	0	0	0
57	2O	2	0	0	0	0
57	2P	2	0	0	0	0
57	2Q	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2R	2	0	0	0	0
57	2S	1	0	0	0	0
57	2T	4	0	0	0	0
57	2U	2	0	0	0	0
57	2V	2	0	0	0	0
57	2W	2	0	0	0	0
57	2X	2	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	238	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2g	1	0	0	0	0
57	2j	1	0	0	0	0
57	2l	3	0	0	0	0
57	2p	1	0	0	0	0
57	2q	2	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	2	0	0	0	0
57	2w	7	0	0	0	0
57	2x	6	0	0	0	0
57	2y	4	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	1A	72	0	0	0	0
59	2A	72	0	0	0	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	1	0
61	2d	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1w	11	0	8	1	0
62	2w	11	0	8	1	0
63	1x	10	0	10	0	0
63	2x	10	0	10	0	0
64	10	11	0	0	0	0
64	11	12	0	0	0	0
64	12	4	0	0	0	0
64	13	5	0	0	0	0
64	14	1	0	0	0	0
64	15	6	0	0	0	0
64	16	3	0	0	0	0
64	17	7	0	0	1	0
64	18	12	0	0	1	0
64	1A	2019	0	0	71	0
64	1B	62	0	0	2	0
64	1D	27	0	0	0	0
64	1E	25	0	0	1	0
64	1F	18	0	0	3	0
64	1G	2	0	0	0	0
64	1H	2	0	0	0	0
64	1N	5	0	0	0	0
64	1O	6	0	0	1	0
64	1P	21	0	0	2	0
64	1Q	9	0	0	0	0
64	1R	11	0	0	0	0
64	1S	3	0	0	0	0
64	1T	7	0	0	0	0
64	1U	11	0	0	0	0
64	1V	7	0	0	0	0
64	1W	8	0	0	0	0
64	1X	4	0	0	0	0
64	1Y	3	0	0	1	0
64	1Z	1	0	0	0	0
64	1a	391	0	0	25	0
64	1b	1	0	0	0	0
64	1d	1	0	0	0	0
64	1e	1	0	0	0	0
64	1f	1	0	0	0	0
64	1g	1	0	0	0	0
64	1j	1	0	0	0	0
64	1l	5	0	0	0	0
64	1m	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	1n	1	0	0	0	0
64	1o	1	0	0	0	0
64	1p	1	0	0	0	0
64	1q	2	0	0	0	0
64	1t	1	0	0	0	0
64	1u	1	0	0	1	0
64	1v	5	0	0	0	0
64	1w	13	0	0	0	0
64	1x	12	0	0	0	0
64	1y	1	0	0	0	0
64	20	1	0	0	0	0
64	21	11	0	0	0	0
64	22	1	0	0	0	0
64	23	3	0	0	1	0
64	25	2	0	0	1	0
64	27	4	0	0	0	0
64	28	3	0	0	0	0
64	29	1	0	0	0	0
64	2A	1149	0	0	63	0
64	2B	20	0	0	2	0
64	2D	20	0	0	0	0
64	2E	14	0	0	0	0
64	2F	12	0	0	0	0
64	2I	1	0	0	1	0
64	2O	1	0	0	0	0
64	2P	12	0	0	0	0
64	2Q	1	0	0	0	0
64	2R	4	0	0	0	0
64	2T	5	0	0	0	0
64	2U	3	0	0	0	0
64	2W	3	0	0	0	0
64	2X	1	0	0	0	0
64	2Y	1	0	0	0	0
64	2a	288	0	0	20	0
64	2c	1	0	0	0	0
64	2d	3	0	0	0	0
64	2e	2	0	0	0	0
64	2j	1	0	0	0	0
64	2l	6	0	0	0	0
64	2n	1	0	0	0	0
64	2p	2	0	0	0	0
64	2q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	2r	1	0	0	0	0
64	2t	2	0	0	0	0
64	2v	2	0	0	0	0
64	2w	3	0	0	0	0
64	2x	9	0	0	2	0
64	2y	5	0	0	0	0
All	All	300368	0	196742	3230	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 3230 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.28	1.32
1:1A:1082:U:O4	1:1A:1086:A:N1	1.97	0.98
56:2y:18:G:H22	56:2y:55:PSU:HN3	1.09	0.98
1:1A:1054:A:H61	1:1A:1105:U:H3	1.06	0.98
29:17:24:THR:HG22	29:17:27:GLY:H	1.30	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	25	34
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	25	34
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	25	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	2F	201/210 (96%)	191 (95%)	7 (4%)	3 (2%)	8	11
6	1G	179/182 (98%)	168 (94%)	11 (6%)	0	100	100
6	2G	179/182 (98%)	156 (87%)	19 (11%)	4 (2%)	5	5
7	1H	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
7	2H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	22	29
8	1I	144/148 (97%)	129 (90%)	14 (10%)	1 (1%)	19	26
8	2I	144/148 (97%)	97 (67%)	36 (25%)	11 (8%)	1	0
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	23
11	1P	147/150 (98%)	132 (90%)	11 (8%)	4 (3%)	4	3
11	2P	147/150 (98%)	131 (89%)	10 (7%)	6 (4%)	2	1
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	19	26
13	1R	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	97 (90%)	9 (8%)	2 (2%)	6	7
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	117 (91%)	12 (9%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	92 (93%)	4 (4%)	3 (3%)	3	2
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	13	18
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	5	5
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	12	15
20	1Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	6	7
20	2Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	13	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	1Z	148/206 (72%)	131 (88%)	14 (10%)	3 (2%)	6	6
21	2Z	156/206 (76%)	134 (86%)	17 (11%)	5 (3%)	3	2
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	12	15
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12	15
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	57 (100%)	0	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	56 (84%)	6 (9%)	5 (8%)	1	0
26	24	67/71 (94%)	54 (81%)	10 (15%)	3 (4%)	2	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	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	229/256 (90%)	198 (86%)	24 (10%)	7 (3%)	3	2
33	2b	229/256 (90%)	189 (82%)	32 (14%)	8 (4%)	3	1
34	1c	204/239 (85%)	187 (92%)	14 (7%)	3 (2%)	8	11
34	2c	204/239 (85%)	172 (84%)	28 (14%)	4 (2%)	6	6
35	1d	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	25	34
35	2d	206/209 (99%)	194 (94%)	10 (5%)	2 (1%)	13	18
36	1e	146/162 (90%)	131 (90%)	9 (6%)	6 (4%)	2	1
36	2e	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	19	26
37	1f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	13	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	141 (92%)	11 (7%)	1 (1%)	19	26
38	2g	153/156 (98%)	141 (92%)	10 (6%)	2 (1%)	10	13
39	1h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	19	26
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16	23
40	2i	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	16	23
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	2	1
41	2j	94/105 (90%)	80 (85%)	10 (11%)	4 (4%)	2	1
42	1k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	14	21
42	2k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	7	8
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	114 (94%)	6 (5%)	1 (1%)	16	23
44	2m	120/126 (95%)	107 (89%)	10 (8%)	3 (2%)	4	4
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	11	14
47	1p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	10	13
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	11	14
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	1
51	2t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	5	6
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11370/12128 (94%)	10516 (92%)	725 (6%)	129 (1%)	12	15

5 of 129 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	44	GLY
21	1Z	53	ILE
23	11	3	LYS
26	14	47	GLN
26	14	62	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	201 (94%)	14 (6%)	14	18
3	2D	215/218 (99%)	197 (92%)	18 (8%)	9	11
4	1E	164/166 (99%)	158 (96%)	6 (4%)	29	42
4	2E	164/166 (99%)	151 (92%)	13 (8%)	10	13
5	1F	160/166 (96%)	144 (90%)	16 (10%)	6	7
5	2F	159/166 (96%)	149 (94%)	10 (6%)	15	19
6	1G	143/156 (92%)	128 (90%)	15 (10%)	5	6
6	2G	143/156 (92%)	122 (85%)	21 (15%)	2	2
7	1H	144/148 (97%)	134 (93%)	10 (7%)	13	16
7	2H	144/148 (97%)	130 (90%)	14 (10%)	6	7
8	1I	113/124 (91%)	97 (86%)	16 (14%)	2	2
8	2I	105/124 (85%)	83 (79%)	22 (21%)	1	0
9	1N	118/119 (99%)	109 (92%)	9 (8%)	11	14
9	2N	118/119 (99%)	107 (91%)	11 (9%)	7	8
10	1O	100/100 (100%)	96 (96%)	4 (4%)	27	40
10	2O	100/100 (100%)	96 (96%)	4 (4%)	27	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	1P	115/116 (99%)	106 (92%)	9 (8%)	10	13
11	2P	115/116 (99%)	108 (94%)	7 (6%)	15	20
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	9	12
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	23	34
13	1R	101/101 (100%)	95 (94%)	6 (6%)	16	21
13	2R	101/101 (100%)	99 (98%)	2 (2%)	50	69
14	1S	86/88 (98%)	82 (95%)	4 (5%)	22	32
14	2S	85/88 (97%)	74 (87%)	11 (13%)	3	3
15	1T	115/127 (91%)	109 (95%)	6 (5%)	19	27
15	2T	113/127 (89%)	105 (93%)	8 (7%)	12	16
16	1U	93/94 (99%)	88 (95%)	5 (5%)	18	25
16	2U	93/94 (99%)	88 (95%)	5 (5%)	18	25
17	1V	80/82 (98%)	74 (92%)	6 (8%)	11	15
17	2V	80/82 (98%)	74 (92%)	6 (8%)	11	15
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33	48
18	2W	90/92 (98%)	85 (94%)	5 (6%)	17	24
19	1X	77/78 (99%)	74 (96%)	3 (4%)	27	41
19	2X	77/78 (99%)	74 (96%)	3 (4%)	27	41
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	4	4
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	9	12
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	8	9
21	2Z	137/179 (76%)	118 (86%)	19 (14%)	3	2
22	10	65/67 (97%)	64 (98%)	1 (2%)	60	76
22	20	65/67 (97%)	63 (97%)	2 (3%)	35	50
23	11	80/83 (96%)	79 (99%)	1 (1%)	65	79
23	21	80/83 (96%)	75 (94%)	5 (6%)	15	19
24	12	65/67 (97%)	64 (98%)	1 (2%)	60	76
24	22	65/67 (97%)	63 (97%)	2 (3%)	35	50
25	13	51/52 (98%)	47 (92%)	4 (8%)	10	13
25	23	50/52 (96%)	47 (94%)	3 (6%)	16	21
26	14	59/63 (94%)	50 (85%)	9 (15%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	24	53/63 (84%)	42 (79%)	11 (21%)	1	0
27	15	50/52 (96%)	47 (94%)	3 (6%)	16	21
27	25	50/52 (96%)	46 (92%)	4 (8%)	10	12
28	16	51/52 (98%)	48 (94%)	3 (6%)	16	21
28	26	50/52 (96%)	45 (90%)	5 (10%)	6	7
29	17	41/42 (98%)	36 (88%)	5 (12%)	4	3
29	27	41/42 (98%)	38 (93%)	3 (7%)	11	15
30	18	54/55 (98%)	50 (93%)	4 (7%)	11	15
30	28	54/55 (98%)	49 (91%)	5 (9%)	7	8
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	31 (91%)	3 (9%)	8	10
33	1b	192/220 (87%)	168 (88%)	24 (12%)	3	3
33	2b	187/220 (85%)	168 (90%)	19 (10%)	6	6
34	1c	142/188 (76%)	130 (92%)	12 (8%)	8	11
34	2c	140/188 (74%)	130 (93%)	10 (7%)	12	16
35	1d	169/181 (93%)	150 (89%)	19 (11%)	5	5
35	2d	173/181 (96%)	154 (89%)	19 (11%)	5	5
36	1e	113/123 (92%)	103 (91%)	10 (9%)	8	10
36	2e	114/123 (93%)	101 (89%)	13 (11%)	4	4
37	1f	84/90 (93%)	75 (89%)	9 (11%)	5	6
37	2f	85/90 (94%)	79 (93%)	6 (7%)	12	16
38	1g	119/127 (94%)	109 (92%)	10 (8%)	9	11
38	2g	120/127 (94%)	111 (92%)	9 (8%)	11	15
39	1h	114/119 (96%)	104 (91%)	10 (9%)	8	10
39	2h	114/119 (96%)	104 (91%)	10 (9%)	8	10
40	1i	90/99 (91%)	75 (83%)	15 (17%)	2	1
40	2i	89/99 (90%)	81 (91%)	8 (9%)	8	9
41	1j	66/92 (72%)	54 (82%)	12 (18%)	1	1
41	2j	69/92 (75%)	58 (84%)	11 (16%)	2	1
42	1k	82/99 (83%)	73 (89%)	9 (11%)	5	5
42	2k	83/99 (84%)	76 (92%)	7 (8%)	9	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	1l	96/108 (89%)	90 (94%)	6 (6%)	15	19
43	2l	96/108 (89%)	93 (97%)	3 (3%)	35	50
44	1m	93/101 (92%)	84 (90%)	9 (10%)	6	7
44	2m	92/101 (91%)	76 (83%)	16 (17%)	1	1
45	1n	49/50 (98%)	44 (90%)	5 (10%)	6	6
45	2n	49/50 (98%)	46 (94%)	3 (6%)	15	20
46	1o	78/80 (98%)	75 (96%)	3 (4%)	28	41
46	2o	78/80 (98%)	75 (96%)	3 (4%)	28	41
47	1p	69/74 (93%)	62 (90%)	7 (10%)	6	7
47	2p	68/74 (92%)	60 (88%)	8 (12%)	4	4
48	1q	94/97 (97%)	87 (93%)	7 (7%)	11	15
48	2q	94/97 (97%)	90 (96%)	4 (4%)	25	36
49	1r	59/77 (77%)	51 (86%)	8 (14%)	3	2
49	2r	59/77 (77%)	54 (92%)	5 (8%)	8	11
50	1s	69/80 (86%)	63 (91%)	6 (9%)	8	10
50	2s	67/80 (84%)	60 (90%)	7 (10%)	5	6
51	1t	70/82 (85%)	66 (94%)	4 (6%)	17	23
51	2t	70/82 (85%)	68 (97%)	2 (3%)	37	54
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8527 (92%)	776 (8%)	9	12

5 of 776 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	2I	87	LYS
23	2I	40	ARG
8	2I	145	VAL
8	2I	82	ARG
15	2T	72	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 136 such sidechains are listed below:

Mol	Chain	Res	Type
38	2g	110	GLN
40	2i	117	HIS
48	2q	26	GLN
43	1l	8	ASN
41	1j	56	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	427 (14%)	26 (0%)
1	2A	2791/2915 (95%)	443 (15%)	28 (1%)
2	1B	119/121 (98%)	13 (10%)	0
2	2B	118/121 (97%)	19 (16%)	0
32	1a	1497/1521 (98%)	231 (15%)	0
32	2a	1501/1521 (98%)	267 (17%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1w	71/76 (93%)	21 (29%)	0
54	2w	68/76 (89%)	25 (36%)	0
55	1x	75/77 (97%)	6 (8%)	0
55	2x	75/77 (97%)	7 (9%)	0
56	1y	72/76 (94%)	32 (44%)	0
56	2y	70/76 (92%)	27 (38%)	0
All	All	9345/9620 (97%)	1525 (16%)	54 (0%)

5 of 1525 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	G
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C

5 of 54 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	228	A
1	2A	746	A
1	2A	2126	A
1	2A	249	C
1	2A	271(M)	G

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

88 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$
55	8AN	2x	76	57,63,55	17,24,25	1.12	2 (11%)	13,35,38	3.01	3 (23%)
54	4SU	1w	8	54	18,21,22	1.85	4 (22%)	25,30,33	1.80	4 (16%)
1	5MU	1A	1915	1	19,22,23	1.41	5 (26%)	27,32,35	2.21	6 (22%)
1	OMG	1A	2251	1,57,55	19,26,27	0.90	1 (5%)	21,38,41	1.12	3 (14%)
32	5MC	2a	967	32	19,22,23	1.71	3 (15%)	26,32,35	1.16	3 (11%)
43	0TD	2l	92	43	8,9,10	4.57	2 (25%)	6,11,13	4.80	2 (33%)
54	8AN	2w	76	54,1,62	17,24,25	1.38	4 (23%)	13,35,38	2.01	2 (15%)
55	PSU	2x	55	55	18,21,22	1.39	2 (11%)	21,30,33	1.99	3 (14%)
54	G7M	2w	46	54	20,26,27	1.21	1 (5%)	16,39,42	0.88	0
32	5MC	2a	1400	32	19,22,23	1.56	3 (15%)	26,32,35	1.19	3 (11%)
1	OMU	2A	2552	1,57	19,22,23	1.10	1 (5%)	25,31,34	1.79	5 (20%)
1	5MU	2A	1939	1,57	19,22,23	1.44	6 (31%)	27,32,35	2.28	6 (22%)
54	PSU	1w	55	54	18,21,22	1.40	2 (11%)	21,30,33	2.03	4 (19%)
54	PSU	2w	39	54	18,21,22	1.41	2 (11%)	21,30,33	1.85	4 (19%)
56	PSU	2y	55	56	18,21,22	1.44	3 (16%)	21,30,33	1.98	4 (19%)
1	OMG	2A	2251	1,55	19,26,27	0.91	1 (5%)	21,38,41	1.14	3 (14%)
54	PSU	2w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.84	3 (14%)
32	4OC	2a	1402	32	20,23,24	0.75	0	25,32,35	0.99	1 (4%)
1	2MA	1A	2503	1,57	18,25,26	0.70	0	20,37,40	2.11	3 (15%)
32	MA6	1a	1519	32	19,26,27	1.03	2 (10%)	18,38,41	2.09	3 (16%)
1	PSU	1A	2605	1,57	18,21,22	1.47	3 (16%)	21,30,33	1.81	3 (14%)
56	G7M	1y	46	56	20,26,27	1.30	1 (5%)	16,39,42	0.55	0
56	MIA	2y	37	56	17,24,32	1.00	1 (5%)	16,35,47	1.26	2 (12%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
56	4SU	1y	8	56	18,21,22	1.76	5 (27%)	25,30,33	1.90	5 (20%)
55	4SU	1x	8	55	18,21,22	2.17	6 (33%)	25,30,33	1.63	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	2a	966	32	20,27,28	1.28	3 (15%)	19,40,43	1.07	1 (5%)
54	G7M	1w	46	54	20,26,27	1.24	2 (10%)	16,39,42	0.64	0
32	MA6	1a	1518	32	19,26,27	1.03	2 (10%)	18,38,41	1.93	3 (16%)
56	PSU	2y	39	56	18,21,22	1.41	2 (11%)	21,30,33	1.65	3 (14%)
55	4SU	2x	8	55	18,21,22	1.99	7 (38%)	25,30,33	1.33	4 (16%)
55	5MU	2x	54	55	19,22,23	1.39	5 (26%)	27,32,35	2.28	6 (22%)
32	M2G	1a	966	32	20,27,28	1.44	3 (15%)	19,40,43	1.04	2 (10%)
1	PSU	2A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	2.06	3 (14%)
32	MA6	2a	1519	32	19,26,27	1.03	2 (10%)	18,38,41	2.06	3 (16%)
1	5MC	2A	1962	1	19,22,23	1.60	3 (15%)	26,32,35	1.12	2 (7%)
56	4SU	2y	8	56	18,21,22	1.86	5 (27%)	25,30,33	1.85	4 (16%)
1	PSU	1A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	1.99	4 (19%)
54	PSU	1w	32	54	18,21,22	1.40	3 (16%)	21,30,33	1.91	4 (19%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.28	1 (6%)
1	5MC	2A	1942	1	19,22,23	1.64	3 (15%)	26,32,35	1.13	2 (7%)
1	5MU	2A	1915	1	19,22,23	1.43	5 (26%)	27,32,35	2.19	6 (22%)
1	PSU	2A	2605	1	18,21,22	1.33	2 (11%)	21,30,33	2.03	4 (19%)
32	MA6	2a	1518	32	19,26,27	0.99	2 (10%)	18,38,41	2.01	3 (16%)
32	5MC	1a	1407	32	19,22,23	1.68	2 (10%)	26,32,35	1.10	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.65	3 (15%)	26,32,35	1.20	2 (7%)
56	PSU	2y	32	56	18,21,22	1.38	2 (11%)	21,30,33	2.01	4 (19%)
56	PSU	1y	55	56	18,21,22	1.34	2 (11%)	21,30,33	2.06	3 (14%)
1	OMU	1A	2552	1	19,22,23	1.21	3 (15%)	25,31,34	1.82	5 (20%)
32	2MG	2a	1207	32	18,26,27	0.91	1 (5%)	16,38,41	1.49	3 (18%)
55	5MC	2x	32	55	19,22,23	1.64	3 (15%)	26,32,35	1.28	3 (11%)
32	PSU	2a	516	32	18,21,22	1.32	2 (11%)	21,30,33	2.06	4 (19%)
54	8AN	1w	76	54,1,62	17,24,25	1.40	4 (23%)	13,35,38	2.07	2 (15%)
54	PSU	1w	39	54	18,21,22	1.35	2 (11%)	21,30,33	2.07	4 (19%)
54	5MU	1w	54	54	19,22,23	1.43	5 (26%)	27,32,35	1.96	6 (22%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.23	3 (11%)
1	2MA	2A	2503	1,57	18,25,26	0.73	0	20,37,40	2.11	4 (20%)
32	4OC	1a	1402	32	20,23,24	0.76	0	25,32,35	0.96	1 (4%)
56	MIA	1y	37	56	17,24,32	1.04	1 (5%)	16,35,47	1.27	2 (12%)
54	MIA	1w	37	54	24,31,32	2.14	3 (12%)	22,44,47	2.61	7 (31%)
54	4SU	2w	8	54	18,21,22	1.81	5 (27%)	25,30,33	2.50	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	G7M	2a	527	32	20,26,27	1.21	2 (10%)	16,39,42	0.56	0
32	5MC	2a	1407	57,32	19,22,23	1.69	3 (15%)	26,32,35	1.21	3 (11%)
1	PSU	1A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.00	5 (23%)
32	UR3	1a	1498	32	19,22,23	0.96	1 (5%)	26,32,35	1.72	4 (15%)
56	G7M	2y	46	56	20,26,27	1.34	2 (10%)	16,39,42	0.56	0
55	5MC	1x	32	55	19,22,23	1.68	3 (15%)	26,32,35	1.21	3 (11%)
32	G7M	1a	527	57,32	20,26,27	1.22	2 (10%)	16,39,42	0.49	0
32	UR3	2a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.75	3 (11%)
1	5MC	1A	1962	1,57	19,22,23	1.71	3 (15%)	26,32,35	1.11	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.90	0
32	PSU	1a	516	32	18,21,22	1.37	2 (11%)	21,30,33	1.95	5 (23%)
54	MIA	2w	37	54	19,27,32	1.80	3 (15%)	18,39,47	1.58	5 (27%)
55	5MU	1x	54	57,55	19,22,23	1.43	5 (26%)	27,32,35	2.00	6 (22%)
32	5MC	1a	967	32	19,22,23	1.71	3 (15%)	26,32,35	1.19	2 (7%)
56	PSU	1y	32	56	18,21,22	1.35	2 (11%)	21,30,33	1.89	4 (19%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.03	4 (19%)
54	PSU	2w	55	54	18,21,22	1.37	2 (11%)	21,30,33	2.03	3 (14%)
56	5MU	2y	54	56	19,22,23	1.41	4 (21%)	27,32,35	1.93	5 (18%)
32	5MC	2a	1404	32	19,22,23	1.75	3 (15%)	26,32,35	1.16	2 (7%)
1	5MC	1A	1942	1	19,22,23	1.74	3 (15%)	26,32,35	1.25	3 (11%)
56	PSU	1y	39	56	18,21,22	1.46	3 (16%)	21,30,33	1.77	4 (19%)
1	5MU	1A	1939	1,57	19,22,23	1.48	6 (31%)	27,32,35	2.19	6 (22%)
55	8AN	1x	76	57,63,55	17,24,25	1.36	3 (17%)	13,35,38	3.04	3 (23%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.00	1 (4%)
43	0TD	1l	92	43	8,9,10	4.52	1 (12%)	6,11,13	2.59	2 (33%)
56	5MU	1y	54	56	19,22,23	1.43	5 (26%)	27,32,35	2.28	9 (33%)
54	5MU	2w	54	54	19,22,23	1.30	4 (21%)	27,32,35	2.04	7 (25%)

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
55	8AN	2x	76	57,63,55	-	3/3/25/26	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,57,55	-	0/5/27/28	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
54	8AN	2w	76	54,1,62	-	0/3/25/26	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	0/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	4/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
1	2MA	1A	2503	1,57	-	1/3/25/26	0/3/3/3
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
56	G7M	1y	46	56	-	2/3/25/26	0/3/3/3
56	MIA	2y	37	56	-	1/3/25/34	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	2/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/9/27/28	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	8AN	1w	76	54,1,62	-	1/3/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	2/3/25/26	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
56	MIA	1y	37	56	-	2/3/25/34	0/3/3/3
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	2/3/25/26	0/3/3/3
32	5MC	2a	1407	57,32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	1/3/25/26	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	57,32	-	3/3/25/26	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,57	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	4/7/29/34	0/3/3/3
55	5MU	1x	54	57,55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	57,63,55	-	3/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2

The worst 5 of 229 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.39	1.69	1.82
43	1l	92	0TD	CB-SB	-12.31	1.69	1.82
54	1w	37	MIA	C2-S10	-6.82	1.70	1.75
54	1w	37	MIA	C13-C14	6.74	1.52	1.32
1	1A	1942	5MC	C5-C4	6.46	1.49	1.44

The worst 5 of 293 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	11.38	122.83	102.36
54	1w	37	MIA	C12-C13-C14	-9.28	110.36	127.01
55	1x	76	8AN	C4'-O4'-C1'	-8.27	102.35	109.92
54	2w	8	4SU	C4-N3-C2	-7.76	119.88	127.31
1	1A	2503	2MA	C2-N3-C4	7.73	121.70	115.46

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C12-C13-C14-C16
56	1y	46	G7M	C4'-C5'-O5'-P
54	2w	37	MIA	C5-C6-N6-C12
54	2w	37	MIA	N1-C6-N6-C12

There are no ring outliers.

28 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2x	76	8AN	2	0
1	1A	2251	OMG	1	0
32	2a	967	5MC	2	0
43	2l	92	0TD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2w	76	8AN	1	0
54	2w	46	G7M	1	0
54	2w	39	PSU	2	0
56	2y	55	PSU	5	0
1	2A	2251	OMG	1	0
32	2a	1402	4OC	1	0
32	1a	1519	MA6	2	0
56	1y	46	G7M	1	0
56	2y	37	MIA	1	0
56	1y	8	4SU	1	0
55	1x	8	4SU	2	0
32	2a	966	M2G	1	0
32	1a	1518	MA6	2	0
56	2y	39	PSU	1	0
32	2a	1519	MA6	2	0
32	2a	1518	MA6	3	0
56	1y	55	PSU	1	0
1	2A	2503	2MA	1	0
32	1a	1402	4OC	1	0
56	1y	37	MIA	3	0
54	1w	37	MIA	1	0
56	2y	46	G7M	3	0
1	1A	1939	5MU	1	0
55	1x	76	8AN	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2794 ligands modelled in this entry, 2786 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	A1AE0	2A	3863	-	77,77,77	2.37	14 (18%)	107,113,113	2.09	16 (14%)
62	PHE	1w	109	54	10,11,12	1.60	1 (10%)	8,13,15	0.56	0
59	A1AE0	1A	4110	-	77,77,77	2.28	13 (16%)	107,113,113	2.02	24 (22%)
62	PHE	2w	108	54	10,11,12	1.63	1 (10%)	8,13,15	0.54	0
61	SF4	2d	303	35	0,12,12	-	-	-		
61	SF4	1d	302	35	0,12,12	-	-	-		
63	FME	1x	115	55	8,9,10	0.45	0	8,9,11	1.29	1 (12%)
63	FME	2x	107	55	8,9,10	0.39	0	8,9,11	1.11	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
59	A1AE0	2A	3863	-	-	11/88/121/121	0/6/6/6
62	PHE	1w	109	54	-	1/5/6/8	0/1/1/1
59	A1AE0	1A	4110	-	-	12/88/121/121	0/6/6/6
62	PHE	2w	108	54	-	2/5/6/8	0/1/1/1
61	SF4	2d	303	35	-	-	0/6/5/5
61	SF4	1d	302	35	-	-	0/6/5/5
63	FME	1x	115	55	-	0/7/9/11	-
63	FME	2x	107	55	-	0/7/9/11	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	2A	3863	A1AE0	CAG-CAF	-12.45	1.41	1.53
59	1A	4110	A1AE0	CAG-CAF	-11.70	1.42	1.53
59	2A	3863	A1AE0	CAB-CAF	-6.97	1.40	1.52
59	1A	4110	A1AE0	OBR-NBJ	6.66	1.56	1.40
59	2A	3863	A1AE0	CAJ-CAI	-6.21	1.38	1.51

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	2A	3863	A1AE0	CAB-CAF-NBJ	-13.77	116.06	126.21
59	1A	4110	A1AE0	CAB-CAF-NBJ	-11.49	117.74	126.21
59	2A	3863	A1AE0	CAB-CAF-CAG	6.21	125.96	119.34
59	2A	3863	A1AE0	OBB-CBT-NBV	4.99	119.14	111.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1A	4110	A1AE0	CCN-CCM-NCL	-4.77	111.33	118.87

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	4110	A1AE0	NBJ-CAF-CAG-CBI
59	2A	3863	A1AE0	CAF-NBJ-OBR-CBS
62	1w	109	PHE	O-C-CA-CB
62	2w	108	PHE	C-CA-CB-CG
59	2A	3863	A1AE0	CBY-CBZ-CCA-CCB

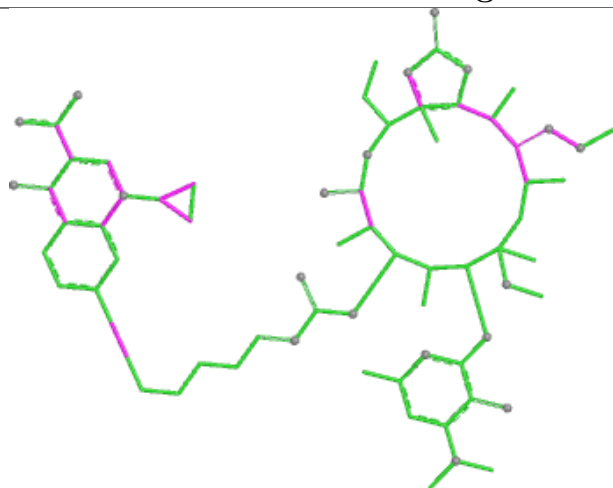
There are no ring outliers.

3 monomers are involved in 3 short contacts:

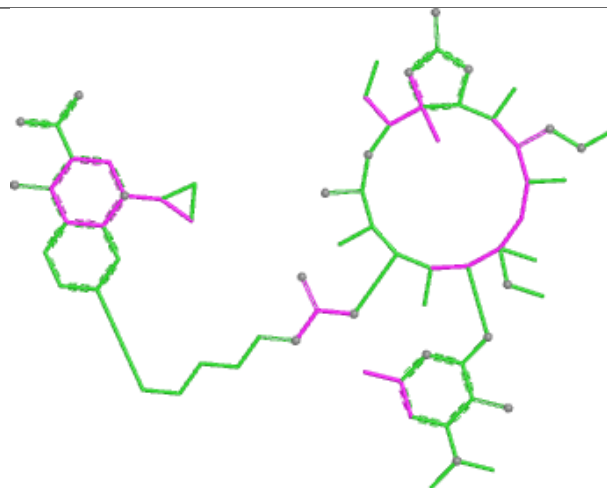
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	1w	109	PHE	1	0
62	2w	108	PHE	1	0
61	1d	302	SF4	1	0

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

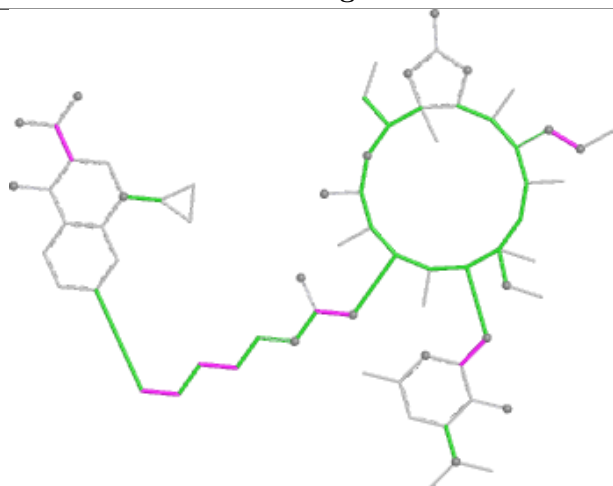
Ligand A1AE0 2A 3863



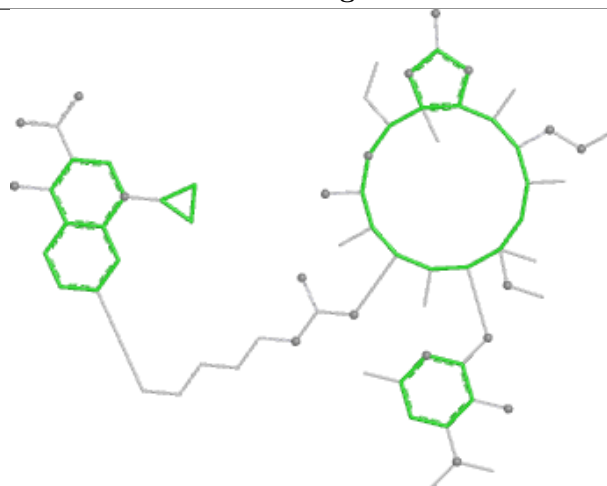
Bond lengths



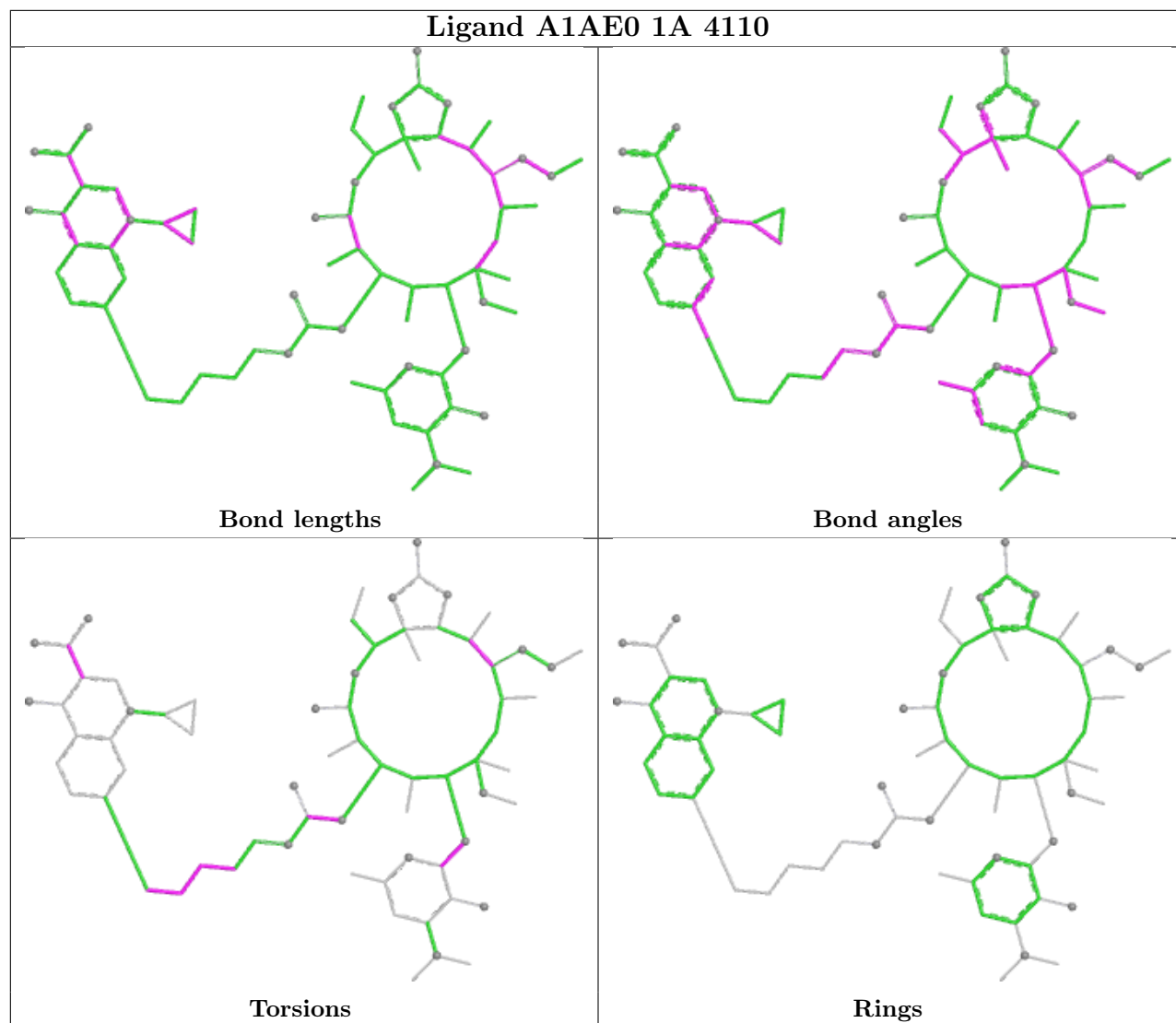
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.52	146 (5%) 34 39	18, 34, 91, 102	0
1	2A	2789/2915 (95%)	-0.03	139 (4%) 35 40	31, 54, 89, 104	0
2	1B	120/121 (99%)	-0.41	0 100 100	30, 47, 62, 84	0
2	2B	120/121 (99%)	0.52	0 100 100	56, 70, 78, 89	0
3	1D	275/276 (99%)	-0.28	2 (0%) 84 86	20, 36, 48, 75	0
3	2D	275/276 (99%)	0.13	3 (1%) 77 80	29, 45, 58, 78	0
4	1E	204/206 (99%)	-0.31	0 100 100	17, 37, 58, 67	0
4	2E	204/206 (99%)	0.37	3 (1%) 71 75	34, 57, 69, 78	0
5	1F	203/210 (96%)	-0.14	1 (0%) 87 90	20, 39, 62, 78	0
5	2F	203/210 (96%)	0.36	2 (0%) 79 82	33, 61, 76, 80	0
6	1G	181/182 (99%)	0.41	9 (4%) 35 40	38, 54, 68, 85	0
6	2G	181/182 (99%)	1.03	17 (9%) 15 19	52, 70, 79, 85	0
7	1H	174/180 (96%)	0.27	4 (2%) 61 65	38, 51, 63, 70	0
7	2H	174/180 (96%)	1.36	33 (18%) 4 5	68, 78, 87, 92	0
8	1I	146/148 (98%)	0.80	7 (4%) 36 42	44, 68, 76, 80	0
8	2I	146/148 (98%)	3.07	90 (61%) 0 0	52, 81, 91, 95	0
9	1N	140/140 (100%)	-0.26	1 (0%) 84 86	24, 37, 57, 72	0
9	2N	140/140 (100%)	0.68	7 (5%) 35 40	46, 61, 74, 80	0
10	1O	122/122 (100%)	-0.27	0 100 100	24, 38, 53, 61	0
10	2O	122/122 (100%)	0.35	0 100 100	46, 56, 66, 69	0
11	1P	149/150 (99%)	0.01	2 (1%) 74 77	18, 44, 65, 73	0
11	2P	149/150 (99%)	0.70	9 (6%) 29 33	35, 63, 77, 84	0
12	1Q	141/141 (100%)	-0.15	0 100 100	23, 39, 52, 66	0
12	2Q	141/141 (100%)	0.70	8 (5%) 30 34	44, 61, 72, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.40	0 100 100	24, 32, 47, 51	0
13	2R	118/118 (100%)	0.12	2 (1%) 69 72	40, 49, 59, 67	0
14	1S	110/112 (98%)	0.07	0 100 100	35, 46, 59, 64	0
14	2S	110/112 (98%)	1.03	8 (7%) 22 26	57, 66, 74, 79	0
15	1T	131/146 (89%)	-0.00	4 (3%) 51 57	28, 42, 63, 76	0
15	2T	131/146 (89%)	0.59	3 (2%) 61 65	48, 58, 71, 75	0
16	1U	116/118 (98%)	-0.52	0 100 100	19, 29, 44, 56	0
16	2U	116/118 (98%)	0.47	2 (1%) 69 72	38, 56, 69, 76	0
17	1V	101/101 (100%)	-0.39	0 100 100	22, 36, 52, 64	0
17	2V	101/101 (100%)	0.56	1 (0%) 79 82	39, 65, 72, 77	0
18	1W	112/113 (99%)	-0.45	0 100 100	21, 29, 48, 74	0
18	2W	112/113 (99%)	0.23	2 (1%) 67 71	38, 47, 62, 88	0
19	1X	95/96 (98%)	-0.14	2 (2%) 63 68	26, 37, 62, 77	0
19	2X	95/96 (98%)	0.47	4 (4%) 41 47	41, 54, 70, 82	0
20	1Y	107/110 (97%)	0.17	2 (1%) 66 69	34, 47, 64, 76	0
20	2Y	107/110 (97%)	1.19	11 (10%) 13 16	55, 67, 77, 82	0
21	1Z	154/206 (74%)	0.74	18 (11%) 10 13	36, 60, 82, 87	0
21	2Z	160/206 (77%)	1.47	35 (21%) 3 4	61, 76, 85, 91	0
22	10	83/85 (97%)	-0.15	0 100 100	22, 34, 47, 59	0
22	20	83/85 (97%)	0.70	3 (3%) 46 52	42, 57, 66, 74	0
23	11	97/98 (98%)	0.06	1 (1%) 79 82	25, 42, 67, 72	0
23	21	97/98 (98%)	0.40	5 (5%) 34 39	36, 52, 70, 74	0
24	12	70/72 (97%)	0.05	2 (2%) 54 58	33, 45, 56, 71	0
24	22	70/72 (97%)	0.50	1 (1%) 73 76	52, 64, 71, 77	0
25	13	59/60 (98%)	-0.22	1 (1%) 69 72	24, 33, 56, 74	0
25	23	59/60 (98%)	0.54	3 (5%) 34 39	50, 58, 71, 76	0
26	14	69/71 (97%)	1.09	14 (20%) 3 4	46, 70, 84, 90	0
26	24	69/71 (97%)	1.32	13 (18%) 4 5	68, 78, 86, 88	0
27	15	59/60 (98%)	-0.36	1 (1%) 69 72	18, 31, 52, 59	0
27	25	59/60 (98%)	0.10	0 100 100	35, 48, 64, 79	0
28	16	53/54 (98%)	-0.22	0 100 100	30, 40, 55, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.35	1 (1%) 66 69	44, 55, 63, 67	0
29	17	48/49 (97%)	-0.26	2 (4%) 41 47	21, 27, 51, 62	0
29	27	48/49 (97%)	0.14	4 (8%) 19 22	28, 38, 59, 70	0
30	18	64/65 (98%)	-0.34	0 100 100	26, 32, 38, 53	0
30	28	64/65 (98%)	0.37	0 100 100	42, 50, 58, 61	0
31	19	37/37 (100%)	-0.10	0 100 100	27, 36, 51, 56	0
31	29	37/37 (100%)	0.89	2 (5%) 32 36	55, 63, 70, 76	0
32	1a	1488/1521 (97%)	0.20	48 (3%) 50 56	33, 61, 87, 101	0
32	2a	1491/1521 (98%)	0.44	62 (4%) 41 47	44, 69, 89, 102	0
33	1b	231/256 (90%)	1.08	30 (12%) 9 11	59, 72, 82, 88	0
33	2b	231/256 (90%)	1.31	42 (18%) 4 5	62, 77, 83, 89	0
34	1c	206/239 (86%)	0.91	19 (9%) 16 19	54, 67, 78, 83	0
34	2c	206/239 (86%)	1.44	52 (25%) 2 3	67, 75, 83, 86	0
35	1d	208/209 (99%)	1.08	21 (10%) 14 17	54, 64, 74, 83	0
35	2d	208/209 (99%)	0.66	8 (3%) 44 50	53, 63, 71, 80	0
36	1e	148/162 (91%)	0.61	9 (6%) 28 32	47, 59, 69, 78	0
36	2e	148/162 (91%)	1.02	10 (6%) 25 28	55, 68, 75, 83	0
37	1f	100/101 (99%)	0.44	0 100 100	52, 62, 70, 74	0
37	2f	100/101 (99%)	0.57	0 100 100	51, 61, 71, 79	0
38	1g	155/156 (99%)	0.68	9 (5%) 30 34	55, 66, 79, 83	0
38	2g	155/156 (99%)	1.01	18 (11%) 11 13	65, 73, 80, 84	0
39	1h	137/138 (99%)	0.57	1 (0%) 84 86	50, 61, 68, 72	0
39	2h	137/138 (99%)	0.98	9 (6%) 26 29	56, 68, 73, 80	0
40	1i	127/128 (99%)	1.20	15 (11%) 10 12	50, 71, 78, 81	0
40	2i	127/128 (99%)	1.85	50 (39%) 1 1	64, 78, 83, 85	0
41	1j	97/105 (92%)	1.38	19 (19%) 4 5	53, 72, 81, 85	0
41	2j	96/105 (91%)	1.95	39 (40%) 1 1	67, 79, 85, 90	0
42	1k	114/129 (88%)	0.53	3 (2%) 57 61	37, 62, 71, 80	0
42	2k	114/129 (88%)	0.64	5 (4%) 39 45	49, 68, 75, 78	0
43	1l	121/132 (91%)	0.24	4 (3%) 49 55	42, 50, 62, 69	0
43	2l	121/132 (91%)	0.56	7 (5%) 30 34	50, 59, 69, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.81	10 (8%) 19 23	51, 64, 73, 83	0
44	2m	122/126 (96%)	1.67	33 (27%) 2 2	64, 74, 79, 83	0
45	1n	60/61 (98%)	0.96	2 (3%) 49 55	55, 61, 69, 72	0
45	2n	60/61 (98%)	2.25	31 (51%) 0 0	68, 75, 81, 85	0
46	1o	88/89 (98%)	0.66	4 (4%) 39 44	44, 60, 70, 71	0
46	2o	88/89 (98%)	0.62	2 (2%) 61 65	53, 65, 74, 78	0
47	1p	82/88 (93%)	1.18	9 (10%) 12 14	52, 65, 72, 78	0
47	2p	82/88 (93%)	0.87	3 (3%) 45 51	57, 64, 72, 75	0
48	1q	99/105 (94%)	0.78	3 (3%) 52 58	52, 63, 72, 77	0
48	2q	99/105 (94%)	0.88	6 (6%) 28 32	56, 67, 73, 77	0
49	1r	68/88 (77%)	0.61	1 (1%) 71 75	53, 62, 73, 76	0
49	2r	68/88 (77%)	0.44	2 (2%) 54 58	54, 64, 71, 74	0
50	1s	83/93 (89%)	0.86	7 (8%) 18 22	58, 67, 75, 79	0
50	2s	83/93 (89%)	1.65	25 (30%) 1 2	71, 78, 84, 91	0
51	1t	96/106 (90%)	1.03	9 (9%) 15 19	54, 65, 73, 77	0
51	2t	96/106 (90%)	0.86	7 (7%) 22 26	56, 65, 74, 77	0
52	1u	23/27 (85%)	1.06	1 (4%) 40 46	55, 62, 66, 71	0
52	2u	23/27 (85%)	2.08	10 (43%) 1 1	68, 73, 76, 79	0
53	1v	13/24 (54%)	0.87	4 (30%) 1 1	43, 51, 89, 92	0
53	2v	13/24 (54%)	1.47	4 (30%) 1 1	60, 66, 92, 103	0
54	1w	66/76 (86%)	1.14	10 (15%) 6 8	25, 79, 92, 95	0
54	2w	64/76 (84%)	1.30	13 (20%) 3 4	44, 86, 93, 98	0
55	1x	72/77 (93%)	0.14	1 (1%) 73 76	25, 57, 77, 86	0
55	2x	72/77 (93%)	0.40	1 (1%) 73 76	40, 69, 79, 92	0
56	1y	67/76 (88%)	1.97	27 (40%) 1 1	59, 95, 98, 102	0
56	2y	66/76 (86%)	2.04	28 (42%) 1 1	69, 96, 101, 102	0
All	All	20873/21748 (95%)	0.33	1363 (6%) 26 30	17, 59, 84, 104	0

The worst 5 of 1363 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	10.5
44	2m	124	PRO	10.0

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Mol	Chain	Res	Type	RSRZ
8	2I	97	ILE	9.9
8	2I	107	VAL	8.8
8	2I	92	VAL	8.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MIA	2y	37	22/30	0.38	0.20	87,97,104,122	0
56	MIA	1y	37	22/30	0.39	0.18	83,90,102,115	0
56	G7M	2y	46	24/25	0.40	0.17	86,96,103,114	0
56	4SU	2y	8	20/21	0.44	0.18	89,98,105,122	0
56	5MU	2y	54	21/22	0.47	0.17	88,96,107,119	0
56	5MU	1y	54	21/22	0.48	0.16	89,94,99,112	0
56	G7M	1y	46	24/25	0.54	0.15	89,95,99,107	0
56	PSU	1y	55	20/21	0.56	0.16	90,95,98,113	0
56	PSU	2y	55	20/21	0.58	0.14	90,96,103,111	0
56	PSU	2y	32	20/21	0.60	0.15	88,92,101,116	0
56	PSU	2y	39	20/21	0.61	0.15	84,92,100,112	0
56	4SU	1y	8	20/21	0.61	0.15	90,96,113,122	0
56	PSU	1y	32	20/21	0.67	0.14	84,90,102,108	0
54	G7M	1w	46	24/25	0.68	0.15	73,80,104,124	0
54	G7M	2w	46	24/25	0.72	0.15	78,87,99,110	0
56	PSU	1y	39	20/21	0.72	0.12	79,88,95,99	0
54	4SU	2w	8	20/21	0.83	0.12	75,83,93,101	0
54	PSU	2w	55	20/21	0.85	0.11	73,79,87,88	0
55	4SU	2x	8	20/21	0.86	0.13	68,74,81,83	0
54	4SU	1w	8	20/21	0.86	0.13	69,79,85,86	0
54	5MU	2w	54	21/22	0.87	0.11	65,72,82,82	0
55	5MU	2x	54	21/22	0.88	0.14	70,76,78,79	0
32	2MG	2a	1207	24/25	0.88	0.12	62,78,81,81	0
55	PSU	1x	55	20/21	0.90	0.11	54,59,70,77	0
55	5MU	1x	54	21/22	0.90	0.10	55,62,69,76	0
54	PSU	2w	32	20/21	0.90	0.14	66,75,81,84	0
55	PSU	2x	55	20/21	0.91	0.11	68,72,82,83	0
54	MIA	2w	37	25/30	0.91	0.14	52,66,76,90	0
54	PSU	1w	55	20/21	0.91	0.09	59,66,74,76	0
43	0TD	2l	92	10/11	0.91	0.13	53,58,64,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	2MG	1a	1207	24/25	0.92	0.10	59,65,68,71	0
32	5MC	2a	967	21/22	0.92	0.14	58,61,69,73	0
55	5MC	2x	32	21/22	0.92	0.14	63,66,68,73	0
54	MIA	1w	37	29/30	0.92	0.15	38,52,64,87	0
1	PSU	2A	1917	20/21	0.93	0.10	51,60,68,69	0
32	G7M	2a	527	24/25	0.93	0.11	52,59,64,68	0
32	M2G	2a	966	25/26	0.93	0.15	51,63,75,78	0
54	PSU	1w	32	20/21	0.93	0.12	56,62,72,73	0
43	0TD	1l	92	10/11	0.93	0.11	49,51,53,68	0
32	5MC	2a	1400	21/22	0.93	0.13	60,63,68,74	0
55	4SU	1x	8	20/21	0.93	0.10	47,58,63,64	0
1	5MU	2A	1915	21/22	0.93	0.10	57,62,66,67	0
32	M2G	1a	966	25/26	0.94	0.11	43,49,56,58	0
32	5MC	2a	1404	21/22	0.94	0.10	43,50,53,55	0
32	PSU	2a	516	20/21	0.94	0.10	53,62,68,69	0
55	5MC	1x	32	21/22	0.94	0.12	49,53,59,68	0
54	5MU	1w	54	21/22	0.95	0.08	45,57,61,63	0
54	PSU	2w	39	20/21	0.95	0.11	60,70,79,80	0
54	PSU	1w	39	20/21	0.95	0.10	46,59,66,69	0
32	5MC	2a	1407	21/22	0.95	0.09	44,51,55,62	0
32	MA6	2a	1518	24/25	0.95	0.11	47,54,59,61	0
1	PSU	1A	1917	20/21	0.95	0.09	36,44,51,52	0
1	OMC	2A	1920	21/22	0.95	0.09	51,57,61,65	0
1	5MC	2A	1942	21/22	0.95	0.09	45,56,61,65	0
32	5MC	1a	1400	21/22	0.96	0.09	40,48,53,55	0
32	MA6	2a	1519	24/25	0.96	0.10	48,56,59,62	0
32	PSU	1a	516	20/21	0.96	0.09	39,51,57,57	0
1	PSU	2A	1911	20/21	0.96	0.08	46,56,59,62	0
55	8AN	2x	76	22/23	0.96	0.09	34,40,47,49	0
32	G7M	1a	527	24/25	0.96	0.09	42,46,50,53	0
1	5MU	1A	1915	21/22	0.96	0.10	43,49,52,53	0
32	5MC	1a	967	21/22	0.96	0.10	42,49,57,59	0
32	4OC	2a	1402	22/23	0.96	0.10	52,56,60,65	0
1	5MC	1A	1942	21/22	0.96	0.08	29,37,40,53	0
1	5MC	2A	1962	21/22	0.96	0.09	34,47,54,58	0
54	8AN	2w	76	22/23	0.96	0.09	29,38,42,43	0
32	UR3	2a	1498	21/22	0.97	0.09	45,50,54,55	0
1	OMU	2A	2552	21/22	0.97	0.07	39,44,47,52	0
1	PSU	2A	2605	20/21	0.97	0.07	30,36,40,40	0
55	8AN	1x	76	22/23	0.97	0.07	17,23,29,37	0
1	OMC	1A	1920	21/22	0.97	0.07	32,39,43,46	0
1	PSU	1A	1911	20/21	0.97	0.07	31,40,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	4OC	1a	1402	22/23	0.97	0.08	38,42,47,50	0
32	5MC	1a	1404	21/22	0.97	0.08	31,38,42,43	0
1	5MU	2A	1939	21/22	0.97	0.08	33,38,41,44	0
32	5MC	1a	1407	21/22	0.97	0.07	31,39,42,43	0
32	MA6	1a	1519	24/25	0.97	0.09	34,39,44,45	0
1	2MA	2A	2503	23/24	0.97	0.09	26,36,40,41	0
32	UR3	1a	1498	21/22	0.98	0.07	33,38,43,45	0
32	MA6	1a	1518	24/25	0.98	0.08	31,38,42,43	0
1	PSU	1A	2605	20/21	0.98	0.05	20,24,26,27	0
1	5MU	1A	1939	21/22	0.98	0.05	20,26,30,35	0
54	8AN	1w	76	22/23	0.98	0.07	17,21,23,24	0
1	5MC	1A	1962	21/22	0.98	0.06	23,31,33,41	0
1	OMG	1A	2251	24/25	0.98	0.06	20,24,25,26	0
1	2MA	1A	2503	23/24	0.98	0.06	15,19,21,23	0
1	OMG	2A	2251	24/25	0.98	0.07	35,38,42,42	0
1	OMU	1A	2552	21/22	0.99	0.06	21,26,31,31	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($\text{\AA}^2$)	Q<0.9
57	MG	1a	1603	1/1	0.54	0.20	67,67,67,67	0
57	MG	1B	221	1/1	0.56	0.22	66,66,66,66	0
57	MG	2y	104	1/1	0.57	0.33	86,86,86,86	0
57	MG	2A	3763	1/1	0.60	0.23	64,64,64,64	0
57	MG	2A	3544	1/1	0.60	0.24	58,58,58,58	0
57	MG	1A	3946	1/1	0.61	0.34	80,80,80,80	0
57	MG	1A	3702	1/1	0.62	0.20	56,56,56,56	0
57	MG	2w	107	1/1	0.63	0.27	78,78,78,78	0
57	MG	2A	3653	1/1	0.64	0.23	72,72,72,72	0
57	MG	2A	3168	1/1	0.64	0.25	78,78,78,78	0
57	MG	1A	3764	1/1	0.65	0.14	23,23,23,23	0
57	MG	2A	3861	1/1	0.65	0.38	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3613	1/1	0.65	0.22	68,68,68,68	0
57	MG	2A	3182	1/1	0.65	0.27	75,75,75,75	0
57	MG	2A	3811	1/1	0.66	0.24	72,72,72,72	0
57	MG	2A	3320	1/1	0.66	0.32	72,72,72,72	0
57	MG	2A	3272	1/1	0.66	0.30	74,74,74,74	0
57	MG	2A	3597	1/1	0.66	0.20	60,60,60,60	0
57	MG	2A	3700	1/1	0.67	0.19	56,56,56,56	0
57	MG	1A	4023	1/1	0.67	0.20	57,57,57,57	0
57	MG	1A	4043	1/1	0.67	0.16	65,65,65,65	0
57	MG	2a	3168	1/1	0.68	0.24	70,70,70,70	0
57	MG	2A	3371	1/1	0.68	0.19	73,73,73,73	0
57	MG	2a	3093	1/1	0.68	0.29	82,82,82,82	0
57	MG	2A	3648	1/1	0.69	0.18	60,60,60,60	0
57	MG	2B	212	1/1	0.70	0.21	73,73,73,73	0
57	MG	2a	3015	1/1	0.70	0.19	70,70,70,70	0
57	MG	1A	4072	1/1	0.70	0.24	40,40,40,40	0
57	MG	2A	3093	1/1	0.70	0.20	78,78,78,78	0
57	MG	2a	3224	1/1	0.70	0.26	69,69,69,69	0
57	MG	1A	4099	1/1	0.70	0.20	66,66,66,66	0
57	MG	2x	106	1/1	0.70	0.28	68,68,68,68	0
57	MG	1A	3876	1/1	0.70	0.19	29,29,29,29	0
57	MG	1w	108	1/1	0.71	0.30	78,78,78,78	0
57	MG	2a	3020	1/1	0.71	0.27	71,71,71,71	0
57	MG	2A	3277	1/1	0.71	0.20	66,66,66,66	0
57	MG	2W	201	1/1	0.71	0.24	72,72,72,72	0
57	MG	2B	203	1/1	0.72	0.21	76,76,76,76	0
57	MG	1G	205	1/1	0.72	0.16	53,53,53,53	0
57	MG	2a	3215	1/1	0.72	0.17	78,78,78,78	0
57	MG	2B	215	1/1	0.72	0.26	78,78,78,78	0
57	MG	2w	102	1/1	0.72	0.24	76,76,76,76	0
57	MG	1a	1787	1/1	0.72	0.14	74,74,74,74	0
57	MG	2A	3839	1/1	0.72	0.16	85,85,85,85	0
57	MG	2A	3703	1/1	0.72	0.17	65,65,65,65	0
57	MG	2A	3832	1/1	0.73	0.20	85,85,85,85	0
57	MG	2A	3273	1/1	0.73	0.18	61,61,61,61	0
57	MG	2A	3842	1/1	0.73	0.30	71,71,71,71	0
57	MG	2A	3670	1/1	0.73	0.15	81,81,81,81	0
57	MG	25	107	1/1	0.73	0.23	76,76,76,76	0
57	MG	2A	3339	1/1	0.74	0.15	68,68,68,68	0
57	MG	1A	3525	1/1	0.74	0.15	55,55,55,55	0
57	MG	2A	3669	1/1	0.74	0.14	68,68,68,68	0
57	MG	2j	201	1/1	0.74	0.23	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3393	1/1	0.74	0.17	61,61,61,61	0
57	MG	1A	3741	1/1	0.74	0.15	70,70,70,70	0
57	MG	1A	4016	1/1	0.74	0.12	70,70,70,70	0
57	MG	2A	3739	1/1	0.74	0.23	61,61,61,61	0
57	MG	1F	303	1/1	0.75	0.19	68,68,68,68	0
57	MG	2A	3310	1/1	0.75	0.20	64,64,64,64	0
57	MG	2A	3247	1/1	0.75	0.11	83,83,83,83	0
57	MG	2A	3634	1/1	0.75	0.22	74,74,74,74	0
57	MG	2A	3730	1/1	0.75	0.21	69,69,69,69	0
57	MG	1a	1682	1/1	0.75	0.13	68,68,68,68	0
57	MG	1A	3999	1/1	0.75	0.13	83,83,83,83	0
57	MG	1A	4078	1/1	0.76	0.29	73,73,73,73	0
57	MG	2a	3204	1/1	0.76	0.21	71,71,71,71	0
57	MG	2A	3269	1/1	0.76	0.17	68,68,68,68	0
57	MG	2A	3105	1/1	0.76	0.15	70,70,70,70	0
57	MG	18	103	1/1	0.76	0.20	59,59,59,59	0
57	MG	2A	3717	1/1	0.76	0.17	37,37,37,37	0
57	MG	2A	3086	1/1	0.76	0.15	79,79,79,79	0
57	MG	2A	3665	1/1	0.76	0.22	72,72,72,72	0
57	MG	2a	3122	1/1	0.76	0.17	73,73,73,73	0
57	MG	1A	3228	1/1	0.77	0.33	71,71,71,71	0
57	MG	2a	3115	1/1	0.77	0.26	79,79,79,79	0
57	MG	2A	3846	1/1	0.77	0.20	63,63,63,63	0
57	MG	2A	3615	1/1	0.77	0.18	67,67,67,67	0
57	MG	2a	3191	1/1	0.77	0.27	66,66,66,66	0
57	MG	1A	4083	1/1	0.77	0.17	62,62,62,62	0
57	MG	1A	3783	1/1	0.77	0.20	82,82,82,82	0
57	MG	1A	3027	1/1	0.77	0.30	67,67,67,67	0
57	MG	1B	228	1/1	0.77	0.12	70,70,70,70	0
57	MG	1A	3900	1/1	0.77	0.12	45,45,45,45	0
57	MG	2a	3013	1/1	0.77	0.12	66,66,66,66	0
57	MG	1A	3504	1/1	0.77	0.15	72,72,72,72	0
57	MG	2A	3687	1/1	0.77	0.19	70,70,70,70	0
57	MG	1a	1746	1/1	0.78	0.29	61,61,61,61	0
57	MG	1A	3829	1/1	0.78	0.12	53,53,53,53	0
57	MG	1A	3969	1/1	0.78	0.18	69,69,69,69	0
57	MG	2B	204	1/1	0.78	0.18	71,71,71,71	0
57	MG	2A	3734	1/1	0.78	0.14	41,41,41,41	0
57	MG	10	107	1/1	0.78	0.29	58,58,58,58	0
57	MG	1A	4103	1/1	0.78	0.13	48,48,48,48	0
57	MG	2A	3769	1/1	0.78	0.14	55,55,55,55	0
57	MG	2p	101	1/1	0.78	0.27	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3860	1/1	0.78	0.14	44,44,44,44	0
57	MG	1A	3922	1/1	0.78	0.13	50,50,50,50	0
57	MG	2A	3690	1/1	0.78	0.12	53,53,53,53	0
57	MG	2y	101	1/1	0.78	0.17	79,79,79,79	0
57	MG	2A	3632	1/1	0.78	0.16	65,65,65,65	0
57	MG	1A	3936	1/1	0.79	0.16	66,66,66,66	0
57	MG	2a	3028	1/1	0.79	0.27	74,74,74,74	0
57	MG	2A	3594	1/1	0.79	0.22	62,62,62,62	0
57	MG	2A	3834	1/1	0.79	0.16	55,55,55,55	0
57	MG	2A	3063	1/1	0.79	0.15	64,64,64,64	0
57	MG	2a	3155	1/1	0.79	0.12	66,66,66,66	0
57	MG	1A	3601	1/1	0.79	0.12	45,45,45,45	0
57	MG	2A	3845	1/1	0.79	0.19	62,62,62,62	0
57	MG	1A	3918	1/1	0.79	0.12	31,31,31,31	0
57	MG	2A	3713	1/1	0.79	0.17	72,72,72,72	0
57	MG	2A	3097	1/1	0.79	0.25	77,77,77,77	0
57	MG	2a	3228	1/1	0.79	0.31	71,71,71,71	0
57	MG	2A	3723	1/1	0.79	0.16	49,49,49,49	0
57	MG	1a	1708	1/1	0.79	0.34	78,78,78,78	0
57	MG	1A	3893	1/1	0.79	0.12	50,50,50,50	0
57	MG	1B	207	1/1	0.79	0.13	64,64,64,64	0
57	MG	2A	3751	1/1	0.79	0.12	39,39,39,39	0
57	MG	2A	3354	1/1	0.79	0.14	63,63,63,63	0
57	MG	2A	3224	1/1	0.79	0.26	61,61,61,61	0
57	MG	1A	3992	1/1	0.80	0.17	36,36,36,36	0
57	MG	1A	3934	1/1	0.80	0.13	30,30,30,30	0
57	MG	1a	1601	1/1	0.80	0.22	65,65,65,65	0
57	MG	2A	3417	1/1	0.80	0.24	64,64,64,64	0
57	MG	2a	3169	1/1	0.80	0.20	58,58,58,58	0
57	MG	2a	3184	1/1	0.80	0.20	70,70,70,70	0
57	MG	2A	3506	1/1	0.80	0.16	50,50,50,50	0
57	MG	1A	3550	1/1	0.80	0.26	62,62,62,62	0
57	MG	2E	302	1/1	0.80	0.14	73,73,73,73	0
57	MG	2a	3217	1/1	0.80	0.15	63,63,63,63	0
57	MG	2A	3797	1/1	0.80	0.12	31,31,31,31	0
57	MG	2X	101	1/1	0.80	0.17	63,63,63,63	0
57	MG	1a	1675	1/1	0.80	0.17	68,68,68,68	0
57	MG	2a	3008	1/1	0.80	0.28	73,73,73,73	0
57	MG	1A	3727	1/1	0.80	0.19	61,61,61,61	0
57	MG	1A	3632	1/1	0.80	0.19	46,46,46,46	0
57	MG	2A	3289	1/1	0.80	0.29	76,76,76,76	0
57	MG	2A	3128	1/1	0.80	0.20	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1O	205	1/1	0.80	0.26	66,66,66,66	0
57	MG	1A	3675	1/1	0.81	0.16	61,61,61,61	0
57	MG	2A	3084	1/1	0.81	0.29	67,67,67,67	0
57	MG	2A	3621	1/1	0.81	0.23	68,68,68,68	0
57	MG	1A	4075	1/1	0.81	0.25	55,55,55,55	0
57	MG	1B	229	1/1	0.81	0.21	70,70,70,70	0
57	MG	1A	3475	1/1	0.81	0.13	57,57,57,57	0
57	MG	1A	4019	1/1	0.81	0.14	71,71,71,71	0
57	MG	1A	3292	1/1	0.81	0.12	61,61,61,61	0
57	MG	1A	3795	1/1	0.81	0.11	56,56,56,56	0
57	MG	2a	3225	1/1	0.81	0.19	75,75,75,75	0
57	MG	1a	1799	1/1	0.81	0.35	62,62,62,62	0
57	MG	2A	3479	1/1	0.81	0.13	35,35,35,35	0
57	MG	2A	3481	1/1	0.81	0.18	71,71,71,71	0
57	MG	1a	1805	1/1	0.81	0.15	65,65,65,65	0
57	MG	1A	4046	1/1	0.81	0.16	51,51,51,51	0
57	MG	2a	3098	1/1	0.81	0.24	68,68,68,68	0
57	MG	1x	108	1/1	0.81	0.36	72,72,72,72	0
57	MG	2A	3046	1/1	0.81	0.22	71,71,71,71	0
57	MG	2A	3684	1/1	0.82	0.18	54,54,54,54	0
57	MG	1A	3584	1/1	0.82	0.18	60,60,60,60	0
57	MG	1A	3304	1/1	0.82	0.22	50,50,50,50	0
57	MG	1A	3988	1/1	0.82	0.12	49,49,49,49	0
57	MG	1a	1772	1/1	0.82	0.13	46,46,46,46	0
57	MG	1A	3823	1/1	0.82	0.15	58,58,58,58	0
57	MG	1A	3449	1/1	0.82	0.15	64,64,64,64	0
57	MG	2A	3286	1/1	0.82	0.32	71,71,71,71	0
57	MG	2a	3197	1/1	0.82	0.26	63,63,63,63	0
57	MG	2a	3201	1/1	0.82	0.15	62,62,62,62	0
57	MG	2A	3100	1/1	0.82	0.21	65,65,65,65	0
57	MG	2A	3300	1/1	0.82	0.18	63,63,63,63	0
57	MG	2a	3216	1/1	0.82	0.27	61,61,61,61	0
57	MG	1A	3759	1/1	0.82	0.11	27,27,27,27	0
57	MG	1w	107	1/1	0.82	0.13	77,77,77,77	0
57	MG	2A	3331	1/1	0.82	0.30	64,64,64,64	0
57	MG	1a	1670	1/1	0.82	0.32	74,74,74,74	0
57	MG	2A	3341	1/1	0.82	0.20	61,61,61,61	0
57	MG	1A	3551	1/1	0.82	0.23	62,62,62,62	0
57	MG	2A	3829	1/1	0.82	0.17	67,67,67,67	0
57	MG	2A	3223	1/1	0.82	0.17	58,58,58,58	0
57	MG	2a	3041	1/1	0.82	0.17	72,72,72,72	0
57	MG	2a	3043	1/1	0.82	0.14	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3374	1/1	0.82	0.33	75,75,75,75	0
57	MG	1A	3455	1/1	0.83	0.25	70,70,70,70	0
57	MG	2A	3667	1/1	0.83	0.19	67,67,67,67	0
57	MG	2A	3295	1/1	0.83	0.20	62,62,62,62	0
57	MG	27	102	1/1	0.83	0.15	60,60,60,60	0
57	MG	2a	3002	1/1	0.83	0.19	75,75,75,75	0
57	MG	2a	3004	1/1	0.83	0.19	60,60,60,60	0
57	MG	2A	3060	1/1	0.83	0.12	66,66,66,66	0
57	MG	2a	3012	1/1	0.83	0.22	71,71,71,71	0
57	MG	1a	1604	1/1	0.83	0.18	59,59,59,59	0
57	MG	1a	1665	1/1	0.83	0.27	62,62,62,62	0
57	MG	1a	1667	1/1	0.83	0.18	64,64,64,64	0
57	MG	1A	3686	1/1	0.83	0.15	64,64,64,64	0
57	MG	2A	3340	1/1	0.83	0.28	70,70,70,70	0
57	MG	1A	3343	1/1	0.83	0.12	60,60,60,60	0
57	MG	1a	1681	1/1	0.83	0.24	62,62,62,62	0
57	MG	1A	4031	1/1	0.83	0.11	34,34,34,34	0
57	MG	2A	3108	1/1	0.83	0.20	52,52,52,52	0
57	MG	2a	3116	1/1	0.83	0.26	58,58,58,58	0
57	MG	2A	3113	1/1	0.83	0.23	59,59,59,59	0
57	MG	2a	3140	1/1	0.83	0.12	71,71,71,71	0
57	MG	1a	1687	1/1	0.83	0.28	71,71,71,71	0
57	MG	1A	3713	1/1	0.83	0.11	47,47,47,47	0
57	MG	2A	3759	1/1	0.83	0.15	59,59,59,59	0
57	MG	2a	3171	1/1	0.83	0.21	69,69,69,69	0
57	MG	2A	3489	1/1	0.83	0.15	55,55,55,55	0
57	MG	1A	3499	1/1	0.83	0.17	55,55,55,55	0
57	MG	2A	3781	1/1	0.83	0.12	44,44,44,44	0
57	MG	2A	3187	1/1	0.83	0.17	63,63,63,63	0
57	MG	2A	3549	1/1	0.83	0.11	60,60,60,60	0
57	MG	2a	3206	1/1	0.83	0.21	71,71,71,71	0
57	MG	2A	3550	1/1	0.83	0.22	72,72,72,72	0
57	MG	2A	3583	1/1	0.83	0.12	30,30,30,30	0
57	MG	2A	3584	1/1	0.83	0.14	46,46,46,46	0
57	MG	1E	305	1/1	0.83	0.17	49,49,49,49	0
57	MG	1A	3425	1/1	0.83	0.12	49,49,49,49	0
57	MG	1A	3612	1/1	0.83	0.13	67,67,67,67	0
57	MG	2A	3248	1/1	0.83	0.14	70,70,70,70	0
57	MG	1A	3367	1/1	0.83	0.33	52,52,52,52	0
57	MG	1A	4080	1/1	0.83	0.14	67,67,67,67	0
57	MG	1A	3908	1/1	0.83	0.11	26,26,26,26	0
57	MG	1A	4090	1/1	0.83	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3649	1/1	0.83	0.30	70,70,70,70	0
57	MG	2A	3035	1/1	0.83	0.14	66,66,66,66	0
57	MG	2A	3347	1/1	0.84	0.15	65,65,65,65	0
57	MG	2A	3348	1/1	0.84	0.12	65,65,65,65	0
57	MG	2A	3173	1/1	0.84	0.18	52,52,52,52	0
57	MG	1q	201	1/1	0.84	0.14	57,57,57,57	0
57	MG	1v	101	1/1	0.84	0.31	78,78,78,78	0
57	MG	2A	3399	1/1	0.84	0.29	67,67,67,67	0
57	MG	2A	3205	1/1	0.84	0.21	71,71,71,71	0
57	MG	2a	3034	1/1	0.84	0.46	75,75,75,75	0
57	MG	1A	3402	1/1	0.84	0.14	54,54,54,54	0
57	MG	1A	3897	1/1	0.84	0.25	39,39,39,39	0
57	MG	2a	3051	1/1	0.84	0.27	72,72,72,72	0
57	MG	2a	3092	1/1	0.84	0.31	78,78,78,78	0
57	MG	1A	3635	1/1	0.84	0.15	63,63,63,63	0
57	MG	1A	3659	1/1	0.84	0.12	28,28,28,28	0
57	MG	2A	3259	1/1	0.84	0.18	71,71,71,71	0
57	MG	2A	3268	1/1	0.84	0.28	61,61,61,61	0
57	MG	2a	3118	1/1	0.84	0.29	77,77,77,77	0
57	MG	2A	3764	1/1	0.84	0.11	66,66,66,66	0
57	MG	1A	4021	1/1	0.84	0.16	50,50,50,50	0
57	MG	2a	3151	1/1	0.84	0.15	66,66,66,66	0
57	MG	1a	1668	1/1	0.84	0.21	67,67,67,67	0
57	MG	2A	3791	1/1	0.84	0.15	80,80,80,80	0
57	MG	1A	3672	1/1	0.84	0.14	47,47,47,47	0
57	MG	2A	3586	1/1	0.84	0.21	44,44,44,44	0
57	MG	2a	3182	1/1	0.84	0.16	67,67,67,67	0
57	MG	1B	214	1/1	0.84	0.13	66,66,66,66	0
57	MG	2a	3189	1/1	0.84	0.22	70,70,70,70	0
57	MG	2A	3283	1/1	0.84	0.17	58,58,58,58	0
57	MG	2A	3612	1/1	0.84	0.13	47,47,47,47	0
57	MG	2a	3200	1/1	0.84	0.15	79,79,79,79	0
57	MG	2A	3284	1/1	0.84	0.15	69,69,69,69	0
57	MG	1A	4026	1/1	0.84	0.16	57,57,57,57	0
57	MG	1A	3380	1/1	0.84	0.30	41,41,41,41	0
57	MG	2A	3625	1/1	0.84	0.16	67,67,67,67	0
57	MG	2A	3860	1/1	0.84	0.14	71,71,71,71	0
57	MG	1A	4033	1/1	0.84	0.10	58,58,58,58	0
57	MG	1A	3205	1/1	0.84	0.14	72,72,72,72	0
57	MG	1A	3690	1/1	0.84	0.10	31,31,31,31	0
57	MG	2a	3226	1/1	0.84	0.15	67,67,67,67	0
57	MG	1A	4050	1/1	0.84	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3650	1/1	0.84	0.15	68,68,68,68	0
57	MG	2A	3322	1/1	0.84	0.20	71,71,71,71	0
57	MG	2A	3327	1/1	0.84	0.29	66,66,66,66	0
57	MG	1A	3401	1/1	0.84	0.28	71,71,71,71	0
57	MG	1A	3707	1/1	0.84	0.19	59,59,59,59	0
57	MG	2A	3166	1/1	0.84	0.20	74,74,74,74	0
57	MG	1A	3535	1/1	0.84	0.23	63,63,63,63	0
57	MG	1A	3515	1/1	0.85	0.10	67,67,67,67	0
57	MG	1a	1726	1/1	0.85	0.20	71,71,71,71	0
57	MG	1A	3766	1/1	0.85	0.12	21,21,21,21	0
57	MG	2A	3321	1/1	0.85	0.13	51,51,51,51	0
57	MG	1A	3290	1/1	0.85	0.27	51,51,51,51	0
57	MG	2a	3009	1/1	0.85	0.30	73,73,73,73	0
57	MG	2A	3157	1/1	0.85	0.19	65,65,65,65	0
57	MG	1G	203	1/1	0.85	0.08	66,66,66,66	0
57	MG	1A	4049	1/1	0.85	0.14	56,56,56,56	0
57	MG	1A	3790	1/1	0.85	0.10	19,19,19,19	0
57	MG	2A	3174	1/1	0.85	0.20	66,66,66,66	0
57	MG	2A	3689	1/1	0.85	0.13	46,46,46,46	0
57	MG	2a	3037	1/1	0.85	0.23	61,61,61,61	0
57	MG	2A	3346	1/1	0.85	0.21	71,71,71,71	0
57	MG	2a	3042	1/1	0.85	0.19	59,59,59,59	0
57	MG	1a	1817	1/1	0.85	0.13	65,65,65,65	0
57	MG	2a	3044	1/1	0.85	0.20	69,69,69,69	0
57	MG	2a	3046	1/1	0.85	0.15	79,79,79,79	0
57	MG	1A	3344	1/1	0.85	0.15	57,57,57,57	0
57	MG	2a	3067	1/1	0.85	0.25	62,62,62,62	0
57	MG	2A	3195	1/1	0.85	0.15	50,50,50,50	0
57	MG	2A	3714	1/1	0.85	0.14	62,62,62,62	0
57	MG	2A	3361	1/1	0.85	0.13	59,59,59,59	0
57	MG	2A	3367	1/1	0.85	0.16	68,68,68,68	0
57	MG	1A	3977	1/1	0.85	0.14	59,59,59,59	0
57	MG	1A	3982	1/1	0.85	0.09	22,22,22,22	0
57	MG	1A	4079	1/1	0.85	0.13	54,54,54,54	0
57	MG	2A	3406	1/1	0.85	0.31	66,66,66,66	0
57	MG	2A	3242	1/1	0.85	0.19	64,64,64,64	0
57	MG	2A	3419	1/1	0.85	0.35	66,66,66,66	0
57	MG	2A	3420	1/1	0.85	0.26	60,60,60,60	0
57	MG	2A	3443	1/1	0.85	0.25	67,67,67,67	0
57	MG	2A	3770	1/1	0.85	0.14	65,65,65,65	0
57	MG	2A	3771	1/1	0.85	0.13	80,80,80,80	0
57	MG	2A	3246	1/1	0.85	0.21	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1x	106	1/1	0.85	0.20	57,57,57,57	0
57	MG	1A	3448	1/1	0.85	0.21	74,74,74,74	0
57	MG	2A	3254	1/1	0.85	0.19	58,58,58,58	0
57	MG	2A	3511	1/1	0.85	0.18	60,60,60,60	0
57	MG	2A	3016	1/1	0.85	0.16	59,59,59,59	0
57	MG	2A	3020	1/1	0.85	0.27	67,67,67,67	0
57	MG	2A	3836	1/1	0.85	0.12	37,37,37,37	0
57	MG	1A	3364	1/1	0.85	0.20	56,56,56,56	0
57	MG	1A	3699	1/1	0.85	0.13	32,32,32,32	0
57	MG	1A	3555	1/1	0.85	0.17	60,60,60,60	0
57	MG	2A	3275	1/1	0.85	0.17	62,62,62,62	0
57	MG	1A	3035	1/1	0.85	0.10	47,47,47,47	0
57	MG	2A	3279	1/1	0.85	0.26	71,71,71,71	0
57	MG	2A	3281	1/1	0.85	0.13	64,64,64,64	0
57	MG	2A	3282	1/1	0.85	0.22	66,66,66,66	0
57	MG	2l	203	1/1	0.85	0.10	70,70,70,70	0
57	MG	1a	1674	1/1	0.85	0.15	43,43,43,43	0
57	MG	2t	201	1/1	0.85	0.21	59,59,59,59	0
57	MG	1A	3294	1/1	0.85	0.26	60,60,60,60	0
57	MG	1A	3493	1/1	0.85	0.15	66,66,66,66	0
57	MG	1A	3068	1/1	0.85	0.12	55,55,55,55	0
57	MG	1A	3339	1/1	0.85	0.20	64,64,64,64	0
57	MG	2Z	301	1/1	0.85	0.10	75,75,75,75	0
57	MG	2A	3582	1/1	0.86	0.07	34,34,34,34	0
57	MG	1A	3602	1/1	0.86	0.09	24,24,24,24	0
57	MG	1A	4107	1/1	0.86	0.33	66,66,66,66	0
57	MG	1A	3704	1/1	0.86	0.16	53,53,53,53	0
57	MG	2A	3589	1/1	0.86	0.18	67,67,67,67	0
57	MG	1B	213	1/1	0.86	0.27	64,64,64,64	0
57	MG	1a	1679	1/1	0.86	0.11	56,56,56,56	0
57	MG	2A	3288	1/1	0.86	0.23	65,65,65,65	0
57	MG	25	101	1/1	0.86	0.22	62,62,62,62	0
57	MG	1A	3944	1/1	0.86	0.09	60,60,60,60	0
57	MG	2A	3290	1/1	0.86	0.13	63,63,63,63	0
57	MG	1A	3827	1/1	0.86	0.12	37,37,37,37	0
57	MG	2A	3624	1/1	0.86	0.15	70,70,70,70	0
57	MG	2A	3110	1/1	0.86	0.32	63,63,63,63	0
57	MG	1B	224	1/1	0.86	0.12	55,55,55,55	0
57	MG	2A	3312	1/1	0.86	0.28	62,62,62,62	0
57	MG	2A	3117	1/1	0.86	0.11	68,68,68,68	0
57	MG	1A	3465	1/1	0.86	0.17	64,64,64,64	0
57	MG	1A	3971	1/1	0.86	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3856	1/1	0.86	0.12	50,50,50,50	0
57	MG	2a	3033	1/1	0.86	0.22	63,63,63,63	0
57	MG	2A	3330	1/1	0.86	0.13	76,76,76,76	0
57	MG	1A	4051	1/1	0.86	0.14	62,62,62,62	0
57	MG	2a	3038	1/1	0.86	0.28	58,58,58,58	0
57	MG	2A	3338	1/1	0.86	0.13	65,65,65,65	0
57	MG	1A	4066	1/1	0.86	0.13	56,56,56,56	0
57	MG	2A	3676	1/1	0.86	0.15	60,60,60,60	0
57	MG	2A	3681	1/1	0.86	0.14	38,38,38,38	0
57	MG	1a	1798	1/1	0.86	0.20	73,73,73,73	0
57	MG	1A	3026	1/1	0.86	0.13	44,44,44,44	0
57	MG	2a	3054	1/1	0.86	0.14	70,70,70,70	0
57	MG	1A	3093	1/1	0.86	0.13	55,55,55,55	0
57	MG	2a	3091	1/1	0.86	0.09	69,69,69,69	0
57	MG	2A	3194	1/1	0.86	0.23	58,58,58,58	0
57	MG	1a	1809	1/1	0.86	0.15	81,81,81,81	0
57	MG	2A	3701	1/1	0.86	0.12	64,64,64,64	0
57	MG	2A	3349	1/1	0.86	0.22	54,54,54,54	0
57	MG	2A	3352	1/1	0.86	0.15	46,46,46,46	0
57	MG	1A	3100	1/1	0.86	0.14	69,69,69,69	0
57	MG	2a	3119	1/1	0.86	0.19	60,60,60,60	0
57	MG	2A	3355	1/1	0.86	0.16	70,70,70,70	0
57	MG	1f	202	1/1	0.86	0.26	65,65,65,65	0
57	MG	2a	3147	1/1	0.86	0.10	58,58,58,58	0
57	MG	1h	201	1/1	0.86	0.13	70,70,70,70	0
57	MG	2A	3232	1/1	0.86	0.09	49,49,49,49	0
57	MG	2a	3156	1/1	0.86	0.14	64,64,64,64	0
57	MG	2a	3158	1/1	0.86	0.12	64,64,64,64	0
57	MG	2a	3162	1/1	0.86	0.16	52,52,52,52	0
57	MG	2a	3165	1/1	0.86	0.13	66,66,66,66	0
57	MG	1l	202	1/1	0.86	0.10	57,57,57,57	0
57	MG	2A	3393	1/1	0.86	0.19	54,54,54,54	0
57	MG	2A	3754	1/1	0.86	0.14	70,70,70,70	0
57	MG	2A	3245	1/1	0.86	0.25	67,67,67,67	0
57	MG	1A	3552	1/1	0.86	0.32	55,55,55,55	0
57	MG	1A	3400	1/1	0.86	0.15	53,53,53,53	0
57	MG	1A	3514	1/1	0.86	0.14	71,71,71,71	0
57	MG	1A	3588	1/1	0.86	0.23	50,50,50,50	0
57	MG	1a	1609	1/1	0.86	0.28	62,62,62,62	0
57	MG	2A	3779	1/1	0.86	0.17	52,52,52,52	0
57	MG	2A	3261	1/1	0.86	0.28	66,66,66,66	0
57	MG	1a	1617	1/1	0.86	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3485	1/1	0.86	0.22	63,63,63,63	0
57	MG	2A	3801	1/1	0.86	0.12	40,40,40,40	0
57	MG	2A	3808	1/1	0.86	0.11	71,71,71,71	0
57	MG	1a	1624	1/1	0.86	0.26	68,68,68,68	0
57	MG	2A	3814	1/1	0.86	0.11	49,49,49,49	0
57	MG	2A	3495	1/1	0.86	0.09	59,59,59,59	0
57	MG	1a	1641	1/1	0.86	0.20	69,69,69,69	0
57	MG	1a	1654	1/1	0.86	0.18	57,57,57,57	0
57	MG	2A	3524	1/1	0.86	0.11	60,60,60,60	0
57	MG	1a	1657	1/1	0.86	0.19	63,63,63,63	0
57	MG	1A	4091	1/1	0.86	0.20	58,58,58,58	0
57	MG	2v	102	1/1	0.86	0.10	69,69,69,69	0
57	MG	1A	3320	1/1	0.86	0.19	51,51,51,51	0
57	MG	2A	3570	1/1	0.86	0.09	30,30,30,30	0
57	MG	2A	3858	1/1	0.86	0.10	63,63,63,63	0
57	MG	2A	3573	1/1	0.86	0.12	54,54,54,54	0
57	MG	2A	3576	1/1	0.86	0.14	55,55,55,55	0
57	MG	2A	3574	1/1	0.87	0.15	54,54,54,54	0
57	MG	2B	206	1/1	0.87	0.23	61,61,61,61	0
57	MG	2A	3054	1/1	0.87	0.31	66,66,66,66	0
57	MG	1A	4097	1/1	0.87	0.15	67,67,67,67	0
57	MG	1A	3865	1/1	0.87	0.16	32,32,32,32	0
57	MG	2U	202	1/1	0.87	0.09	57,57,57,57	0
57	MG	1A	4101	1/1	0.87	0.08	72,72,72,72	0
57	MG	1A	3872	1/1	0.87	0.15	59,59,59,59	0
57	MG	1A	3735	1/1	0.87	0.08	17,17,17,17	0
57	MG	2A	3294	1/1	0.87	0.34	54,54,54,54	0
57	MG	25	102	1/1	0.87	0.24	52,52,52,52	0
57	MG	1A	4008	1/1	0.87	0.10	39,39,39,39	0
57	MG	2A	3296	1/1	0.87	0.12	62,62,62,62	0
57	MG	2A	3098	1/1	0.87	0.20	63,63,63,63	0
57	MG	2A	3614	1/1	0.87	0.13	41,41,41,41	0
57	MG	2A	3301	1/1	0.87	0.31	49,49,49,49	0
57	MG	1A	3877	1/1	0.87	0.09	25,25,25,25	0
57	MG	1A	3884	1/1	0.87	0.12	29,29,29,29	0
57	MG	1A	3890	1/1	0.87	0.17	31,31,31,31	0
57	MG	2a	3014	1/1	0.87	0.18	64,64,64,64	0
57	MG	2A	3631	1/1	0.87	0.14	61,61,61,61	0
57	MG	2a	3016	1/1	0.87	0.16	73,73,73,73	0
57	MG	2a	3018	1/1	0.87	0.25	81,81,81,81	0
57	MG	1A	3024	1/1	0.87	0.24	61,61,61,61	0
57	MG	2a	3027	1/1	0.87	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1703	1/1	0.87	0.32	63,63,63,63	0
57	MG	2a	3030	1/1	0.87	0.20	68,68,68,68	0
57	MG	1B	225	1/1	0.87	0.11	51,51,51,51	0
57	MG	2A	3329	1/1	0.87	0.23	73,73,73,73	0
57	MG	1a	1715	1/1	0.87	0.21	63,63,63,63	0
57	MG	1A	3743	1/1	0.87	0.10	34,34,34,34	0
57	MG	2A	3663	1/1	0.87	0.12	65,65,65,65	0
57	MG	2A	3333	1/1	0.87	0.16	69,69,69,69	0
57	MG	1a	1730	1/1	0.87	0.17	65,65,65,65	0
57	MG	1A	3746	1/1	0.87	0.10	42,42,42,42	0
57	MG	2a	3045	1/1	0.87	0.18	70,70,70,70	0
57	MG	1a	1763	1/1	0.87	0.14	59,59,59,59	0
57	MG	1a	1771	1/1	0.87	0.12	65,65,65,65	0
57	MG	1A	3092	1/1	0.87	0.12	41,41,41,41	0
57	MG	2a	3057	1/1	0.87	0.19	68,68,68,68	0
57	MG	1E	311	1/1	0.87	0.19	66,66,66,66	0
57	MG	2a	3080	1/1	0.87	0.17	65,65,65,65	0
57	MG	2a	3083	1/1	0.87	0.19	58,58,58,58	0
57	MG	2A	3192	1/1	0.87	0.15	67,67,67,67	0
57	MG	1A	3594	1/1	0.87	0.10	43,43,43,43	0
57	MG	1A	3540	1/1	0.87	0.23	60,60,60,60	0
57	MG	2A	3204	1/1	0.87	0.12	54,54,54,54	0
57	MG	2a	3101	1/1	0.87	0.25	68,68,68,68	0
57	MG	2a	3106	1/1	0.87	0.32	67,67,67,67	0
57	MG	1A	3351	1/1	0.87	0.12	57,57,57,57	0
57	MG	2A	3357	1/1	0.87	0.20	60,60,60,60	0
57	MG	2A	3704	1/1	0.87	0.11	59,59,59,59	0
57	MG	2A	3219	1/1	0.87	0.23	60,60,60,60	0
57	MG	2A	3363	1/1	0.87	0.12	68,68,68,68	0
57	MG	2a	3137	1/1	0.87	0.09	89,89,89,89	0
57	MG	1A	3935	1/1	0.87	0.11	31,31,31,31	0
57	MG	1A	3325	1/1	0.87	0.14	51,51,51,51	0
57	MG	13	104	1/1	0.87	0.12	53,53,53,53	0
57	MG	2A	3375	1/1	0.87	0.08	70,70,70,70	0
57	MG	2A	3380	1/1	0.87	0.18	64,64,64,64	0
57	MG	1A	3631	1/1	0.87	0.12	41,41,41,41	0
57	MG	2A	3244	1/1	0.87	0.17	75,75,75,75	0
57	MG	2a	3163	1/1	0.87	0.26	53,53,53,53	0
57	MG	1A	3463	1/1	0.87	0.29	72,72,72,72	0
57	MG	2A	3412	1/1	0.87	0.32	63,63,63,63	0
57	MG	2A	3416	1/1	0.87	0.19	57,57,57,57	0
57	MG	2a	3170	1/1	0.87	0.21	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3953	1/1	0.87	0.10	27,27,27,27	0
57	MG	1A	3020	1/1	0.87	0.16	45,45,45,45	0
57	MG	1w	105	1/1	0.87	0.17	75,75,75,75	0
57	MG	2A	3776	1/1	0.87	0.10	57,57,57,57	0
57	MG	2a	3190	1/1	0.87	0.11	54,54,54,54	0
57	MG	2A	3424	1/1	0.87	0.30	73,73,73,73	0
57	MG	1A	3726	1/1	0.87	0.15	67,67,67,67	0
57	MG	2A	3455	1/1	0.87	0.14	70,70,70,70	0
57	MG	2A	3457	1/1	0.87	0.17	58,58,58,58	0
57	MG	1A	3575	1/1	0.87	0.13	51,51,51,51	0
57	MG	2A	3260	1/1	0.87	0.17	59,59,59,59	0
57	MG	2a	3211	1/1	0.87	0.12	69,69,69,69	0
57	MG	1x	103	1/1	0.87	0.13	59,59,59,59	0
57	MG	2A	3266	1/1	0.87	0.13	69,69,69,69	0
57	MG	2A	3490	1/1	0.87	0.16	53,53,53,53	0
57	MG	2a	3223	1/1	0.87	0.14	74,74,74,74	0
57	MG	1A	3980	1/1	0.87	0.09	26,26,26,26	0
57	MG	2A	3502	1/1	0.87	0.27	68,68,68,68	0
57	MG	1a	1630	1/1	0.87	0.15	59,59,59,59	0
57	MG	1a	1639	1/1	0.87	0.14	60,60,60,60	0
57	MG	2A	3840	1/1	0.87	0.13	51,51,51,51	0
57	MG	2A	3019	1/1	0.87	0.20	63,63,63,63	0
57	MG	1A	4084	1/1	0.87	0.15	61,61,61,61	0
57	MG	2A	3032	1/1	0.87	0.16	69,69,69,69	0
57	MG	2v	101	1/1	0.87	0.28	62,62,62,62	0
57	MG	2A	3853	1/1	0.87	0.16	56,56,56,56	0
57	MG	2w	101	1/1	0.87	0.17	56,56,56,56	0
57	MG	2A	3854	1/1	0.87	0.16	61,61,61,61	0
57	MG	2w	103	1/1	0.87	0.17	77,77,77,77	0
57	MG	2w	106	1/1	0.87	0.12	62,62,62,62	0
57	MG	1A	3728	1/1	0.87	0.10	51,51,51,51	0
57	MG	2x	103	1/1	0.87	0.21	62,62,62,62	0
57	MG	2A	3562	1/1	0.87	0.23	60,60,60,60	0
57	MG	1A	3985	1/1	0.87	0.21	60,60,60,60	0
57	MG	2A	3053	1/1	0.87	0.16	62,62,62,62	0
57	MG	2A	3674	1/1	0.88	0.09	31,31,31,31	0
57	MG	1A	3677	1/1	0.88	0.08	41,41,41,41	0
57	MG	1A	3289	1/1	0.88	0.13	44,44,44,44	0
57	MG	2A	3404	1/1	0.88	0.18	57,57,57,57	0
57	MG	2a	3021	1/1	0.88	0.17	68,68,68,68	0
57	MG	2A	3090	1/1	0.88	0.13	40,40,40,40	0
57	MG	1A	3424	1/1	0.88	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4045	1/1	0.88	0.08	13,13,13,13	0
57	MG	2A	3699	1/1	0.88	0.14	71,71,71,71	0
57	MG	1a	1741	1/1	0.88	0.26	76,76,76,76	0
57	MG	1A	3486	1/1	0.88	0.10	55,55,55,55	0
57	MG	1a	1761	1/1	0.88	0.12	77,77,77,77	0
57	MG	1A	3050	1/1	0.88	0.15	45,45,45,45	0
57	MG	2A	3285	1/1	0.88	0.24	74,74,74,74	0
57	MG	2A	3445	1/1	0.88	0.14	62,62,62,62	0
57	MG	2A	3716	1/1	0.88	0.16	65,65,65,65	0
57	MG	2A	3452	1/1	0.88	0.10	53,53,53,53	0
57	MG	1N	201	1/1	0.88	0.21	70,70,70,70	0
57	MG	2A	3727	1/1	0.88	0.20	56,56,56,56	0
57	MG	1A	3937	1/1	0.88	0.16	55,55,55,55	0
57	MG	2A	3471	1/1	0.88	0.18	50,50,50,50	0
57	MG	2A	3473	1/1	0.88	0.26	64,64,64,64	0
57	MG	2A	3741	1/1	0.88	0.20	55,55,55,55	0
57	MG	2A	3478	1/1	0.88	0.11	46,46,46,46	0
57	MG	2a	3087	1/1	0.88	0.27	63,63,63,63	0
57	MG	2a	3088	1/1	0.88	0.21	60,60,60,60	0
57	MG	2a	3089	1/1	0.88	0.16	51,51,51,51	0
57	MG	1A	3618	1/1	0.88	0.15	54,54,54,54	0
57	MG	2A	3119	1/1	0.88	0.25	62,62,62,62	0
57	MG	2A	3761	1/1	0.88	0.14	53,53,53,53	0
57	MG	1A	4060	1/1	0.88	0.10	54,54,54,54	0
57	MG	2a	3099	1/1	0.88	0.15	59,59,59,59	0
57	MG	1A	3825	1/1	0.88	0.14	59,59,59,59	0
57	MG	2A	3768	1/1	0.88	0.09	73,73,73,73	0
57	MG	2a	3107	1/1	0.88	0.08	61,61,61,61	0
57	MG	1A	3951	1/1	0.88	0.09	37,37,37,37	0
57	MG	1A	3625	1/1	0.88	0.09	20,20,20,20	0
57	MG	1A	3446	1/1	0.88	0.14	49,49,49,49	0
57	MG	2A	3773	1/1	0.88	0.12	48,48,48,48	0
57	MG	2A	3303	1/1	0.88	0.17	61,61,61,61	0
57	MG	2a	3131	1/1	0.88	0.13	75,75,75,75	0
57	MG	2a	3132	1/1	0.88	0.11	72,72,72,72	0
57	MG	1A	3718	1/1	0.88	0.12	55,55,55,55	0
57	MG	2A	3512	1/1	0.88	0.10	35,35,35,35	0
57	MG	1A	3972	1/1	0.88	0.10	63,63,63,63	0
57	MG	1A	3975	1/1	0.88	0.10	61,61,61,61	0
57	MG	1m	3002	1/1	0.88	0.14	53,53,53,53	0
57	MG	1A	3719	1/1	0.88	0.12	69,69,69,69	0
57	MG	2A	3560	1/1	0.88	0.10	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3326	1/1	0.88	0.17	72,72,72,72	0
57	MG	1A	3391	1/1	0.88	0.08	41,41,41,41	0
57	MG	2A	3572	1/1	0.88	0.18	66,66,66,66	0
57	MG	2A	3196	1/1	0.88	0.10	52,52,52,52	0
57	MG	2A	3197	1/1	0.88	0.16	52,52,52,52	0
57	MG	1A	3868	1/1	0.88	0.32	35,35,35,35	0
57	MG	1A	3347	1/1	0.88	0.13	62,62,62,62	0
57	MG	2a	3174	1/1	0.88	0.27	56,56,56,56	0
57	MG	2a	3179	1/1	0.88	0.24	67,67,67,67	0
57	MG	2A	3337	1/1	0.88	0.10	58,58,58,58	0
57	MG	2a	3183	1/1	0.88	0.16	66,66,66,66	0
57	MG	2A	3844	1/1	0.88	0.14	66,66,66,66	0
57	MG	2a	3185	1/1	0.88	0.17	80,80,80,80	0
57	MG	2a	3186	1/1	0.88	0.18	54,54,54,54	0
57	MG	2A	3216	1/1	0.88	0.22	62,62,62,62	0
57	MG	1A	3636	1/1	0.88	0.12	60,60,60,60	0
57	MG	1A	3637	1/1	0.88	0.12	22,22,22,22	0
57	MG	1A	3998	1/1	0.88	0.08	61,61,61,61	0
57	MG	2A	3856	1/1	0.88	0.12	59,59,59,59	0
57	MG	2A	3225	1/1	0.88	0.27	40,40,40,40	0
57	MG	2A	3604	1/1	0.88	0.17	42,42,42,42	0
57	MG	1A	3646	1/1	0.88	0.12	44,44,44,44	0
57	MG	2a	3208	1/1	0.88	0.14	50,50,50,50	0
57	MG	2a	3209	1/1	0.88	0.23	72,72,72,72	0
57	MG	2B	201	1/1	0.88	0.17	70,70,70,70	0
57	MG	1x	112	1/1	0.88	0.12	66,66,66,66	0
57	MG	2A	3012	1/1	0.88	0.12	68,68,68,68	0
57	MG	2A	3351	1/1	0.88	0.08	70,70,70,70	0
57	MG	2a	3222	1/1	0.88	0.16	61,61,61,61	0
57	MG	1A	4002	1/1	0.88	0.07	23,23,23,23	0
57	MG	1a	1671	1/1	0.88	0.13	54,54,54,54	0
57	MG	1A	3252	1/1	0.88	0.12	56,56,56,56	0
57	MG	2R	201	1/1	0.88	0.11	55,55,55,55	0
57	MG	2S	3900	1/1	0.88	0.12	69,69,69,69	0
57	MG	2a	3237	1/1	0.88	0.15	58,58,58,58	0
57	MG	2A	3627	1/1	0.88	0.13	67,67,67,67	0
57	MG	1A	3283	1/1	0.88	0.14	57,57,57,57	0
57	MG	2A	3360	1/1	0.88	0.11	61,61,61,61	0
57	MG	1B	216	1/1	0.88	0.14	48,48,48,48	0
57	MG	2A	3646	1/1	0.88	0.13	60,60,60,60	0
57	MG	2A	3038	1/1	0.88	0.20	55,55,55,55	0
57	MG	1A	3748	1/1	0.88	0.09	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3752	1/1	0.88	0.08	16,16,16,16	0
57	MG	1A	3905	1/1	0.88	0.14	30,30,30,30	0
57	MG	1a	1691	1/1	0.88	0.28	61,61,61,61	0
57	MG	2A	3377	1/1	0.88	0.11	67,67,67,67	0
57	MG	2A	3666	1/1	0.88	0.11	49,49,49,49	0
57	MG	1A	3589	1/1	0.88	0.23	59,59,59,59	0
57	MG	2A	3381	1/1	0.88	0.14	64,64,64,64	0
57	MG	2y	102	1/1	0.88	0.11	74,74,74,74	0
57	MG	2A	3392	1/1	0.88	0.22	36,36,36,36	0
57	MG	2A	3642	1/1	0.89	0.13	52,52,52,52	0
57	MG	2a	3011	1/1	0.89	0.29	66,66,66,66	0
57	MG	2A	3645	1/1	0.89	0.13	46,46,46,46	0
57	MG	2A	3155	1/1	0.89	0.19	57,57,57,57	0
57	MG	1a	1732	1/1	0.89	0.14	62,62,62,62	0
57	MG	1a	1733	1/1	0.89	0.08	54,54,54,54	0
57	MG	1a	1740	1/1	0.89	0.08	66,66,66,66	0
57	MG	1A	3494	1/1	0.89	0.13	63,63,63,63	0
57	MG	2A	3655	1/1	0.89	0.15	60,60,60,60	0
57	MG	2A	3660	1/1	0.89	0.15	43,43,43,43	0
57	MG	2a	3026	1/1	0.89	0.37	62,62,62,62	0
57	MG	1A	3751	1/1	0.89	0.11	43,43,43,43	0
57	MG	1a	1748	1/1	0.89	0.15	51,51,51,51	0
57	MG	1B	230	1/1	0.89	0.08	67,67,67,67	0
57	MG	2a	3032	1/1	0.89	0.17	70,70,70,70	0
57	MG	2A	3189	1/1	0.89	0.17	66,66,66,66	0
57	MG	1a	1762	1/1	0.89	0.09	76,76,76,76	0
57	MG	2a	3035	1/1	0.89	0.26	66,66,66,66	0
57	MG	2a	3036	1/1	0.89	0.12	55,55,55,55	0
57	MG	2A	3359	1/1	0.89	0.21	60,60,60,60	0
57	MG	1D	312	1/1	0.89	0.18	40,40,40,40	0
57	MG	1A	3055	1/1	0.89	0.11	47,47,47,47	0
57	MG	1A	3679	1/1	0.89	0.12	62,62,62,62	0
57	MG	2A	3683	1/1	0.89	0.15	50,50,50,50	0
57	MG	2A	3366	1/1	0.89	0.10	51,51,51,51	0
57	MG	2A	3686	1/1	0.89	0.13	56,56,56,56	0
57	MG	1a	1778	1/1	0.89	0.07	65,65,65,65	0
57	MG	2A	3200	1/1	0.89	0.15	66,66,66,66	0
57	MG	2a	3052	1/1	0.89	0.20	74,74,74,74	0
57	MG	1A	4032	1/1	0.89	0.23	61,61,61,61	0
57	MG	1a	1789	1/1	0.89	0.09	64,64,64,64	0
57	MG	1a	1792	1/1	0.89	0.12	59,59,59,59	0
57	MG	2a	3069	1/1	0.89	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3761	1/1	0.89	0.09	38,38,38,38	0
57	MG	1G	204	1/1	0.89	0.09	71,71,71,71	0
57	MG	2A	3383	1/1	0.89	0.09	69,69,69,69	0
57	MG	2A	3709	1/1	0.89	0.10	73,73,73,73	0
57	MG	1a	1801	1/1	0.89	0.15	58,58,58,58	0
57	MG	1A	3909	1/1	0.89	0.10	30,30,30,30	0
57	MG	2A	3394	1/1	0.89	0.25	48,48,48,48	0
57	MG	1A	3246	1/1	0.89	0.09	57,57,57,57	0
57	MG	2a	3094	1/1	0.89	0.09	69,69,69,69	0
57	MG	2A	3238	1/1	0.89	0.13	58,58,58,58	0
57	MG	1a	1813	1/1	0.89	0.15	73,73,73,73	0
57	MG	1A	3089	1/1	0.89	0.15	51,51,51,51	0
57	MG	1Y	201	1/1	0.89	0.13	52,52,52,52	0
57	MG	2A	3736	1/1	0.89	0.15	67,67,67,67	0
57	MG	1Z	303	1/1	0.89	0.12	49,49,49,49	0
57	MG	1A	3124	1/1	0.89	0.12	49,49,49,49	0
57	MG	1A	3517	1/1	0.89	0.10	61,61,61,61	0
57	MG	2A	3250	1/1	0.89	0.32	64,64,64,64	0
57	MG	1A	3792	1/1	0.89	0.08	39,39,39,39	0
57	MG	2a	3127	1/1	0.89	0.09	67,67,67,67	0
57	MG	2A	3255	1/1	0.89	0.18	64,64,64,64	0
57	MG	2A	3257	1/1	0.89	0.32	70,70,70,70	0
57	MG	2A	3258	1/1	0.89	0.19	62,62,62,62	0
57	MG	1A	3160	1/1	0.89	0.20	58,58,58,58	0
57	MG	1A	4061	1/1	0.89	0.08	20,20,20,20	0
57	MG	1A	3801	1/1	0.89	0.14	52,52,52,52	0
57	MG	1A	3705	1/1	0.89	0.12	49,49,49,49	0
57	MG	1A	3528	1/1	0.89	0.16	44,44,44,44	0
57	MG	1A	3626	1/1	0.89	0.17	55,55,55,55	0
57	MG	2a	3159	1/1	0.89	0.10	62,62,62,62	0
57	MG	1A	3828	1/1	0.89	0.08	34,34,34,34	0
57	MG	1a	1638	1/1	0.89	0.37	62,62,62,62	0
57	MG	1A	3399	1/1	0.89	0.23	44,44,44,44	0
57	MG	2a	3166	1/1	0.89	0.29	67,67,67,67	0
57	MG	2A	3493	1/1	0.89	0.21	71,71,71,71	0
57	MG	1A	3830	1/1	0.89	0.14	55,55,55,55	0
57	MG	2A	3018	1/1	0.89	0.18	48,48,48,48	0
57	MG	1A	3840	1/1	0.89	0.08	56,56,56,56	0
57	MG	1A	3849	1/1	0.89	0.10	26,26,26,26	0
57	MG	2A	3817	1/1	0.89	0.06	49,49,49,49	0
57	MG	1a	1658	1/1	0.89	0.11	52,52,52,52	0
57	MG	1a	1664	1/1	0.89	0.24	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3543	1/1	0.89	0.16	72,72,72,72	0
57	MG	1A	3850	1/1	0.89	0.07	33,33,33,33	0
57	MG	1A	3178	1/1	0.89	0.24	49,49,49,49	0
57	MG	2a	3187	1/1	0.89	0.14	60,60,60,60	0
57	MG	1A	3984	1/1	0.89	0.10	28,28,28,28	0
57	MG	1A	3857	1/1	0.89	0.12	67,67,67,67	0
57	MG	2A	3058	1/1	0.89	0.20	55,55,55,55	0
57	MG	2a	3192	1/1	0.89	0.21	63,63,63,63	0
57	MG	2a	3196	1/1	0.89	0.12	62,62,62,62	0
57	MG	2A	3569	1/1	0.89	0.18	61,61,61,61	0
57	MG	1A	3464	1/1	0.89	0.13	58,58,58,58	0
57	MG	2A	3849	1/1	0.89	0.12	55,55,55,55	0
57	MG	2a	3202	1/1	0.89	0.30	67,67,67,67	0
57	MG	2A	3851	1/1	0.89	0.14	59,59,59,59	0
57	MG	1A	4105	1/1	0.89	0.13	55,55,55,55	0
57	MG	2A	3064	1/1	0.89	0.10	45,45,45,45	0
57	MG	2A	3070	1/1	0.89	0.22	70,70,70,70	0
57	MG	2a	3210	1/1	0.89	0.33	65,65,65,65	0
57	MG	2A	3575	1/1	0.89	0.15	62,62,62,62	0
57	MG	1A	3181	1/1	0.89	0.15	65,65,65,65	0
57	MG	2A	3578	1/1	0.89	0.11	39,39,39,39	0
57	MG	2A	3862	1/1	0.89	0.09	70,70,70,70	0
57	MG	2A	3579	1/1	0.89	0.10	61,61,61,61	0
57	MG	2A	3302	1/1	0.89	0.14	53,53,53,53	0
57	MG	1A	3062	1/1	0.89	0.08	52,52,52,52	0
57	MG	2A	3307	1/1	0.89	0.15	66,66,66,66	0
57	MG	1A	3731	1/1	0.89	0.07	48,48,48,48	0
57	MG	2B	213	1/1	0.89	0.18	64,64,64,64	0
57	MG	1A	3421	1/1	0.89	0.20	64,64,64,64	0
57	MG	2A	3318	1/1	0.89	0.13	57,57,57,57	0
57	MG	1a	1685	1/1	0.89	0.27	56,56,56,56	0
57	MG	1A	3492	1/1	0.89	0.09	58,58,58,58	0
57	MG	2r	101	1/1	0.89	0.19	72,72,72,72	0
57	MG	1B	217	1/1	0.89	0.08	50,50,50,50	0
57	MG	1a	1701	1/1	0.89	0.28	61,61,61,61	0
57	MG	1B	220	1/1	0.89	0.08	59,59,59,59	0
57	MG	1A	4012	1/1	0.89	0.11	56,56,56,56	0
57	MG	1B	223	1/1	0.89	0.14	54,54,54,54	0
57	MG	1a	1720	1/1	0.89	0.21	37,37,37,37	0
57	MG	1A	3423	1/1	0.89	0.12	52,52,52,52	0
57	MG	1A	3674	1/1	0.89	0.10	30,30,30,30	0
57	MG	2x	102	1/1	0.89	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3135	1/1	0.89	0.12	60,60,60,60	0
57	MG	2A	3138	1/1	0.89	0.22	51,51,51,51	0
57	MG	2a	3005	1/1	0.89	0.21	69,69,69,69	0
57	MG	2a	3007	1/1	0.89	0.26	69,69,69,69	0
57	MG	2A	3148	1/1	0.89	0.21	69,69,69,69	0
57	MG	1A	3349	1/1	0.90	0.11	73,73,73,73	0
57	MG	1A	3802	1/1	0.90	0.15	49,49,49,49	0
57	MG	2A	3677	1/1	0.90	0.18	68,68,68,68	0
57	MG	2a	3023	1/1	0.90	0.11	56,56,56,56	0
57	MG	1A	3809	1/1	0.90	0.10	49,49,49,49	0
57	MG	1A	3820	1/1	0.90	0.13	51,51,51,51	0
57	MG	1A	4044	1/1	0.90	0.17	60,60,60,60	0
57	MG	2A	3685	1/1	0.90	0.09	44,44,44,44	0
57	MG	2A	3405	1/1	0.90	0.36	60,60,60,60	0
57	MG	1A	3633	1/1	0.90	0.09	20,20,20,20	0
57	MG	2A	3411	1/1	0.90	0.21	52,52,52,52	0
57	MG	1B	231	1/1	0.90	0.10	56,56,56,56	0
57	MG	2A	3024	1/1	0.90	0.21	57,57,57,57	0
57	MG	1A	3169	1/1	0.90	0.09	43,43,43,43	0
57	MG	1A	3473	1/1	0.90	0.19	34,34,34,34	0
57	MG	2A	3702	1/1	0.90	0.09	37,37,37,37	0
57	MG	1A	3291	1/1	0.90	0.09	61,61,61,61	0
57	MG	1a	1692	1/1	0.90	0.22	53,53,53,53	0
57	MG	2A	3429	1/1	0.90	0.31	44,44,44,44	0
57	MG	1E	313	1/1	0.90	0.12	55,55,55,55	0
57	MG	1A	3476	1/1	0.90	0.18	57,57,57,57	0
57	MG	2a	3047	1/1	0.90	0.14	66,66,66,66	0
57	MG	2A	3447	1/1	0.90	0.28	60,60,60,60	0
57	MG	1A	3479	1/1	0.90	0.12	38,38,38,38	0
57	MG	1A	3836	1/1	0.90	0.08	67,67,67,67	0
57	MG	2A	3061	1/1	0.90	0.20	59,59,59,59	0
57	MG	2a	3058	1/1	0.90	0.07	60,60,60,60	0
57	MG	2A	3728	1/1	0.90	0.12	60,60,60,60	0
57	MG	1A	3970	1/1	0.90	0.11	40,40,40,40	0
57	MG	2a	3072	1/1	0.90	0.20	48,48,48,48	0
57	MG	2a	3077	1/1	0.90	0.20	55,55,55,55	0
57	MG	2a	3079	1/1	0.90	0.26	64,64,64,64	0
57	MG	1a	1722	1/1	0.90	0.15	56,56,56,56	0
57	MG	2A	3069	1/1	0.90	0.09	47,47,47,47	0
57	MG	2a	3085	1/1	0.90	0.15	78,78,78,78	0
57	MG	1A	4068	1/1	0.90	0.14	38,38,38,38	0
57	MG	2A	3480	1/1	0.90	0.21	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3075	1/1	0.90	0.15	48,48,48,48	0
57	MG	2A	3081	1/1	0.90	0.11	55,55,55,55	0
57	MG	2A	3757	1/1	0.90	0.11	64,64,64,64	0
57	MG	2A	3488	1/1	0.90	0.11	59,59,59,59	0
57	MG	1O	204	1/1	0.90	0.11	63,63,63,63	0
57	MG	2a	3096	1/1	0.90	0.10	60,60,60,60	0
57	MG	1A	3331	1/1	0.90	0.08	52,52,52,52	0
57	MG	2A	3491	1/1	0.90	0.12	59,59,59,59	0
57	MG	2A	3287	1/1	0.90	0.22	59,59,59,59	0
57	MG	2a	3102	1/1	0.90	0.17	68,68,68,68	0
57	MG	2A	3494	1/1	0.90	0.07	35,35,35,35	0
57	MG	1T	202	1/1	0.90	0.13	49,49,49,49	0
57	MG	2a	3110	1/1	0.90	0.13	59,59,59,59	0
57	MG	1a	1739	1/1	0.90	0.19	59,59,59,59	0
57	MG	2A	3772	1/1	0.90	0.10	44,44,44,44	0
57	MG	2A	3095	1/1	0.90	0.15	55,55,55,55	0
57	MG	2A	3096	1/1	0.90	0.20	69,69,69,69	0
57	MG	1A	3377	1/1	0.90	0.11	55,55,55,55	0
57	MG	2a	3123	1/1	0.90	0.19	61,61,61,61	0
57	MG	2a	3125	1/1	0.90	0.20	66,66,66,66	0
57	MG	2A	3517	1/1	0.90	0.10	42,42,42,42	0
57	MG	1A	3974	1/1	0.90	0.08	66,66,66,66	0
57	MG	10	102	1/1	0.90	0.18	46,46,46,46	0
57	MG	2A	3800	1/1	0.90	0.09	63,63,63,63	0
57	MG	10	104	1/1	0.90	0.14	62,62,62,62	0
57	MG	2a	3141	1/1	0.90	0.08	53,53,53,53	0
57	MG	2A	3805	1/1	0.90	0.09	64,64,64,64	0
57	MG	2A	3548	1/1	0.90	0.14	45,45,45,45	0
57	MG	2a	3154	1/1	0.90	0.09	67,67,67,67	0
57	MG	2A	3810	1/1	0.90	0.13	42,42,42,42	0
57	MG	1a	1759	1/1	0.90	0.17	80,80,80,80	0
57	MG	1A	3256	1/1	0.90	0.12	63,63,63,63	0
57	MG	11	103	1/1	0.90	0.07	69,69,69,69	0
57	MG	2A	3819	1/1	0.90	0.14	55,55,55,55	0
57	MG	2A	3824	1/1	0.90	0.12	60,60,60,60	0
57	MG	2A	3826	1/1	0.90	0.11	57,57,57,57	0
57	MG	2A	3828	1/1	0.90	0.08	43,43,43,43	0
57	MG	12	101	1/1	0.90	0.12	55,55,55,55	0
57	MG	1A	3445	1/1	0.90	0.13	62,62,62,62	0
57	MG	2A	3315	1/1	0.90	0.15	58,58,58,58	0
57	MG	17	104	1/1	0.90	0.13	51,51,51,51	0
57	MG	18	101	1/1	0.90	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3244	1/1	0.90	0.14	55,55,55,55	0
57	MG	1A	3682	1/1	0.90	0.10	32,32,32,32	0
57	MG	1A	3501	1/1	0.90	0.14	51,51,51,51	0
57	MG	1A	3753	1/1	0.90	0.13	46,46,46,46	0
57	MG	1A	3689	1/1	0.90	0.10	34,34,34,34	0
57	MG	2A	3581	1/1	0.90	0.15	57,57,57,57	0
57	MG	1A	3991	1/1	0.90	0.12	55,55,55,55	0
57	MG	1A	3301	1/1	0.90	0.30	53,53,53,53	0
57	MG	1a	1806	1/1	0.90	0.10	60,60,60,60	0
57	MG	2A	3336	1/1	0.90	0.08	59,59,59,59	0
57	MG	2A	3180	1/1	0.90	0.17	59,59,59,59	0
57	MG	2a	3193	1/1	0.90	0.12	67,67,67,67	0
57	MG	1A	3695	1/1	0.90	0.08	24,24,24,24	0
57	MG	1A	3883	1/1	0.90	0.11	25,25,25,25	0
57	MG	2A	3188	1/1	0.90	0.26	60,60,60,60	0
57	MG	1A	3395	1/1	0.90	0.15	46,46,46,46	0
57	MG	1b	301	1/1	0.90	0.12	64,64,64,64	0
57	MG	1e	201	1/1	0.90	0.11	67,67,67,67	0
57	MG	1B	202	1/1	0.90	0.29	60,60,60,60	0
57	MG	2B	210	1/1	0.90	0.08	70,70,70,70	0
57	MG	2A	3618	1/1	0.90	0.26	65,65,65,65	0
57	MG	2A	3619	1/1	0.90	0.15	41,41,41,41	0
57	MG	1a	1644	1/1	0.90	0.14	60,60,60,60	0
57	MG	2a	3214	1/1	0.90	0.21	60,60,60,60	0
57	MG	1l	201	1/1	0.90	0.08	61,61,61,61	0
57	MG	2E	306	1/1	0.90	0.14	56,56,56,56	0
57	MG	1a	1650	1/1	0.90	0.26	62,62,62,62	0
57	MG	2a	3220	1/1	0.90	0.10	72,72,72,72	0
57	MG	2R	202	1/1	0.90	0.12	56,56,56,56	0
57	MG	1a	1652	1/1	0.90	0.18	45,45,45,45	0
57	MG	2U	201	1/1	0.90	0.22	52,52,52,52	0
57	MG	1A	3773	1/1	0.90	0.12	32,32,32,32	0
57	MG	2A	3211	1/1	0.90	0.18	61,61,61,61	0
57	MG	2a	3227	1/1	0.90	0.20	61,61,61,61	0
57	MG	1t	201	1/1	0.90	0.15	56,56,56,56	0
57	MG	2a	3235	1/1	0.90	0.09	80,80,80,80	0
57	MG	1A	3452	1/1	0.90	0.10	44,44,44,44	0
57	MG	21	102	1/1	0.90	0.36	51,51,51,51	0
57	MG	1A	3785	1/1	0.90	0.13	55,55,55,55	0
57	MG	1A	3453	1/1	0.90	0.18	56,56,56,56	0
57	MG	1A	3791	1/1	0.90	0.10	38,38,38,38	0
57	MG	26	101	1/1	0.90	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3226	1/1	0.90	0.17	55,55,55,55	0
57	MG	2A	3370	1/1	0.90	0.29	62,62,62,62	0
57	MG	1x	101	1/1	0.90	0.29	62,62,62,62	0
57	MG	2A	3372	1/1	0.90	0.16	63,63,63,63	0
57	MG	1A	3098	1/1	0.90	0.13	63,63,63,63	0
57	MG	2A	3239	1/1	0.90	0.17	63,63,63,63	0
57	MG	1x	104	1/1	0.90	0.17	62,62,62,62	0
57	MG	2A	3243	1/1	0.90	0.20	61,61,61,61	0
57	MG	1x	105	1/1	0.90	0.21	56,56,56,56	0
57	MG	2A	3668	1/1	0.90	0.12	61,61,61,61	0
57	MG	1A	3348	1/1	0.90	0.17	61,61,61,61	0
57	MG	2A	3384	1/1	0.90	0.16	59,59,59,59	0
57	MG	2A	3671	1/1	0.90	0.13	64,64,64,64	0
59	A1AE0	1A	4110	72/72	0.90	0.14	14,30,64,67	0
57	MG	1A	3467	1/1	0.91	0.14	49,49,49,49	0
57	MG	2A	3609	1/1	0.91	0.15	48,48,48,48	0
57	MG	2A	3611	1/1	0.91	0.11	39,39,39,39	0
57	MG	1A	4000	1/1	0.91	0.17	43,43,43,43	0
57	MG	2A	3102	1/1	0.91	0.09	52,52,52,52	0
57	MG	1A	3853	1/1	0.91	0.09	45,45,45,45	0
57	MG	1E	309	1/1	0.91	0.09	26,26,26,26	0
57	MG	1A	4005	1/1	0.91	0.08	24,24,24,24	0
57	MG	29	101	1/1	0.91	0.24	68,68,68,68	0
57	MG	1A	4007	1/1	0.91	0.08	40,40,40,40	0
57	MG	2A	3114	1/1	0.91	0.17	58,58,58,58	0
57	MG	1A	3470	1/1	0.91	0.18	39,39,39,39	0
57	MG	1F	311	1/1	0.91	0.25	37,37,37,37	0
57	MG	2A	3121	1/1	0.91	0.08	56,56,56,56	0
57	MG	1F	312	1/1	0.91	0.11	45,45,45,45	0
57	MG	2A	3132	1/1	0.91	0.14	50,50,50,50	0
57	MG	1a	1751	1/1	0.91	0.14	64,64,64,64	0
57	MG	2A	3636	1/1	0.91	0.12	52,52,52,52	0
57	MG	1A	4010	1/1	0.91	0.12	45,45,45,45	0
57	MG	2A	3146	1/1	0.91	0.20	48,48,48,48	0
57	MG	1A	3231	1/1	0.91	0.10	64,64,64,64	0
57	MG	1A	3859	1/1	0.91	0.10	45,45,45,45	0
57	MG	1A	4018	1/1	0.91	0.10	47,47,47,47	0
57	MG	1a	1767	1/1	0.91	0.10	66,66,66,66	0
57	MG	2a	3022	1/1	0.91	0.30	68,68,68,68	0
57	MG	1A	3729	1/1	0.91	0.08	53,53,53,53	0
57	MG	2a	3024	1/1	0.91	0.12	58,58,58,58	0
57	MG	2a	3025	1/1	0.91	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3654	1/1	0.91	0.15	44,44,44,44	0
57	MG	1A	3863	1/1	0.91	0.18	36,36,36,36	0
57	MG	2A	3658	1/1	0.91	0.12	53,53,53,53	0
57	MG	2A	3659	1/1	0.91	0.11	50,50,50,50	0
57	MG	2a	3031	1/1	0.91	0.22	59,59,59,59	0
57	MG	1A	3306	1/1	0.91	0.20	55,55,55,55	0
57	MG	2A	3176	1/1	0.91	0.13	56,56,56,56	0
57	MG	1a	1780	1/1	0.91	0.11	76,76,76,76	0
57	MG	1A	3316	1/1	0.91	0.10	50,50,50,50	0
57	MG	2A	3362	1/1	0.91	0.09	64,64,64,64	0
57	MG	2A	3184	1/1	0.91	0.11	59,59,59,59	0
57	MG	2A	3186	1/1	0.91	0.18	65,65,65,65	0
57	MG	2a	3039	1/1	0.91	0.12	64,64,64,64	0
57	MG	1Z	301	1/1	0.91	0.14	55,55,55,55	0
57	MG	2A	3369	1/1	0.91	0.17	52,52,52,52	0
57	MG	1A	4030	1/1	0.91	0.13	55,55,55,55	0
57	MG	2A	3675	1/1	0.91	0.17	66,66,66,66	0
57	MG	1A	3243	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3125	1/1	0.91	0.11	42,42,42,42	0
57	MG	1A	3179	1/1	0.91	0.16	55,55,55,55	0
57	MG	1a	1803	1/1	0.91	0.19	51,51,51,51	0
57	MG	1l	102	1/1	0.91	0.09	46,46,46,46	0
57	MG	1A	3880	1/1	0.91	0.09	36,36,36,36	0
57	MG	2A	3198	1/1	0.91	0.11	53,53,53,53	0
57	MG	1A	3336	1/1	0.91	0.16	59,59,59,59	0
57	MG	2a	3064	1/1	0.91	0.20	58,58,58,58	0
57	MG	1A	3407	1/1	0.91	0.11	62,62,62,62	0
57	MG	1a	1814	1/1	0.91	0.08	61,61,61,61	0
57	MG	2a	3070	1/1	0.91	0.09	66,66,66,66	0
57	MG	2A	3691	1/1	0.91	0.10	42,42,42,42	0
57	MG	2A	3696	1/1	0.91	0.11	59,59,59,59	0
57	MG	2A	3207	1/1	0.91	0.23	61,61,61,61	0
57	MG	2A	3210	1/1	0.91	0.15	58,58,58,58	0
57	MG	2A	3396	1/1	0.91	0.22	56,56,56,56	0
57	MG	2A	3398	1/1	0.91	0.15	62,62,62,62	0
57	MG	2a	3086	1/1	0.91	0.30	63,63,63,63	0
57	MG	15	3205	1/1	0.91	0.14	33,33,33,33	0
57	MG	2A	3214	1/1	0.91	0.13	60,60,60,60	0
57	MG	2A	3705	1/1	0.91	0.12	40,40,40,40	0
57	MG	2A	3706	1/1	0.91	0.11	57,57,57,57	0
57	MG	1A	3886	1/1	0.91	0.07	30,30,30,30	0
57	MG	2A	3218	1/1	0.91	0.29	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3410	1/1	0.91	0.19	53,53,53,53	0
57	MG	1d	301	1/1	0.91	0.38	64,64,64,64	0
57	MG	1A	3411	1/1	0.91	0.12	53,53,53,53	0
57	MG	2A	3720	1/1	0.91	0.10	35,35,35,35	0
57	MG	2A	3722	1/1	0.91	0.18	39,39,39,39	0
57	MG	2A	3413	1/1	0.91	0.19	55,55,55,55	0
57	MG	18	102	1/1	0.91	0.10	34,34,34,34	0
57	MG	1A	3415	1/1	0.91	0.24	55,55,55,55	0
57	MG	2A	3729	1/1	0.91	0.14	52,52,52,52	0
57	MG	1A	3145	1/1	0.91	0.24	32,32,32,32	0
57	MG	1A	3508	1/1	0.91	0.25	44,44,44,44	0
57	MG	2A	3421	1/1	0.91	0.28	56,56,56,56	0
57	MG	2A	3738	1/1	0.91	0.09	63,63,63,63	0
57	MG	2A	3423	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3904	1/1	0.91	0.11	29,29,29,29	0
57	MG	2A	3427	1/1	0.91	0.21	61,61,61,61	0
57	MG	1a	1605	1/1	0.91	0.10	58,58,58,58	0
57	MG	2A	3440	1/1	0.91	0.16	56,56,56,56	0
57	MG	2A	3758	1/1	0.91	0.12	64,64,64,64	0
57	MG	1A	3657	1/1	0.91	0.11	50,50,50,50	0
57	MG	1A	3765	1/1	0.91	0.09	50,50,50,50	0
57	MG	2A	3446	1/1	0.91	0.21	59,59,59,59	0
57	MG	1a	1622	1/1	0.91	0.16	55,55,55,55	0
57	MG	2A	3767	1/1	0.91	0.10	63,63,63,63	0
57	MG	2A	3450	1/1	0.91	0.08	53,53,53,53	0
57	MG	1w	106	1/1	0.91	0.20	65,65,65,65	0
57	MG	1A	3342	1/1	0.91	0.23	62,62,62,62	0
57	MG	1a	1628	1/1	0.91	0.25	54,54,54,54	0
57	MG	2A	3467	1/1	0.91	0.11	47,47,47,47	0
57	MG	1A	4073	1/1	0.91	0.11	55,55,55,55	0
57	MG	2A	3249	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3475	1/1	0.91	0.10	48,48,48,48	0
57	MG	2A	3477	1/1	0.91	0.08	45,45,45,45	0
57	MG	1A	3910	1/1	0.91	0.12	34,34,34,34	0
57	MG	2A	3794	1/1	0.91	0.08	52,52,52,52	0
57	MG	1A	3663	1/1	0.91	0.09	31,31,31,31	0
57	MG	1A	3182	1/1	0.91	0.08	31,31,31,31	0
57	MG	2a	3172	1/1	0.91	0.10	66,66,66,66	0
57	MG	1A	3260	1/1	0.91	0.06	45,45,45,45	0
57	MG	2A	3804	1/1	0.91	0.10	56,56,56,56	0
57	MG	1A	3521	1/1	0.91	0.09	44,44,44,44	0
57	MG	1A	3439	1/1	0.91	0.13	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3443	1/1	0.91	0.15	52,52,52,52	0
57	MG	1A	3534	1/1	0.91	0.17	52,52,52,52	0
57	MG	1A	4096	1/1	0.91	0.14	55,55,55,55	0
57	MG	1A	3683	1/1	0.91	0.12	19,19,19,19	0
57	MG	1A	3947	1/1	0.91	0.11	57,57,57,57	0
57	MG	2A	3822	1/1	0.91	0.09	56,56,56,56	0
57	MG	1a	1666	1/1	0.91	0.22	60,60,60,60	0
57	MG	1A	3263	1/1	0.91	0.15	48,48,48,48	0
57	MG	2A	3033	1/1	0.91	0.16	52,52,52,52	0
57	MG	2A	3507	1/1	0.91	0.10	53,53,53,53	0
57	MG	2A	3510	1/1	0.91	0.10	44,44,44,44	0
57	MG	2A	3276	1/1	0.91	0.09	51,51,51,51	0
57	MG	1A	3537	1/1	0.91	0.10	52,52,52,52	0
57	MG	2A	3838	1/1	0.91	0.10	57,57,57,57	0
57	MG	2A	3516	1/1	0.91	0.10	51,51,51,51	0
57	MG	2a	3205	1/1	0.91	0.11	69,69,69,69	0
57	MG	1A	3954	1/1	0.91	0.11	45,45,45,45	0
57	MG	1A	3819	1/1	0.91	0.07	41,41,41,41	0
57	MG	2A	3050	1/1	0.91	0.21	64,64,64,64	0
57	MG	2A	3052	1/1	0.91	0.23	63,63,63,63	0
57	MG	1A	4108	1/1	0.91	0.26	59,59,59,59	0
57	MG	2a	3213	1/1	0.91	0.25	59,59,59,59	0
57	MG	1A	3185	1/1	0.91	0.11	40,40,40,40	0
57	MG	2A	3850	1/1	0.91	0.12	54,54,54,54	0
57	MG	1A	3821	1/1	0.91	0.14	48,48,48,48	0
57	MG	1A	3189	1/1	0.91	0.10	47,47,47,47	0
57	MG	1A	3019	1/1	0.91	0.16	49,49,49,49	0
57	MG	2A	3565	1/1	0.91	0.10	63,63,63,63	0
57	MG	2A	3568	1/1	0.91	0.15	57,57,57,57	0
57	MG	2A	3859	1/1	0.91	0.15	79,79,79,79	0
57	MG	1a	1684	1/1	0.91	0.31	49,49,49,49	0
57	MG	1A	3363	1/1	0.91	0.16	51,51,51,51	0
57	MG	1A	3214	1/1	0.91	0.09	48,48,48,48	0
57	MG	1a	1688	1/1	0.91	0.36	62,62,62,62	0
57	MG	2a	3229	1/1	0.91	0.23	65,65,65,65	0
57	MG	1a	1689	1/1	0.91	0.19	58,58,58,58	0
57	MG	2A	3298	1/1	0.91	0.14	49,49,49,49	0
57	MG	2g	201	1/1	0.91	0.20	69,69,69,69	0
57	MG	2A	3078	1/1	0.91	0.21	60,60,60,60	0
57	MG	2A	3079	1/1	0.91	0.12	49,49,49,49	0
57	MG	1A	3365	1/1	0.91	0.12	54,54,54,54	0
57	MG	1A	3582	1/1	0.91	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2B	214	1/1	0.91	0.08	63,63,63,63	0
57	MG	2A	3306	1/1	0.91	0.11	64,64,64,64	0
57	MG	2D	305	1/1	0.91	0.24	55,55,55,55	0
57	MG	1A	3831	1/1	0.91	0.09	42,42,42,42	0
57	MG	1A	3220	1/1	0.91	0.14	39,39,39,39	0
57	MG	2F	308	1/1	0.91	0.20	62,62,62,62	0
57	MG	2P	201	1/1	0.91	0.18	48,48,48,48	0
57	MG	1A	3221	1/1	0.91	0.14	43,43,43,43	0
57	MG	2A	3587	1/1	0.91	0.07	41,41,41,41	0
57	MG	1A	3846	1/1	0.91	0.10	61,61,61,61	0
57	MG	2T	202	1/1	0.91	0.14	66,66,66,66	0
57	MG	1A	3847	1/1	0.91	0.08	59,59,59,59	0
57	MG	1A	3082	1/1	0.91	0.09	35,35,35,35	0
57	MG	2y	103	1/1	0.91	0.11	84,84,84,84	0
57	MG	2V	201	1/1	0.91	0.20	42,42,42,42	0
57	MG	2A	3598	1/1	0.91	0.15	37,37,37,37	0
57	MG	2A	3292	1/1	0.92	0.19	65,65,65,65	0
57	MG	2E	303	1/1	0.92	0.13	53,53,53,53	0
57	MG	2A	3293	1/1	0.92	0.25	61,61,61,61	0
57	MG	2F	302	1/1	0.92	0.09	64,64,64,64	0
57	MG	2F	305	1/1	0.92	0.12	53,53,53,53	0
57	MG	1a	1660	1/1	0.92	0.10	54,54,54,54	0
57	MG	2G	201	1/1	0.92	0.18	68,68,68,68	0
57	MG	1a	1662	1/1	0.92	0.15	57,57,57,57	0
57	MG	1A	3916	1/1	0.92	0.09	54,54,54,54	0
57	MG	2A	3297	1/1	0.92	0.13	55,55,55,55	0
57	MG	2A	3055	1/1	0.92	0.13	46,46,46,46	0
57	MG	1A	4086	1/1	0.92	0.09	35,35,35,35	0
57	MG	1A	3358	1/1	0.92	0.14	51,51,51,51	0
57	MG	1A	3503	1/1	0.92	0.14	58,58,58,58	0
57	MG	1A	3932	1/1	0.92	0.11	54,54,54,54	0
57	MG	1a	1669	1/1	0.92	0.33	64,64,64,64	0
57	MG	1A	3168	1/1	0.92	0.12	54,54,54,54	0
57	MG	2A	3308	1/1	0.92	0.17	56,56,56,56	0
57	MG	1A	3319	1/1	0.92	0.13	54,54,54,54	0
57	MG	1A	3643	1/1	0.92	0.14	60,60,60,60	0
57	MG	2A	3314	1/1	0.92	0.14	55,55,55,55	0
57	MG	25	103	1/1	0.92	0.12	63,63,63,63	0
57	MG	25	106	1/1	0.92	0.10	52,52,52,52	0
57	MG	1A	3511	1/1	0.92	0.11	54,54,54,54	0
57	MG	2A	3316	1/1	0.92	0.12	69,69,69,69	0
57	MG	1A	3654	1/1	0.92	0.07	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	28	103	1/1	0.92	0.21	46,46,46,46	0
57	MG	1A	4106	1/1	0.92	0.13	49,49,49,49	0
57	MG	1A	3945	1/1	0.92	0.09	53,53,53,53	0
57	MG	2a	3003	1/1	0.92	0.09	71,71,71,71	0
57	MG	2A	3620	1/1	0.92	0.11	47,47,47,47	0
57	MG	1A	3656	1/1	0.92	0.09	54,54,54,54	0
57	MG	1A	3431	1/1	0.92	0.11	61,61,61,61	0
57	MG	1A	3950	1/1	0.92	0.07	42,42,42,42	0
57	MG	1A	3001	1/1	0.92	0.11	38,38,38,38	0
57	MG	1A	3442	1/1	0.92	0.16	69,69,69,69	0
57	MG	1A	3671	1/1	0.92	0.07	25,25,25,25	0
57	MG	2A	3332	1/1	0.92	0.13	62,62,62,62	0
57	MG	2A	3635	1/1	0.92	0.07	31,31,31,31	0
57	MG	1A	3957	1/1	0.92	0.13	53,53,53,53	0
57	MG	1a	1693	1/1	0.92	0.09	47,47,47,47	0
57	MG	1a	1695	1/1	0.92	0.23	60,60,60,60	0
57	MG	2A	3103	1/1	0.92	0.20	51,51,51,51	0
57	MG	1A	3964	1/1	0.92	0.11	51,51,51,51	0
57	MG	2A	3106	1/1	0.92	0.24	57,57,57,57	0
57	MG	1A	3818	1/1	0.92	0.08	28,28,28,28	0
57	MG	2A	3342	1/1	0.92	0.40	66,66,66,66	0
57	MG	1A	3323	1/1	0.92	0.13	49,49,49,49	0
57	MG	1a	1709	1/1	0.92	0.08	55,55,55,55	0
57	MG	2A	3656	1/1	0.92	0.09	67,67,67,67	0
57	MG	1a	1711	1/1	0.92	0.24	64,64,64,64	0
57	MG	1a	1714	1/1	0.92	0.22	54,54,54,54	0
57	MG	1A	3368	1/1	0.92	0.11	48,48,48,48	0
57	MG	1A	3372	1/1	0.92	0.12	48,48,48,48	0
57	MG	2A	3124	1/1	0.92	0.14	58,58,58,58	0
57	MG	1A	3529	1/1	0.92	0.17	48,48,48,48	0
57	MG	1a	1724	1/1	0.92	0.08	57,57,57,57	0
57	MG	1A	3531	1/1	0.92	0.13	36,36,36,36	0
57	MG	2A	3137	1/1	0.92	0.18	57,57,57,57	0
57	MG	1A	3264	1/1	0.92	0.18	64,64,64,64	0
57	MG	2A	3142	1/1	0.92	0.13	51,51,51,51	0
57	MG	2a	3040	1/1	0.92	0.28	71,71,71,71	0
57	MG	2A	3143	1/1	0.92	0.24	62,62,62,62	0
57	MG	1A	3378	1/1	0.92	0.39	49,49,49,49	0
57	MG	1A	3685	1/1	0.92	0.09	29,29,29,29	0
57	MG	1a	1736	1/1	0.92	0.24	65,65,65,65	0
57	MG	2A	3679	1/1	0.92	0.13	59,59,59,59	0
57	MG	1A	3536	1/1	0.92	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3682	1/1	0.92	0.08	38,38,38,38	0
57	MG	2a	3049	1/1	0.92	0.12	64,64,64,64	0
57	MG	2a	3050	1/1	0.92	0.09	61,61,61,61	0
57	MG	2A	3160	1/1	0.92	0.21	68,68,68,68	0
57	MG	2A	3164	1/1	0.92	0.08	62,62,62,62	0
57	MG	1A	3077	1/1	0.92	0.25	42,42,42,42	0
57	MG	1A	3987	1/1	0.92	0.10	56,56,56,56	0
57	MG	2A	3376	1/1	0.92	0.14	60,60,60,60	0
57	MG	1a	1745	1/1	0.92	0.11	48,48,48,48	0
57	MG	2A	3378	1/1	0.92	0.11	63,63,63,63	0
57	MG	1A	3834	1/1	0.92	0.22	55,55,55,55	0
57	MG	2A	3695	1/1	0.92	0.10	56,56,56,56	0
57	MG	1A	3538	1/1	0.92	0.07	53,53,53,53	0
57	MG	2a	3073	1/1	0.92	0.26	63,63,63,63	0
57	MG	1A	3693	1/1	0.92	0.17	54,54,54,54	0
57	MG	1A	3844	1/1	0.92	0.09	20,20,20,20	0
57	MG	2A	3391	1/1	0.92	0.23	54,54,54,54	0
57	MG	1a	1760	1/1	0.92	0.08	55,55,55,55	0
57	MG	2A	3185	1/1	0.92	0.24	63,63,63,63	0
57	MG	1A	3334	1/1	0.92	0.14	42,42,42,42	0
57	MG	1A	3547	1/1	0.92	0.30	49,49,49,49	0
57	MG	1A	3392	1/1	0.92	0.10	34,34,34,34	0
57	MG	1A	3703	1/1	0.92	0.10	52,52,52,52	0
57	MG	2A	3710	1/1	0.92	0.13	58,58,58,58	0
57	MG	1a	1768	1/1	0.92	0.10	38,38,38,38	0
57	MG	1A	3457	1/1	0.92	0.13	68,68,68,68	0
57	MG	2A	3715	1/1	0.92	0.11	76,76,76,76	0
57	MG	1A	3285	1/1	0.92	0.12	53,53,53,53	0
57	MG	2A	3407	1/1	0.92	0.30	57,57,57,57	0
57	MG	2A	3718	1/1	0.92	0.14	54,54,54,54	0
57	MG	2a	3100	1/1	0.92	0.19	61,61,61,61	0
57	MG	1S	202	1/1	0.92	0.10	47,47,47,47	0
57	MG	2A	3721	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3554	1/1	0.92	0.11	41,41,41,41	0
57	MG	1V	202	1/1	0.92	0.25	41,41,41,41	0
57	MG	2a	3109	1/1	0.92	0.15	65,65,65,65	0
57	MG	1V	207	1/1	0.92	0.11	55,55,55,55	0
57	MG	2A	3202	1/1	0.92	0.11	54,54,54,54	0
57	MG	2A	3203	1/1	0.92	0.07	49,49,49,49	0
57	MG	1A	3002	1/1	0.92	0.10	50,50,50,50	0
57	MG	2A	3731	1/1	0.92	0.13	61,61,61,61	0
57	MG	2a	3120	1/1	0.92	0.27	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3121	1/1	0.92	0.23	58,58,58,58	0
57	MG	1A	4013	1/1	0.92	0.09	64,64,64,64	0
57	MG	1A	3569	1/1	0.92	0.09	31,31,31,31	0
57	MG	1A	3861	1/1	0.92	0.13	40,40,40,40	0
57	MG	1A	3862	1/1	0.92	0.21	37,37,37,37	0
57	MG	1a	1804	1/1	0.92	0.18	56,56,56,56	0
57	MG	1A	3398	1/1	0.92	0.21	49,49,49,49	0
57	MG	2A	3437	1/1	0.92	0.12	56,56,56,56	0
57	MG	1A	3581	1/1	0.92	0.09	44,44,44,44	0
57	MG	1A	3217	1/1	0.92	0.11	45,45,45,45	0
57	MG	2A	3220	1/1	0.92	0.09	57,57,57,57	0
57	MG	1A	3869	1/1	0.92	0.09	33,33,33,33	0
57	MG	2a	3152	1/1	0.92	0.08	68,68,68,68	0
57	MG	2A	3762	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3468	1/1	0.92	0.50	51,51,51,51	0
57	MG	2A	3448	1/1	0.92	0.10	45,45,45,45	0
57	MG	2A	3765	1/1	0.92	0.10	58,58,58,58	0
57	MG	2A	3766	1/1	0.92	0.12	68,68,68,68	0
57	MG	14	101	1/1	0.92	0.14	70,70,70,70	0
57	MG	2A	3451	1/1	0.92	0.06	33,33,33,33	0
57	MG	2a	3164	1/1	0.92	0.19	58,58,58,58	0
57	MG	1A	3873	1/1	0.92	0.11	34,34,34,34	0
57	MG	2A	3453	1/1	0.92	0.25	65,65,65,65	0
57	MG	15	3207	1/1	0.92	0.12	36,36,36,36	0
57	MG	2A	3236	1/1	0.92	0.14	58,58,58,58	0
57	MG	2A	3458	1/1	0.92	0.10	53,53,53,53	0
57	MG	2A	3462	1/1	0.92	0.09	48,48,48,48	0
57	MG	2A	3464	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3875	1/1	0.92	0.08	31,31,31,31	0
57	MG	2A	3785	1/1	0.92	0.14	50,50,50,50	0
57	MG	2a	3181	1/1	0.92	0.12	59,59,59,59	0
57	MG	2A	3788	1/1	0.92	0.08	48,48,48,48	0
57	MG	1A	4036	1/1	0.92	0.12	30,30,30,30	0
57	MG	1A	4037	1/1	0.92	0.10	23,23,23,23	0
57	MG	1A	3586	1/1	0.92	0.27	66,66,66,66	0
57	MG	19	101	1/1	0.92	0.19	49,49,49,49	0
57	MG	1A	3247	1/1	0.92	0.13	54,54,54,54	0
57	MG	2A	3803	1/1	0.92	0.17	63,63,63,63	0
57	MG	1A	3879	1/1	0.92	0.13	25,25,25,25	0
57	MG	1A	3250	1/1	0.92	0.09	20,20,20,20	0
57	MG	1A	3738	1/1	0.92	0.06	17,17,17,17	0
57	MG	1w	102	1/1	0.92	0.13	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1w	104	1/1	0.92	0.20	51,51,51,51	0
57	MG	2A	3251	1/1	0.92	0.12	61,61,61,61	0
57	MG	2A	3816	1/1	0.92	0.09	34,34,34,34	0
57	MG	1a	1607	1/1	0.92	0.10	54,54,54,54	0
57	MG	1a	1608	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3148	1/1	0.92	0.10	41,41,41,41	0
57	MG	1a	1614	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3885	1/1	0.92	0.12	23,23,23,23	0
57	MG	1a	1619	1/1	0.92	0.17	49,49,49,49	0
57	MG	2A	3503	1/1	0.92	0.07	33,33,33,33	0
57	MG	2A	3830	1/1	0.92	0.12	60,60,60,60	0
57	MG	2A	3831	1/1	0.92	0.21	46,46,46,46	0
57	MG	2A	3505	1/1	0.92	0.18	58,58,58,58	0
57	MG	2A	3833	1/1	0.92	0.14	48,48,48,48	0
57	MG	1A	3405	1/1	0.92	0.24	58,58,58,58	0
57	MG	2A	3265	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3477	1/1	0.92	0.09	48,48,48,48	0
57	MG	2a	3218	1/1	0.92	0.12	54,54,54,54	0
57	MG	1a	1625	1/1	0.92	0.29	61,61,61,61	0
57	MG	1A	3040	1/1	0.92	0.22	59,59,59,59	0
57	MG	2A	3515	1/1	0.92	0.10	39,39,39,39	0
57	MG	2A	3843	1/1	0.92	0.16	64,64,64,64	0
57	MG	2A	3271	1/1	0.92	0.17	54,54,54,54	0
57	MG	1x	111	1/1	0.92	0.19	67,67,67,67	0
57	MG	1A	4067	1/1	0.92	0.10	49,49,49,49	0
57	MG	2A	3528	1/1	0.92	0.08	51,51,51,51	0
57	MG	2A	3530	1/1	0.92	0.12	42,42,42,42	0
57	MG	2a	3234	1/1	0.92	0.13	64,64,64,64	0
57	MG	2A	3537	1/1	0.92	0.10	31,31,31,31	0
57	MG	2A	3539	1/1	0.92	0.08	32,32,32,32	0
57	MG	2A	3542	1/1	0.92	0.08	44,44,44,44	0
57	MG	1a	1635	1/1	0.92	0.16	66,66,66,66	0
57	MG	1A	3894	1/1	0.92	0.09	56,56,56,56	0
57	MG	1A	3408	1/1	0.92	0.07	42,42,42,42	0
57	MG	2q	201	1/1	0.92	0.09	72,72,72,72	0
57	MG	2q	202	1/1	0.92	0.12	67,67,67,67	0
57	MG	1A	3257	1/1	0.92	0.17	62,62,62,62	0
57	MG	2A	3280	1/1	0.92	0.09	56,56,56,56	0
57	MG	2A	3558	1/1	0.92	0.13	66,66,66,66	0
57	MG	1A	3258	1/1	0.92	0.11	54,54,54,54	0
57	MG	2B	202	1/1	0.92	0.13	59,59,59,59	0
57	MG	1a	1646	1/1	0.92	0.22	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3755	1/1	0.92	0.11	20,20,20,20	0
57	MG	1A	3630	1/1	0.92	0.11	47,47,47,47	0
57	MG	2B	209	1/1	0.92	0.16	53,53,53,53	0
57	MG	1A	3419	1/1	0.92	0.09	51,51,51,51	0
57	MG	1a	1655	1/1	0.92	0.10	55,55,55,55	0
57	MG	2A	3039	1/1	0.92	0.16	67,67,67,67	0
57	MG	1A	4082	1/1	0.92	0.18	58,58,58,58	0
57	MG	2A	3049	1/1	0.92	0.10	62,62,62,62	0
57	MG	2B	218	1/1	0.92	0.10	55,55,55,55	0
57	MG	2B	219	1/1	0.92	0.24	65,65,65,65	0
57	MG	1A	3353	1/1	0.92	0.10	52,52,52,52	0
59	A1AE0	2A	3863	72/72	0.92	0.15	32,46,68,77	0
57	MG	1A	3760	1/1	0.93	0.09	23,23,23,23	0
57	MG	1A	3116	1/1	0.93	0.07	33,33,33,33	0
57	MG	2F	303	1/1	0.93	0.17	52,52,52,52	0
57	MG	2A	3305	1/1	0.93	0.09	59,59,59,59	0
57	MG	1a	1661	1/1	0.93	0.14	56,56,56,56	0
57	MG	2A	3588	1/1	0.93	0.11	40,40,40,40	0
57	MG	2O	202	1/1	0.93	0.15	60,60,60,60	0
57	MG	2A	3062	1/1	0.93	0.26	50,50,50,50	0
57	MG	2A	3591	1/1	0.93	0.15	61,61,61,61	0
57	MG	1A	3763	1/1	0.93	0.06	29,29,29,29	0
57	MG	2A	3595	1/1	0.93	0.11	49,49,49,49	0
57	MG	1A	3297	1/1	0.93	0.18	43,43,43,43	0
57	MG	2A	3311	1/1	0.93	0.13	60,60,60,60	0
57	MG	1A	4089	1/1	0.93	0.12	58,58,58,58	0
57	MG	2A	3607	1/1	0.93	0.09	50,50,50,50	0
57	MG	1A	3496	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3498	1/1	0.93	0.09	44,44,44,44	0
57	MG	1A	4094	1/1	0.93	0.07	41,41,41,41	0
57	MG	1A	3919	1/1	0.93	0.09	48,48,48,48	0
57	MG	2I	103	1/1	0.93	0.08	51,51,51,51	0
57	MG	2A	3319	1/1	0.93	0.22	68,68,68,68	0
57	MG	1A	3770	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3616	1/1	0.93	0.12	44,44,44,44	0
57	MG	25	105	1/1	0.93	0.10	48,48,48,48	0
57	MG	2A	3617	1/1	0.93	0.13	58,58,58,58	0
57	MG	2A	3083	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3199	1/1	0.93	0.06	42,42,42,42	0
57	MG	2A	3323	1/1	0.93	0.11	53,53,53,53	0
57	MG	1A	3302	1/1	0.93	0.09	63,63,63,63	0
57	MG	1A	4102	1/1	0.93	0.08	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3248	1/1	0.93	0.07	59,59,59,59	0
57	MG	1A	3366	1/1	0.93	0.14	45,45,45,45	0
57	MG	1A	3507	1/1	0.93	0.25	43,43,43,43	0
57	MG	1A	3941	1/1	0.93	0.07	56,56,56,56	0
57	MG	2a	3006	1/1	0.93	0.08	64,64,64,64	0
57	MG	2A	3633	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3204	1/1	0.93	0.17	53,53,53,53	0
57	MG	1A	3793	1/1	0.93	0.06	49,49,49,49	0
57	MG	2a	3010	1/1	0.93	0.22	60,60,60,60	0
57	MG	1A	3440	1/1	0.93	0.16	63,63,63,63	0
57	MG	2A	3637	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3639	1/1	0.93	0.07	27,27,27,27	0
57	MG	1a	1690	1/1	0.93	0.22	57,57,57,57	0
57	MG	1A	3512	1/1	0.93	0.13	61,61,61,61	0
57	MG	1A	3806	1/1	0.93	0.14	42,42,42,42	0
57	MG	1A	3513	1/1	0.93	0.11	43,43,43,43	0
57	MG	2A	3344	1/1	0.93	0.18	63,63,63,63	0
57	MG	2A	3345	1/1	0.93	0.13	63,63,63,63	0
57	MG	2A	3111	1/1	0.93	0.25	58,58,58,58	0
57	MG	1A	3811	1/1	0.93	0.09	51,51,51,51	0
57	MG	1a	1699	1/1	0.93	0.29	56,56,56,56	0
57	MG	1A	3647	1/1	0.93	0.07	35,35,35,35	0
57	MG	2A	3350	1/1	0.93	0.07	61,61,61,61	0
57	MG	1B	222	1/1	0.93	0.10	53,53,53,53	0
57	MG	2A	3120	1/1	0.93	0.07	48,48,48,48	0
57	MG	2A	3353	1/1	0.93	0.16	58,58,58,58	0
57	MG	1a	1704	1/1	0.93	0.21	48,48,48,48	0
57	MG	1A	3441	1/1	0.93	0.17	33,33,33,33	0
57	MG	2A	3356	1/1	0.93	0.29	61,61,61,61	0
57	MG	1A	3966	1/1	0.93	0.07	52,52,52,52	0
57	MG	1A	3655	1/1	0.93	0.06	18,18,18,18	0
57	MG	1B	226	1/1	0.93	0.08	42,42,42,42	0
57	MG	1A	3162	1/1	0.93	0.24	32,32,32,32	0
57	MG	1a	1717	1/1	0.93	0.11	56,56,56,56	0
57	MG	2A	3141	1/1	0.93	0.29	72,72,72,72	0
57	MG	2A	3365	1/1	0.93	0.29	64,64,64,64	0
57	MG	2A	3678	1/1	0.93	0.12	56,56,56,56	0
57	MG	1A	3164	1/1	0.93	0.17	33,33,33,33	0
57	MG	1A	3519	1/1	0.93	0.08	47,47,47,47	0
57	MG	2A	3368	1/1	0.93	0.08	53,53,53,53	0
57	MG	1A	3375	1/1	0.93	0.11	35,35,35,35	0
57	MG	1B	235	1/1	0.93	0.08	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3151	1/1	0.93	0.10	49,49,49,49	0
57	MG	1a	1727	1/1	0.93	0.12	54,54,54,54	0
57	MG	1D	309	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3118	1/1	0.93	0.15	41,41,41,41	0
57	MG	1A	3527	1/1	0.93	0.14	38,38,38,38	0
57	MG	1A	3978	1/1	0.93	0.15	60,60,60,60	0
57	MG	2a	3055	1/1	0.93	0.11	58,58,58,58	0
57	MG	2A	3167	1/1	0.93	0.13	66,66,66,66	0
57	MG	1A	3322	1/1	0.93	0.08	46,46,46,46	0
57	MG	2a	3061	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3119	1/1	0.93	0.11	53,53,53,53	0
57	MG	1E	314	1/1	0.93	0.08	39,39,39,39	0
57	MG	2A	3175	1/1	0.93	0.24	65,65,65,65	0
57	MG	2A	3388	1/1	0.93	0.23	46,46,46,46	0
57	MG	2A	3389	1/1	0.93	0.16	38,38,38,38	0
57	MG	2A	3390	1/1	0.93	0.20	44,44,44,44	0
57	MG	2a	3074	1/1	0.93	0.22	50,50,50,50	0
57	MG	2a	3075	1/1	0.93	0.21	61,61,61,61	0
57	MG	1A	3832	1/1	0.93	0.10	39,39,39,39	0
57	MG	2A	3177	1/1	0.93	0.22	56,56,56,56	0
57	MG	1A	3384	1/1	0.93	0.45	42,42,42,42	0
57	MG	1A	3532	1/1	0.93	0.29	51,51,51,51	0
57	MG	1a	1750	1/1	0.93	0.17	61,61,61,61	0
57	MG	1G	202	1/1	0.93	0.17	59,59,59,59	0
57	MG	1a	1756	1/1	0.93	0.15	51,51,51,51	0
57	MG	1A	3087	1/1	0.93	0.16	45,45,45,45	0
57	MG	1A	3989	1/1	0.93	0.13	38,38,38,38	0
57	MG	2a	3090	1/1	0.93	0.10	57,57,57,57	0
57	MG	1A	3841	1/1	0.93	0.13	51,51,51,51	0
57	MG	2A	3190	1/1	0.93	0.13	59,59,59,59	0
57	MG	2A	3408	1/1	0.93	0.18	52,52,52,52	0
57	MG	1A	3842	1/1	0.93	0.11	63,63,63,63	0
57	MG	2A	3193	1/1	0.93	0.16	53,53,53,53	0
57	MG	2A	3726	1/1	0.93	0.09	53,53,53,53	0
57	MG	1N	206	1/1	0.93	0.15	44,44,44,44	0
57	MG	1O	201	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3414	1/1	0.93	0.12	66,66,66,66	0
57	MG	1A	3993	1/1	0.93	0.07	13,13,13,13	0
57	MG	2a	3103	1/1	0.93	0.17	69,69,69,69	0
57	MG	1a	1769	1/1	0.93	0.08	50,50,50,50	0
57	MG	2A	3733	1/1	0.93	0.10	40,40,40,40	0
57	MG	1A	3997	1/1	0.93	0.07	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3735	1/1	0.93	0.16	62,62,62,62	0
57	MG	1R	205	1/1	0.93	0.16	32,32,32,32	0
57	MG	2A	3737	1/1	0.93	0.07	55,55,55,55	0
57	MG	1a	1773	1/1	0.93	0.10	47,47,47,47	0
57	MG	2A	3422	1/1	0.93	0.21	51,51,51,51	0
57	MG	1A	3454	1/1	0.93	0.12	59,59,59,59	0
57	MG	1A	3223	1/1	0.93	0.16	61,61,61,61	0
57	MG	2A	3752	1/1	0.93	0.14	67,67,67,67	0
57	MG	2A	3425	1/1	0.93	0.14	55,55,55,55	0
57	MG	1A	3227	1/1	0.93	0.08	48,48,48,48	0
57	MG	1A	3461	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3209	1/1	0.93	0.26	74,74,74,74	0
57	MG	1A	3539	1/1	0.93	0.08	53,53,53,53	0
57	MG	1A	3851	1/1	0.93	0.08	46,46,46,46	0
57	MG	1Z	302	1/1	0.93	0.08	62,62,62,62	0
57	MG	2A	3215	1/1	0.93	0.16	57,57,57,57	0
57	MG	1A	3335	1/1	0.93	0.14	57,57,57,57	0
57	MG	1a	1802	1/1	0.93	0.15	58,58,58,58	0
57	MG	2A	3449	1/1	0.93	0.16	62,62,62,62	0
57	MG	1A	3541	1/1	0.93	0.16	35,35,35,35	0
57	MG	1A	3543	1/1	0.93	0.10	42,42,42,42	0
57	MG	1A	3546	1/1	0.93	0.11	35,35,35,35	0
57	MG	1A	3268	1/1	0.93	0.11	52,52,52,52	0
57	MG	1a	1808	1/1	0.93	0.11	60,60,60,60	0
57	MG	1A	4017	1/1	0.93	0.07	58,58,58,58	0
57	MG	2A	3229	1/1	0.93	0.29	47,47,47,47	0
57	MG	2A	3230	1/1	0.93	0.12	58,58,58,58	0
57	MG	2A	3463	1/1	0.93	0.08	53,53,53,53	0
57	MG	2A	3784	1/1	0.93	0.16	46,46,46,46	0
57	MG	1A	3549	1/1	0.93	0.20	40,40,40,40	0
57	MG	2A	3233	1/1	0.93	0.08	67,67,67,67	0
57	MG	13	103	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3270	1/1	0.93	0.07	38,38,38,38	0
57	MG	1A	4020	1/1	0.93	0.09	51,51,51,51	0
57	MG	2A	3799	1/1	0.93	0.07	44,44,44,44	0
57	MG	2a	3178	1/1	0.93	0.14	60,60,60,60	0
57	MG	1A	3276	1/1	0.93	0.29	34,34,34,34	0
57	MG	1A	3864	1/1	0.93	0.05	38,38,38,38	0
57	MG	16	102	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	3006	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	4028	1/1	0.93	0.06	41,41,41,41	0
57	MG	2A	3482	1/1	0.93	0.10	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3809	1/1	0.93	0.08	50,50,50,50	0
57	MG	1A	3866	1/1	0.93	0.19	36,36,36,36	0
57	MG	2a	3188	1/1	0.93	0.23	54,54,54,54	0
57	MG	1A	3469	1/1	0.93	0.13	51,51,51,51	0
57	MG	2A	3813	1/1	0.93	0.06	33,33,33,33	0
57	MG	1A	3140	1/1	0.93	0.09	35,35,35,35	0
57	MG	1A	3560	1/1	0.93	0.14	50,50,50,50	0
57	MG	1A	3562	1/1	0.93	0.22	52,52,52,52	0
57	MG	2a	3195	1/1	0.93	0.11	62,62,62,62	0
57	MG	2A	3252	1/1	0.93	0.09	52,52,52,52	0
57	MG	1w	101	1/1	0.93	0.12	43,43,43,43	0
57	MG	2a	3199	1/1	0.93	0.08	59,59,59,59	0
57	MG	1A	3403	1/1	0.93	0.10	50,50,50,50	0
57	MG	2A	3498	1/1	0.93	0.07	39,39,39,39	0
57	MG	2A	3827	1/1	0.93	0.16	60,60,60,60	0
57	MG	2a	3203	1/1	0.93	0.19	51,51,51,51	0
57	MG	2A	3256	1/1	0.93	0.10	55,55,55,55	0
57	MG	1A	3570	1/1	0.93	0.21	33,33,33,33	0
57	MG	1A	3345	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3232	1/1	0.93	0.15	25,25,25,25	0
57	MG	1A	3057	1/1	0.93	0.09	45,45,45,45	0
57	MG	1A	4048	1/1	0.93	0.09	44,44,44,44	0
57	MG	2A	3262	1/1	0.93	0.12	52,52,52,52	0
57	MG	2A	3835	1/1	0.93	0.08	56,56,56,56	0
57	MG	1A	3882	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3513	1/1	0.93	0.05	44,44,44,44	0
57	MG	1a	1618	1/1	0.93	0.10	56,56,56,56	0
57	MG	1A	3110	1/1	0.93	0.11	39,39,39,39	0
57	MG	1a	1621	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	3480	1/1	0.93	0.09	53,53,53,53	0
57	MG	1A	4054	1/1	0.93	0.07	40,40,40,40	0
57	MG	1A	3485	1/1	0.93	0.11	53,53,53,53	0
57	MG	1A	3412	1/1	0.93	0.21	58,58,58,58	0
57	MG	2A	3001	1/1	0.93	0.22	54,54,54,54	0
57	MG	1A	4062	1/1	0.93	0.11	59,59,59,59	0
57	MG	1a	1632	1/1	0.93	0.15	62,62,62,62	0
57	MG	1A	3887	1/1	0.93	0.07	15,15,15,15	0
57	MG	1a	1637	1/1	0.93	0.19	55,55,55,55	0
57	MG	1A	3750	1/1	0.93	0.10	49,49,49,49	0
57	MG	1A	3487	1/1	0.93	0.17	55,55,55,55	0
57	MG	2a	3236	1/1	0.93	0.18	70,70,70,70	0
57	MG	2A	3551	1/1	0.93	0.07	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2d	302	1/1	0.93	0.14	66,66,66,66	0
57	MG	2f	202	1/1	0.93	0.15	62,62,62,62	0
57	MG	2A	3554	1/1	0.93	0.17	55,55,55,55	0
57	MG	2A	3029	1/1	0.93	0.21	54,54,54,54	0
57	MG	1a	1640	1/1	0.93	0.17	58,58,58,58	0
57	MG	2A	3561	1/1	0.93	0.07	45,45,45,45	0
57	MG	1A	4069	1/1	0.93	0.10	30,30,30,30	0
57	MG	1A	3598	1/1	0.93	0.10	26,26,26,26	0
57	MG	2A	3037	1/1	0.93	0.23	57,57,57,57	0
57	MG	1a	1645	1/1	0.93	0.27	61,61,61,61	0
57	MG	2B	207	1/1	0.93	0.10	63,63,63,63	0
57	MG	2B	208	1/1	0.93	0.29	61,61,61,61	0
57	MG	1A	3490	1/1	0.93	0.19	46,46,46,46	0
57	MG	2A	3571	1/1	0.93	0.23	72,72,72,72	0
57	MG	2A	3040	1/1	0.93	0.10	60,60,60,60	0
57	MG	2w	104	1/1	0.93	0.23	51,51,51,51	0
57	MG	2w	105	1/1	0.93	0.14	62,62,62,62	0
57	MG	1A	3899	1/1	0.93	0.11	55,55,55,55	0
57	MG	2A	3047	1/1	0.93	0.09	48,48,48,48	0
57	MG	1A	4077	1/1	0.93	0.07	45,45,45,45	0
57	MG	2B	216	1/1	0.93	0.16	60,60,60,60	0
57	MG	2x	105	1/1	0.93	0.17	60,60,60,60	0
57	MG	1a	1653	1/1	0.93	0.25	55,55,55,55	0
57	MG	1A	3245	1/1	0.93	0.21	39,39,39,39	0
57	MG	2D	301	1/1	0.93	0.15	47,47,47,47	0
57	MG	1A	3902	1/1	0.93	0.13	52,52,52,52	0
57	MG	1a	1656	1/1	0.93	0.11	48,48,48,48	0
57	MG	1A	3606	1/1	0.93	0.09	42,42,42,42	0
57	MG	2E	305	1/1	0.93	0.11	33,33,33,33	0
57	MG	1A	4029	1/1	0.94	0.07	46,46,46,46	0
57	MG	2A	3127	1/1	0.94	0.08	53,53,53,53	0
57	MG	1X	106	1/1	0.94	0.15	46,46,46,46	0
57	MG	2A	3130	1/1	0.94	0.07	42,42,42,42	0
57	MG	1X	108	1/1	0.94	0.13	69,69,69,69	0
57	MG	2T	201	1/1	0.94	0.10	63,63,63,63	0
57	MG	1A	3757	1/1	0.94	0.06	25,25,25,25	0
57	MG	1A	3041	1/1	0.94	0.07	30,30,30,30	0
57	MG	2A	3622	1/1	0.94	0.11	54,54,54,54	0
57	MG	2A	3623	1/1	0.94	0.20	50,50,50,50	0
57	MG	1A	3338	1/1	0.94	0.17	34,34,34,34	0
57	MG	2A	3140	1/1	0.94	0.22	49,49,49,49	0
57	MG	2Y	201	1/1	0.94	0.19	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3626	1/1	0.94	0.13	49,49,49,49	0
57	MG	20	102	1/1	0.94	0.15	70,70,70,70	0
57	MG	21	101	1/1	0.94	0.07	59,59,59,59	0
57	MG	1a	1753	1/1	0.94	0.07	58,58,58,58	0
57	MG	1a	1755	1/1	0.94	0.10	53,53,53,53	0
57	MG	1A	3076	1/1	0.94	0.16	45,45,45,45	0
57	MG	2A	3145	1/1	0.94	0.20	52,52,52,52	0
57	MG	1A	4034	1/1	0.94	0.07	35,35,35,35	0
57	MG	1A	3281	1/1	0.94	0.17	40,40,40,40	0
57	MG	1A	3230	1/1	0.94	0.26	48,48,48,48	0
57	MG	2A	3152	1/1	0.94	0.10	35,35,35,35	0
57	MG	2A	3638	1/1	0.94	0.09	56,56,56,56	0
57	MG	10	108	1/1	0.94	0.09	47,47,47,47	0
57	MG	2A	3644	1/1	0.94	0.12	35,35,35,35	0
57	MG	10	109	1/1	0.94	0.08	41,41,41,41	0
57	MG	11	101	1/1	0.94	0.20	33,33,33,33	0
57	MG	2A	3161	1/1	0.94	0.27	61,61,61,61	0
57	MG	2A	3162	1/1	0.94	0.10	40,40,40,40	0
57	MG	1A	3417	1/1	0.94	0.14	37,37,37,37	0
57	MG	2A	3165	1/1	0.94	0.12	64,64,64,64	0
57	MG	1A	3418	1/1	0.94	0.09	43,43,43,43	0
57	MG	1A	3895	1/1	0.94	0.15	56,56,56,56	0
57	MG	1A	3034	1/1	0.94	0.27	34,34,34,34	0
57	MG	2A	3657	1/1	0.94	0.10	47,47,47,47	0
57	MG	2A	3171	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3287	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3776	1/1	0.94	0.10	26,26,26,26	0
57	MG	2A	3661	1/1	0.94	0.07	69,69,69,69	0
57	MG	1A	3780	1/1	0.94	0.04	32,32,32,32	0
57	MG	1a	1786	1/1	0.94	0.10	71,71,71,71	0
57	MG	1A	3422	1/1	0.94	0.09	60,60,60,60	0
57	MG	1A	3097	1/1	0.94	0.11	50,50,50,50	0
57	MG	1A	3642	1/1	0.94	0.07	48,48,48,48	0
57	MG	1a	1795	1/1	0.94	0.09	48,48,48,48	0
57	MG	2A	3379	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	3240	1/1	0.94	0.09	42,42,42,42	0
57	MG	2A	3673	1/1	0.94	0.07	58,58,58,58	0
57	MG	1A	3128	1/1	0.94	0.09	37,37,37,37	0
57	MG	2A	3382	1/1	0.94	0.13	42,42,42,42	0
57	MG	1A	4064	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	4065	1/1	0.94	0.11	40,40,40,40	0
57	MG	1A	3912	1/1	0.94	0.07	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1602	1/1	0.94	0.06	58,58,58,58	0
57	MG	1A	3915	1/1	0.94	0.10	38,38,38,38	0
57	MG	1A	3350	1/1	0.94	0.10	44,44,44,44	0
57	MG	1a	1807	1/1	0.94	0.09	58,58,58,58	0
57	MG	1A	3652	1/1	0.94	0.07	27,27,27,27	0
57	MG	1A	3653	1/1	0.94	0.07	23,23,23,23	0
57	MG	1a	1812	1/1	0.94	0.21	59,59,59,59	0
57	MG	1A	3435	1/1	0.94	0.16	39,39,39,39	0
57	MG	2A	3199	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3400	1/1	0.94	0.24	46,46,46,46	0
57	MG	2A	3403	1/1	0.94	0.28	59,59,59,59	0
57	MG	1A	3924	1/1	0.94	0.07	37,37,37,37	0
57	MG	1a	1816	1/1	0.94	0.12	53,53,53,53	0
57	MG	1a	1611	1/1	0.94	0.15	44,44,44,44	0
57	MG	1A	3803	1/1	0.94	0.11	35,35,35,35	0
57	MG	1A	3078	1/1	0.94	0.06	24,24,24,24	0
57	MG	2a	3048	1/1	0.94	0.09	67,67,67,67	0
57	MG	1A	3807	1/1	0.94	0.13	51,51,51,51	0
57	MG	2A	3208	1/1	0.94	0.08	62,62,62,62	0
57	MG	1A	3352	1/1	0.94	0.12	54,54,54,54	0
57	MG	1A	3081	1/1	0.94	0.18	39,39,39,39	0
57	MG	2a	3053	1/1	0.94	0.16	58,58,58,58	0
57	MG	1A	3815	1/1	0.94	0.07	26,26,26,26	0
57	MG	2A	3212	1/1	0.94	0.15	44,44,44,44	0
57	MG	1A	3816	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3711	1/1	0.94	0.09	58,58,58,58	0
57	MG	2a	3059	1/1	0.94	0.22	58,58,58,58	0
57	MG	1A	3354	1/1	0.94	0.09	44,44,44,44	0
57	MG	1n	101	1/1	0.94	0.33	59,59,59,59	0
57	MG	2a	3066	1/1	0.94	0.28	71,71,71,71	0
57	MG	1n	102	1/1	0.94	0.15	46,46,46,46	0
57	MG	1a	1626	1/1	0.94	0.16	61,61,61,61	0
57	MG	1A	3661	1/1	0.94	0.07	18,18,18,18	0
57	MG	2a	3071	1/1	0.94	0.12	52,52,52,52	0
57	MG	1a	1629	1/1	0.94	0.12	49,49,49,49	0
57	MG	1A	3355	1/1	0.94	0.09	51,51,51,51	0
57	MG	1a	1631	1/1	0.94	0.18	54,54,54,54	0
57	MG	1A	3949	1/1	0.94	0.10	49,49,49,49	0
57	MG	2a	3076	1/1	0.94	0.14	60,60,60,60	0
57	MG	2A	3430	1/1	0.94	0.17	51,51,51,51	0
57	MG	2a	3078	1/1	0.94	0.20	47,47,47,47	0
57	MG	2A	3724	1/1	0.94	0.10	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3431	1/1	0.94	0.10	60,60,60,60	0
57	MG	2a	3082	1/1	0.94	0.27	52,52,52,52	0
57	MG	2A	3435	1/1	0.94	0.10	68,68,68,68	0
57	MG	2A	3436	1/1	0.94	0.22	63,63,63,63	0
57	MG	2A	3227	1/1	0.94	0.15	46,46,46,46	0
57	MG	2A	3439	1/1	0.94	0.14	42,42,42,42	0
57	MG	1A	3668	1/1	0.94	0.09	24,24,24,24	0
57	MG	2A	3732	1/1	0.94	0.10	33,33,33,33	0
57	MG	1A	3357	1/1	0.94	0.18	42,42,42,42	0
57	MG	2A	3231	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	3952	1/1	0.94	0.09	54,54,54,54	0
57	MG	1A	3824	1/1	0.94	0.07	47,47,47,47	0
57	MG	2A	3234	1/1	0.94	0.10	46,46,46,46	0
57	MG	1A	3191	1/1	0.94	0.20	33,33,33,33	0
57	MG	2A	3237	1/1	0.94	0.18	44,44,44,44	0
57	MG	1x	102	1/1	0.94	0.22	55,55,55,55	0
57	MG	2A	3743	1/1	0.94	0.12	46,46,46,46	0
57	MG	2A	3746	1/1	0.94	0.07	56,56,56,56	0
57	MG	2A	3749	1/1	0.94	0.17	61,61,61,61	0
57	MG	1A	3956	1/1	0.94	0.08	53,53,53,53	0
57	MG	2A	3240	1/1	0.94	0.10	46,46,46,46	0
57	MG	1A	3362	1/1	0.94	0.24	36,36,36,36	0
57	MG	1A	4104	1/1	0.94	0.08	35,35,35,35	0
57	MG	1A	3959	1/1	0.94	0.10	37,37,37,37	0
57	MG	2a	3111	1/1	0.94	0.08	55,55,55,55	0
57	MG	1a	1647	1/1	0.94	0.20	52,52,52,52	0
57	MG	1x	110	1/1	0.94	0.10	23,23,23,23	0
57	MG	1A	3961	1/1	0.94	0.15	55,55,55,55	0
57	MG	1A	3298	1/1	0.94	0.32	55,55,55,55	0
57	MG	1x	113	1/1	0.94	0.07	53,53,53,53	0
57	MG	1A	3450	1/1	0.94	0.14	47,47,47,47	0
57	MG	2A	3002	1/1	0.94	0.19	54,54,54,54	0
57	MG	2A	3476	1/1	0.94	0.11	60,60,60,60	0
57	MG	1B	201	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3195	1/1	0.94	0.08	33,33,33,33	0
57	MG	2a	3128	1/1	0.94	0.09	70,70,70,70	0
57	MG	1A	3109	1/1	0.94	0.13	35,35,35,35	0
57	MG	1A	3303	1/1	0.94	0.09	56,56,56,56	0
57	MG	1A	3152	1/1	0.94	0.26	35,35,35,35	0
57	MG	1A	3251	1/1	0.94	0.07	49,49,49,49	0
57	MG	2A	3484	1/1	0.94	0.11	21,21,21,21	0
57	MG	2a	3146	1/1	0.94	0.10	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3778	1/1	0.94	0.10	64,64,64,64	0
57	MG	1A	3837	1/1	0.94	0.07	58,58,58,58	0
57	MG	1A	3838	1/1	0.94	0.14	54,54,54,54	0
57	MG	1a	1663	1/1	0.94	0.17	55,55,55,55	0
57	MG	1A	3307	1/1	0.94	0.26	58,58,58,58	0
57	MG	2A	3786	1/1	0.94	0.08	38,38,38,38	0
57	MG	2A	3787	1/1	0.94	0.10	51,51,51,51	0
57	MG	2A	3263	1/1	0.94	0.14	60,60,60,60	0
57	MG	2A	3789	1/1	0.94	0.10	37,37,37,37	0
57	MG	2A	3264	1/1	0.94	0.11	63,63,63,63	0
57	MG	1A	3374	1/1	0.94	0.09	63,63,63,63	0
57	MG	2A	3796	1/1	0.94	0.09	57,57,57,57	0
57	MG	1A	3308	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3798	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3309	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3501	1/1	0.94	0.09	54,54,54,54	0
57	MG	1A	3310	1/1	0.94	0.09	48,48,48,48	0
57	MG	2A	3042	1/1	0.94	0.11	43,43,43,43	0
57	MG	2a	3173	1/1	0.94	0.21	58,58,58,58	0
57	MG	1A	3986	1/1	0.94	0.10	48,48,48,48	0
57	MG	2a	3177	1/1	0.94	0.10	58,58,58,58	0
57	MG	1B	227	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3048	1/1	0.94	0.22	66,66,66,66	0
57	MG	1A	3153	1/1	0.94	0.11	40,40,40,40	0
57	MG	1A	3382	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3317	1/1	0.94	0.17	50,50,50,50	0
57	MG	1A	3471	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3514	1/1	0.94	0.08	36,36,36,36	0
57	MG	1B	233	1/1	0.94	0.14	65,65,65,65	0
57	MG	1A	3561	1/1	0.94	0.25	38,38,38,38	0
57	MG	2A	3056	1/1	0.94	0.16	56,56,56,56	0
57	MG	2A	3821	1/1	0.94	0.13	46,46,46,46	0
57	MG	1A	3855	1/1	0.94	0.12	52,52,52,52	0
57	MG	2A	3526	1/1	0.94	0.10	36,36,36,36	0
57	MG	2A	3527	1/1	0.94	0.12	39,39,39,39	0
57	MG	1A	3385	1/1	0.94	0.09	49,49,49,49	0
57	MG	1A	3390	1/1	0.94	0.21	34,34,34,34	0
57	MG	2A	3531	1/1	0.94	0.11	62,62,62,62	0
57	MG	2A	3535	1/1	0.94	0.09	32,32,32,32	0
57	MG	1E	308	1/1	0.94	0.06	47,47,47,47	0
57	MG	1A	3211	1/1	0.94	0.07	44,44,44,44	0
57	MG	2A	3541	1/1	0.94	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3059	1/1	0.94	0.07	36,36,36,36	0
57	MG	2A	3067	1/1	0.94	0.19	48,48,48,48	0
57	MG	1A	3577	1/1	0.94	0.15	50,50,50,50	0
57	MG	1A	4003	1/1	0.94	0.05	22,22,22,22	0
57	MG	1A	4004	1/1	0.94	0.10	34,34,34,34	0
57	MG	2a	3207	1/1	0.94	0.14	57,57,57,57	0
57	MG	1F	304	1/1	0.94	0.08	37,37,37,37	0
57	MG	2A	3841	1/1	0.94	0.10	36,36,36,36	0
57	MG	1a	1696	1/1	0.94	0.12	58,58,58,58	0
57	MG	2A	3552	1/1	0.94	0.08	51,51,51,51	0
57	MG	2A	3080	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3478	1/1	0.94	0.14	47,47,47,47	0
57	MG	1A	3216	1/1	0.94	0.09	44,44,44,44	0
57	MG	2A	3847	1/1	0.94	0.08	57,57,57,57	0
57	MG	2A	3848	1/1	0.94	0.10	52,52,52,52	0
57	MG	1A	3114	1/1	0.94	0.18	25,25,25,25	0
57	MG	2A	3085	1/1	0.94	0.09	48,48,48,48	0
57	MG	2a	3221	1/1	0.94	0.09	59,59,59,59	0
57	MG	1A	3482	1/1	0.94	0.19	49,49,49,49	0
57	MG	2A	3852	1/1	0.94	0.14	64,64,64,64	0
57	MG	2A	3567	1/1	0.94	0.08	47,47,47,47	0
57	MG	2A	3304	1/1	0.94	0.12	54,54,54,54	0
57	MG	2A	3087	1/1	0.94	0.11	59,59,59,59	0
57	MG	2A	3089	1/1	0.94	0.16	48,48,48,48	0
57	MG	1A	3397	1/1	0.94	0.11	43,43,43,43	0
57	MG	2A	3091	1/1	0.94	0.09	43,43,43,43	0
57	MG	2A	3309	1/1	0.94	0.20	57,57,57,57	0
57	MG	1A	3054	1/1	0.94	0.07	51,51,51,51	0
57	MG	1a	1710	1/1	0.94	0.38	62,62,62,62	0
57	MG	1I	201	1/1	0.94	0.07	61,61,61,61	0
57	MG	2d	301	1/1	0.94	0.08	61,61,61,61	0
57	MG	2A	3577	1/1	0.94	0.15	62,62,62,62	0
57	MG	1A	3329	1/1	0.94	0.10	51,51,51,51	0
57	MG	2B	205	1/1	0.94	0.17	59,59,59,59	0
57	MG	1A	3330	1/1	0.94	0.18	53,53,53,53	0
57	MG	2I	201	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3167	1/1	0.94	0.26	34,34,34,34	0
57	MG	2A	3317	1/1	0.94	0.26	49,49,49,49	0
57	MG	2A	3101	1/1	0.94	0.20	69,69,69,69	0
57	MG	1A	3333	1/1	0.94	0.12	45,45,45,45	0
57	MG	2B	211	1/1	0.94	0.19	60,60,60,60	0
57	MG	1A	3267	1/1	0.94	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1723	1/1	0.94	0.07	61,61,61,61	0
57	MG	1P	201	1/1	0.94	0.40	30,30,30,30	0
57	MG	1a	1725	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3590	1/1	0.94	0.11	44,44,44,44	0
57	MG	2B	217	1/1	0.94	0.16	63,63,63,63	0
57	MG	2A	3325	1/1	0.94	0.12	66,66,66,66	0
57	MG	1A	3608	1/1	0.94	0.05	30,30,30,30	0
57	MG	1A	3609	1/1	0.94	0.09	10,10,10,10	0
57	MG	1S	203	1/1	0.94	0.06	51,51,51,51	0
57	MG	2x	101	1/1	0.94	0.18	65,65,65,65	0
57	MG	1T	201	1/1	0.94	0.08	61,61,61,61	0
57	MG	2A	3601	1/1	0.94	0.10	51,51,51,51	0
57	MG	2x	104	1/1	0.94	0.07	44,44,44,44	0
57	MG	2E	304	1/1	0.94	0.11	42,42,42,42	0
57	MG	1A	3117	1/1	0.94	0.24	46,46,46,46	0
57	MG	2A	3118	1/1	0.94	0.19	54,54,54,54	0
57	MG	1U	204	1/1	0.94	0.28	48,48,48,48	0
57	MG	2A	3334	1/1	0.94	0.08	48,48,48,48	0
57	MG	1A	3756	1/1	0.94	0.07	41,41,41,41	0
57	MG	1V	205	1/1	0.94	0.23	56,56,56,56	0
57	MG	2A	3122	1/1	0.94	0.09	60,60,60,60	0
57	MG	2E	301	1/1	0.95	0.09	53,53,53,53	0
57	MG	2A	3014	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3300	1/1	0.95	0.06	45,45,45,45	0
57	MG	1A	3149	1/1	0.95	0.05	29,29,29,29	0
57	MG	1A	3099	1/1	0.95	0.08	50,50,50,50	0
57	MG	1a	1623	1/1	0.95	0.07	46,46,46,46	0
57	MG	2A	3022	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3229	1/1	0.95	0.12	43,43,43,43	0
57	MG	2F	304	1/1	0.95	0.07	42,42,42,42	0
57	MG	2A	3025	1/1	0.95	0.14	60,60,60,60	0
57	MG	2A	3027	1/1	0.95	0.10	55,55,55,55	0
57	MG	2A	3028	1/1	0.95	0.13	41,41,41,41	0
57	MG	1A	3370	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	3025	1/1	0.95	0.15	33,33,33,33	0
57	MG	2P	202	1/1	0.95	0.10	56,56,56,56	0
57	MG	2Q	202	1/1	0.95	0.16	48,48,48,48	0
57	MG	1a	1627	1/1	0.95	0.17	52,52,52,52	0
57	MG	1A	4071	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3891	1/1	0.95	0.09	47,47,47,47	0
57	MG	2A	3592	1/1	0.95	0.08	37,37,37,37	0
57	MG	1A	3737	1/1	0.95	0.08	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3563	1/1	0.95	0.10	35,35,35,35	0
57	MG	2A	3596	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3739	1/1	0.95	0.17	43,43,43,43	0
57	MG	2V	202	1/1	0.95	0.10	55,55,55,55	0
57	MG	1a	1634	1/1	0.95	0.20	49,49,49,49	0
57	MG	2W	202	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3305	1/1	0.95	0.25	49,49,49,49	0
57	MG	2A	3602	1/1	0.95	0.12	60,60,60,60	0
57	MG	1A	3154	1/1	0.95	0.14	43,43,43,43	0
57	MG	20	101	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3744	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3156	1/1	0.95	0.12	27,27,27,27	0
57	MG	1A	3103	1/1	0.95	0.07	26,26,26,26	0
57	MG	1A	3749	1/1	0.95	0.12	52,52,52,52	0
57	MG	1a	1642	1/1	0.95	0.21	57,57,57,57	0
57	MG	1A	3578	1/1	0.95	0.12	39,39,39,39	0
57	MG	1A	3580	1/1	0.95	0.16	33,33,33,33	0
57	MG	25	104	1/1	0.95	0.14	53,53,53,53	0
57	MG	2A	3313	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3161	1/1	0.95	0.17	36,36,36,36	0
57	MG	1A	3106	1/1	0.95	0.27	37,37,37,37	0
57	MG	1A	3913	1/1	0.95	0.09	68,68,68,68	0
57	MG	1a	1651	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	4095	1/1	0.95	0.06	56,56,56,56	0
57	MG	1A	3313	1/1	0.95	0.12	60,60,60,60	0
57	MG	1A	3315	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	4098	1/1	0.95	0.11	66,66,66,66	0
57	MG	1A	3587	1/1	0.95	0.19	50,50,50,50	0
57	MG	1A	3474	1/1	0.95	0.08	34,34,34,34	0
57	MG	2A	3071	1/1	0.95	0.08	44,44,44,44	0
57	MG	2A	3628	1/1	0.95	0.09	66,66,66,66	0
57	MG	1A	3388	1/1	0.95	0.19	30,30,30,30	0
57	MG	2A	3076	1/1	0.95	0.06	46,46,46,46	0
57	MG	2A	3328	1/1	0.95	0.22	68,68,68,68	0
57	MG	1a	1659	1/1	0.95	0.20	66,66,66,66	0
57	MG	1A	3590	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	3593	1/1	0.95	0.07	53,53,53,53	0
57	MG	1A	3108	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3596	1/1	0.95	0.06	37,37,37,37	0
57	MG	1A	3165	1/1	0.95	0.17	51,51,51,51	0
57	MG	2a	3017	1/1	0.95	0.10	63,63,63,63	0
57	MG	2A	3643	1/1	0.95	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3019	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3767	1/1	0.95	0.05	24,24,24,24	0
57	MG	1A	4109	1/1	0.95	0.26	56,56,56,56	0
57	MG	1A	3938	1/1	0.95	0.08	60,60,60,60	0
57	MG	2A	3647	1/1	0.95	0.13	61,61,61,61	0
57	MG	1A	3940	1/1	0.95	0.07	60,60,60,60	0
57	MG	1A	3599	1/1	0.95	0.06	39,39,39,39	0
57	MG	1B	208	1/1	0.95	0.14	59,59,59,59	0
57	MG	2A	3652	1/1	0.95	0.13	56,56,56,56	0
57	MG	2A	3092	1/1	0.95	0.07	56,56,56,56	0
57	MG	2a	3029	1/1	0.95	0.20	46,46,46,46	0
57	MG	1B	209	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3094	1/1	0.95	0.08	49,49,49,49	0
57	MG	1a	1672	1/1	0.95	0.15	55,55,55,55	0
57	MG	1B	211	1/1	0.95	0.13	48,48,48,48	0
57	MG	1B	212	1/1	0.95	0.15	60,60,60,60	0
57	MG	1A	3600	1/1	0.95	0.07	28,28,28,28	0
57	MG	1a	1680	1/1	0.95	0.32	59,59,59,59	0
57	MG	1A	3318	1/1	0.95	0.14	36,36,36,36	0
57	MG	1A	3029	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3781	1/1	0.95	0.06	47,47,47,47	0
57	MG	2A	3104	1/1	0.95	0.13	42,42,42,42	0
57	MG	1A	3394	1/1	0.95	0.06	46,46,46,46	0
57	MG	1a	1686	1/1	0.95	0.22	57,57,57,57	0
57	MG	1A	3607	1/1	0.95	0.08	24,24,24,24	0
57	MG	2A	3109	1/1	0.95	0.25	67,67,67,67	0
57	MG	1A	3786	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3481	1/1	0.95	0.10	57,57,57,57	0
57	MG	2A	3112	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3033	1/1	0.95	0.40	33,33,33,33	0
57	MG	2A	3364	1/1	0.95	0.09	58,58,58,58	0
57	MG	1A	3611	1/1	0.95	0.05	24,24,24,24	0
57	MG	2A	3116	1/1	0.95	0.11	41,41,41,41	0
57	MG	1A	3484	1/1	0.95	0.06	41,41,41,41	0
57	MG	1A	3613	1/1	0.95	0.11	28,28,28,28	0
57	MG	1A	3614	1/1	0.95	0.06	30,30,30,30	0
57	MG	1A	3615	1/1	0.95	0.08	29,29,29,29	0
57	MG	1a	1697	1/1	0.95	0.22	60,60,60,60	0
57	MG	1a	1698	1/1	0.95	0.06	50,50,50,50	0
57	MG	2A	3373	1/1	0.95	0.24	49,49,49,49	0
57	MG	2a	3060	1/1	0.95	0.16	56,56,56,56	0
57	MG	1A	3962	1/1	0.95	0.15	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3125	1/1	0.95	0.11	41,41,41,41	0
57	MG	2A	3126	1/1	0.95	0.17	45,45,45,45	0
57	MG	1A	3396	1/1	0.95	0.09	44,44,44,44	0
57	MG	2A	3693	1/1	0.95	0.15	57,57,57,57	0
57	MG	1a	1702	1/1	0.95	0.06	43,43,43,43	0
57	MG	2A	3129	1/1	0.95	0.04	37,37,37,37	0
57	MG	1A	3624	1/1	0.95	0.07	22,22,22,22	0
57	MG	1B	234	1/1	0.95	0.11	57,57,57,57	0
57	MG	2A	3133	1/1	0.95	0.14	40,40,40,40	0
57	MG	1a	1705	1/1	0.95	0.12	35,35,35,35	0
57	MG	1a	1707	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	3967	1/1	0.95	0.07	68,68,68,68	0
57	MG	1B	236	1/1	0.95	0.07	41,41,41,41	0
57	MG	1A	3968	1/1	0.95	0.09	66,66,66,66	0
57	MG	2A	3707	1/1	0.95	0.10	50,50,50,50	0
57	MG	2A	3708	1/1	0.95	0.13	53,53,53,53	0
57	MG	1A	3249	1/1	0.95	0.19	42,42,42,42	0
57	MG	1a	1713	1/1	0.95	0.15	51,51,51,51	0
57	MG	1A	3112	1/1	0.95	0.17	35,35,35,35	0
57	MG	1E	307	1/1	0.95	0.08	48,48,48,48	0
57	MG	2A	3395	1/1	0.95	0.21	48,48,48,48	0
57	MG	2A	3147	1/1	0.95	0.20	51,51,51,51	0
57	MG	2A	3397	1/1	0.95	0.19	33,33,33,33	0
57	MG	1A	3324	1/1	0.95	0.13	48,48,48,48	0
57	MG	2A	3149	1/1	0.95	0.09	55,55,55,55	0
57	MG	2A	3719	1/1	0.95	0.12	57,57,57,57	0
57	MG	2A	3150	1/1	0.95	0.11	53,53,53,53	0
57	MG	2A	3402	1/1	0.95	0.20	47,47,47,47	0
57	MG	1a	1718	1/1	0.95	0.06	52,52,52,52	0
57	MG	1A	3812	1/1	0.95	0.07	38,38,38,38	0
57	MG	2A	3153	1/1	0.95	0.13	52,52,52,52	0
57	MG	2A	3725	1/1	0.95	0.21	62,62,62,62	0
57	MG	1A	3813	1/1	0.95	0.06	23,23,23,23	0
57	MG	1E	312	1/1	0.95	0.14	33,33,33,33	0
57	MG	2a	3104	1/1	0.95	0.15	67,67,67,67	0
57	MG	2a	3105	1/1	0.95	0.22	56,56,56,56	0
57	MG	1A	3058	1/1	0.95	0.06	29,29,29,29	0
57	MG	1A	3327	1/1	0.95	0.12	46,46,46,46	0
57	MG	2a	3108	1/1	0.95	0.13	52,52,52,52	0
57	MG	1F	302	1/1	0.95	0.19	32,32,32,32	0
57	MG	2A	3163	1/1	0.95	0.12	44,44,44,44	0
57	MG	1A	3084	1/1	0.95	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3113	1/1	0.95	0.28	65,65,65,65	0
57	MG	2a	3114	1/1	0.95	0.19	49,49,49,49	0
57	MG	1A	3253	1/1	0.95	0.10	31,31,31,31	0
57	MG	1a	1731	1/1	0.95	0.12	54,54,54,54	0
57	MG	2a	3117	1/1	0.95	0.21	55,55,55,55	0
57	MG	1F	309	1/1	0.95	0.08	48,48,48,48	0
57	MG	2A	3418	1/1	0.95	0.17	42,42,42,42	0
57	MG	1A	3497	1/1	0.95	0.08	40,40,40,40	0
57	MG	2A	3170	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3255	1/1	0.95	0.12	44,44,44,44	0
57	MG	1F	313	1/1	0.95	0.15	53,53,53,53	0
57	MG	2a	3124	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	3822	1/1	0.95	0.18	43,43,43,43	0
57	MG	2a	3126	1/1	0.95	0.09	61,61,61,61	0
57	MG	1A	3086	1/1	0.95	0.10	38,38,38,38	0
57	MG	1A	3043	1/1	0.95	0.23	34,34,34,34	0
57	MG	2A	3750	1/1	0.95	0.08	64,64,64,64	0
57	MG	1A	3409	1/1	0.95	0.07	53,53,53,53	0
57	MG	2a	3133	1/1	0.95	0.13	60,60,60,60	0
57	MG	2a	3134	1/1	0.95	0.11	59,59,59,59	0
57	MG	2a	3136	1/1	0.95	0.10	71,71,71,71	0
57	MG	2A	3428	1/1	0.95	0.09	54,54,54,54	0
57	MG	2A	3179	1/1	0.95	0.13	44,44,44,44	0
57	MG	2A	3755	1/1	0.95	0.06	42,42,42,42	0
57	MG	1A	3645	1/1	0.95	0.09	41,41,41,41	0
57	MG	1a	1749	1/1	0.95	0.10	58,58,58,58	0
57	MG	2a	3149	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3410	1/1	0.95	0.11	47,47,47,47	0
57	MG	1N	202	1/1	0.95	0.18	42,42,42,42	0
57	MG	1N	203	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3088	1/1	0.95	0.10	40,40,40,40	0
57	MG	1A	3259	1/1	0.95	0.17	56,56,56,56	0
57	MG	2a	3157	1/1	0.95	0.14	53,53,53,53	0
57	MG	1a	1758	1/1	0.95	0.06	60,60,60,60	0
57	MG	1A	3509	1/1	0.95	0.18	36,36,36,36	0
57	MG	2a	3160	1/1	0.95	0.12	46,46,46,46	0
57	MG	2a	3161	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3413	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3833	1/1	0.95	0.06	35,35,35,35	0
57	MG	1P	203	1/1	0.95	0.13	37,37,37,37	0
57	MG	1Q	203	1/1	0.95	0.11	60,60,60,60	0
57	MG	1a	1764	1/1	0.95	0.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3167	1/1	0.95	0.20	49,49,49,49	0
57	MG	1R	202	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3120	1/1	0.95	0.16	37,37,37,37	0
57	MG	1A	4001	1/1	0.95	0.05	30,30,30,30	0
57	MG	1A	3060	1/1	0.95	0.20	56,56,56,56	0
57	MG	1A	3049	1/1	0.95	0.05	13,13,13,13	0
57	MG	1A	3265	1/1	0.95	0.20	48,48,48,48	0
57	MG	2A	3460	1/1	0.95	0.08	46,46,46,46	0
57	MG	1U	202	1/1	0.95	0.17	38,38,38,38	0
57	MG	1A	3839	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3516	1/1	0.95	0.14	70,70,70,70	0
57	MG	2a	3180	1/1	0.95	0.09	62,62,62,62	0
57	MG	2A	3465	1/1	0.95	0.22	52,52,52,52	0
57	MG	2A	3466	1/1	0.95	0.36	63,63,63,63	0
57	MG	1A	3198	1/1	0.95	0.11	31,31,31,31	0
57	MG	2A	3469	1/1	0.95	0.08	51,51,51,51	0
57	MG	1A	3126	1/1	0.95	0.11	66,66,66,66	0
57	MG	1V	208	1/1	0.95	0.11	46,46,46,46	0
57	MG	2A	3474	1/1	0.95	0.09	54,54,54,54	0
57	MG	1a	1794	1/1	0.95	0.06	59,59,59,59	0
57	MG	1W	202	1/1	0.95	0.09	44,44,44,44	0
57	MG	1a	1796	1/1	0.95	0.17	59,59,59,59	0
57	MG	1a	1797	1/1	0.95	0.19	62,62,62,62	0
57	MG	1W	204	1/1	0.95	0.09	34,34,34,34	0
57	MG	2A	3217	1/1	0.95	0.23	57,57,57,57	0
57	MG	1W	205	1/1	0.95	0.15	22,22,22,22	0
57	MG	1a	1800	1/1	0.95	0.11	58,58,58,58	0
57	MG	1A	4011	1/1	0.95	0.05	50,50,50,50	0
57	MG	2A	3221	1/1	0.95	0.16	37,37,37,37	0
57	MG	2A	3222	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3346	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3524	1/1	0.95	0.24	37,37,37,37	0
57	MG	1Y	202	1/1	0.95	0.23	52,52,52,52	0
57	MG	1A	3202	1/1	0.95	0.23	48,48,48,48	0
57	MG	1A	3203	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3427	1/1	0.95	0.07	40,40,40,40	0
57	MG	2A	3823	1/1	0.95	0.08	53,53,53,53	0
57	MG	2A	3497	1/1	0.95	0.06	42,42,42,42	0
57	MG	10	101	1/1	0.95	0.12	45,45,45,45	0
57	MG	1A	3428	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3429	1/1	0.95	0.11	48,48,48,48	0
57	MG	10	105	1/1	0.95	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3854	1/1	0.95	0.09	43,43,43,43	0
57	MG	1A	4022	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3065	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3509	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	4025	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3533	1/1	0.95	0.16	51,51,51,51	0
57	MG	1A	3131	1/1	0.95	0.10	52,52,52,52	0
57	MG	2A	3241	1/1	0.95	0.21	57,57,57,57	0
57	MG	1e	202	1/1	0.95	0.16	51,51,51,51	0
57	MG	1A	3858	1/1	0.95	0.07	21,21,21,21	0
57	MG	1A	3206	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3286	1/1	0.95	0.12	53,53,53,53	0
57	MG	2A	3520	1/1	0.95	0.13	54,54,54,54	0
57	MG	1A	3691	1/1	0.95	0.08	24,24,24,24	0
57	MG	15	3202	1/1	0.95	0.19	34,34,34,34	0
57	MG	2a	3232	1/1	0.95	0.07	47,47,47,47	0
57	MG	2a	3233	1/1	0.95	0.10	43,43,43,43	0
57	MG	15	3203	1/1	0.95	0.22	43,43,43,43	0
57	MG	1A	3209	1/1	0.95	0.07	35,35,35,35	0
57	MG	2A	3529	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3135	1/1	0.95	0.17	44,44,44,44	0
57	MG	2a	3238	1/1	0.95	0.08	59,59,59,59	0
57	MG	15	3208	1/1	0.95	0.07	46,46,46,46	0
57	MG	2A	3533	1/1	0.95	0.08	34,34,34,34	0
57	MG	2e	201	1/1	0.95	0.09	63,63,63,63	0
57	MG	16	101	1/1	0.95	0.14	48,48,48,48	0
57	MG	1A	3698	1/1	0.95	0.08	28,28,28,28	0
57	MG	1A	3138	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3540	1/1	0.95	0.19	59,59,59,59	0
57	MG	2l	202	1/1	0.95	0.07	65,65,65,65	0
57	MG	1A	4039	1/1	0.95	0.05	45,45,45,45	0
57	MG	1A	4041	1/1	0.95	0.06	45,45,45,45	0
57	MG	1A	3444	1/1	0.95	0.18	51,51,51,51	0
57	MG	1A	3139	1/1	0.95	0.07	43,43,43,43	0
57	MG	2A	3545	1/1	0.95	0.11	42,42,42,42	0
57	MG	2A	3546	1/1	0.95	0.07	35,35,35,35	0
57	MG	1A	3094	1/1	0.95	0.17	36,36,36,36	0
57	MG	1A	3870	1/1	0.95	0.14	31,31,31,31	0
57	MG	1A	3447	1/1	0.95	0.08	48,48,48,48	0
57	MG	1A	3361	1/1	0.95	0.15	44,44,44,44	0
57	MG	1A	3711	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3144	1/1	0.95	0.19	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3555	1/1	0.95	0.14	55,55,55,55	0
57	MG	1A	3714	1/1	0.95	0.13	37,37,37,37	0
57	MG	1A	4055	1/1	0.95	0.10	58,58,58,58	0
57	MG	1x	109	1/1	0.95	0.23	59,59,59,59	0
57	MG	1A	4058	1/1	0.95	0.11	13,13,13,13	0
57	MG	1a	1612	1/1	0.95	0.31	64,64,64,64	0
57	MG	1A	3015	1/1	0.95	0.08	32,32,32,32	0
57	MG	1a	1615	1/1	0.95	0.08	57,57,57,57	0
57	MG	1a	1616	1/1	0.95	0.22	60,60,60,60	0
57	MG	1A	3053	1/1	0.95	0.10	45,45,45,45	0
57	MG	2A	3003	1/1	0.95	0.11	46,46,46,46	0
57	MG	2A	3004	1/1	0.95	0.12	51,51,51,51	0
57	MG	2A	3007	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3720	1/1	0.95	0.12	43,43,43,43	0
57	MG	2D	306	1/1	0.95	0.15	55,55,55,55	0
62	PHE	2w	108	11/12	0.95	0.11	36,39,42,44	0
57	MG	1A	3462	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	4074	1/1	0.96	0.13	49,49,49,49	0
57	MG	15	3206	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3127	1/1	0.96	0.12	38,38,38,38	0
57	MG	1A	4076	1/1	0.96	0.06	37,37,37,37	0
57	MG	28	101	1/1	0.96	0.28	53,53,53,53	0
57	MG	1A	3789	1/1	0.96	0.09	20,20,20,20	0
57	MG	2A	3386	1/1	0.96	0.15	37,37,37,37	0
57	MG	2a	3001	1/1	0.96	0.09	63,63,63,63	0
57	MG	2A	3387	1/1	0.96	0.15	48,48,48,48	0
57	MG	2A	3169	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3648	1/1	0.96	0.09	46,46,46,46	0
57	MG	17	101	1/1	0.96	0.11	34,34,34,34	0
57	MG	17	102	1/1	0.96	0.18	30,30,30,30	0
57	MG	2A	3662	1/1	0.96	0.07	32,32,32,32	0
57	MG	1A	3042	1/1	0.96	0.06	22,22,22,22	0
57	MG	1A	3299	1/1	0.96	0.24	54,54,54,54	0
57	MG	1A	4081	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3200	1/1	0.96	0.09	21,21,21,21	0
57	MG	1A	3794	1/1	0.96	0.05	43,43,43,43	0
57	MG	1a	1810	1/1	0.96	0.06	56,56,56,56	0
57	MG	2A	3181	1/1	0.96	0.07	48,48,48,48	0
57	MG	1a	1811	1/1	0.96	0.07	52,52,52,52	0
57	MG	2A	3183	1/1	0.96	0.11	42,42,42,42	0
57	MG	1A	3071	1/1	0.96	0.09	29,29,29,29	0
57	MG	1A	3797	1/1	0.96	0.04	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3132	1/1	0.96	0.08	26,26,26,26	0
57	MG	1A	3073	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3075	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3943	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3805	1/1	0.96	0.08	57,57,57,57	0
57	MG	2A	3409	1/1	0.96	0.19	53,53,53,53	0
57	MG	2A	3191	1/1	0.96	0.22	55,55,55,55	0
57	MG	1A	3004	1/1	0.96	0.05	23,23,23,23	0
57	MG	1A	3207	1/1	0.96	0.12	41,41,41,41	0
57	MG	1f	201	1/1	0.96	0.18	44,44,44,44	0
57	MG	1A	3808	1/1	0.96	0.12	23,23,23,23	0
57	MG	1A	3047	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	4100	1/1	0.96	0.10	63,63,63,63	0
57	MG	1A	3810	1/1	0.96	0.18	30,30,30,30	0
57	MG	1A	3669	1/1	0.96	0.04	19,19,19,19	0
57	MG	1A	3210	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3170	1/1	0.96	0.08	38,38,38,38	0
57	MG	1a	1620	1/1	0.96	0.09	43,43,43,43	0
57	MG	1A	3212	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3312	1/1	0.96	0.22	35,35,35,35	0
57	MG	1A	3175	1/1	0.96	0.11	21,21,21,21	0
57	MG	2A	3426	1/1	0.96	0.22	40,40,40,40	0
57	MG	1A	3215	1/1	0.96	0.11	29,29,29,29	0
57	MG	1w	103	1/1	0.96	0.07	60,60,60,60	0
57	MG	1A	3960	1/1	0.96	0.07	30,30,30,30	0
57	MG	1A	3261	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3483	1/1	0.96	0.13	42,42,42,42	0
57	MG	2A	3213	1/1	0.96	0.17	45,45,45,45	0
57	MG	1B	203	1/1	0.96	0.08	42,42,42,42	0
57	MG	1A	3963	1/1	0.96	0.09	43,43,43,43	0
57	MG	2A	3438	1/1	0.96	0.10	58,58,58,58	0
57	MG	1A	3684	1/1	0.96	0.07	19,19,19,19	0
57	MG	1A	3965	1/1	0.96	0.13	60,60,60,60	0
57	MG	2A	3441	1/1	0.96	0.11	38,38,38,38	0
57	MG	1B	210	1/1	0.96	0.12	48,48,48,48	0
57	MG	2A	3444	1/1	0.96	0.05	25,25,25,25	0
57	MG	1A	3176	1/1	0.96	0.06	34,34,34,34	0
57	MG	2a	3056	1/1	0.96	0.13	39,39,39,39	0
57	MG	1A	3572	1/1	0.96	0.14	61,61,61,61	0
57	MG	1A	3687	1/1	0.96	0.08	26,26,26,26	0
57	MG	1x	107	1/1	0.96	0.19	51,51,51,51	0
57	MG	1A	3826	1/1	0.96	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3048	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3079	1/1	0.96	0.13	39,39,39,39	0
57	MG	1B	218	1/1	0.96	0.15	41,41,41,41	0
57	MG	1B	219	1/1	0.96	0.06	40,40,40,40	0
57	MG	2a	3068	1/1	0.96	0.18	56,56,56,56	0
57	MG	2A	3454	1/1	0.96	0.10	45,45,45,45	0
57	MG	2A	3228	1/1	0.96	0.28	51,51,51,51	0
57	MG	2A	3456	1/1	0.96	0.15	55,55,55,55	0
57	MG	1a	1643	1/1	0.96	0.15	48,48,48,48	0
57	MG	1y	101	1/1	0.96	0.10	58,58,58,58	0
57	MG	2A	3459	1/1	0.96	0.08	38,38,38,38	0
57	MG	1A	3369	1/1	0.96	0.21	33,33,33,33	0
57	MG	1A	3692	1/1	0.96	0.08	21,21,21,21	0
57	MG	1A	3426	1/1	0.96	0.12	36,36,36,36	0
57	MG	1A	3976	1/1	0.96	0.07	49,49,49,49	0
57	MG	2A	3235	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	3694	1/1	0.96	0.09	29,29,29,29	0
57	MG	2A	3008	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3491	1/1	0.96	0.18	36,36,36,36	0
57	MG	2a	3084	1/1	0.96	0.19	34,34,34,34	0
57	MG	2A	3744	1/1	0.96	0.10	62,62,62,62	0
57	MG	2A	3013	1/1	0.96	0.16	40,40,40,40	0
57	MG	1A	3979	1/1	0.96	0.13	24,24,24,24	0
57	MG	2A	3015	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	3266	1/1	0.96	0.12	49,49,49,49	0
57	MG	1A	3371	1/1	0.96	0.08	44,44,44,44	0
57	MG	2A	3753	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3701	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3585	1/1	0.96	0.10	38,38,38,38	0
57	MG	2A	3021	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3080	1/1	0.96	0.12	30,30,30,30	0
57	MG	2a	3097	1/1	0.96	0.11	56,56,56,56	0
57	MG	1B	232	1/1	0.96	0.09	57,57,57,57	0
57	MG	1A	3495	1/1	0.96	0.09	55,55,55,55	0
57	MG	1A	3430	1/1	0.96	0.10	61,61,61,61	0
57	MG	1A	3706	1/1	0.96	0.05	62,62,62,62	0
57	MG	1A	3990	1/1	0.96	0.05	43,43,43,43	0
57	MG	2A	3030	1/1	0.96	0.10	44,44,44,44	0
57	MG	1D	302	1/1	0.96	0.28	49,49,49,49	0
57	MG	1D	303	1/1	0.96	0.16	36,36,36,36	0
57	MG	1D	305	1/1	0.96	0.04	32,32,32,32	0
57	MG	2A	3036	1/1	0.96	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3222	1/1	0.96	0.06	33,33,33,33	0
57	MG	1D	310	1/1	0.96	0.19	30,30,30,30	0
57	MG	1A	3708	1/1	0.96	0.05	13,13,13,13	0
57	MG	2A	3500	1/1	0.96	0.08	32,32,32,32	0
57	MG	2A	3775	1/1	0.96	0.05	45,45,45,45	0
57	MG	1E	302	1/1	0.96	0.07	44,44,44,44	0
57	MG	2A	3777	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3709	1/1	0.96	0.08	49,49,49,49	0
57	MG	2A	3043	1/1	0.96	0.18	53,53,53,53	0
57	MG	2A	3504	1/1	0.96	0.07	65,65,65,65	0
57	MG	2A	3044	1/1	0.96	0.13	42,42,42,42	0
57	MG	2A	3045	1/1	0.96	0.12	26,26,26,26	0
57	MG	2A	3267	1/1	0.96	0.11	55,55,55,55	0
57	MG	2A	3508	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3848	1/1	0.96	0.08	19,19,19,19	0
57	MG	1A	3432	1/1	0.96	0.12	36,36,36,36	0
57	MG	2A	3790	1/1	0.96	0.06	36,36,36,36	0
57	MG	1a	1673	1/1	0.96	0.11	43,43,43,43	0
57	MG	1A	3591	1/1	0.96	0.07	30,30,30,30	0
57	MG	2A	3795	1/1	0.96	0.05	65,65,65,65	0
57	MG	1A	3433	1/1	0.96	0.14	32,32,32,32	0
57	MG	2A	3051	1/1	0.96	0.06	38,38,38,38	0
57	MG	1a	1677	1/1	0.96	0.22	64,64,64,64	0
57	MG	1A	3716	1/1	0.96	0.09	50,50,50,50	0
57	MG	2A	3278	1/1	0.96	0.16	51,51,51,51	0
57	MG	1A	3500	1/1	0.96	0.10	24,24,24,24	0
57	MG	2a	3139	1/1	0.96	0.11	67,67,67,67	0
57	MG	2A	3523	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3595	1/1	0.96	0.07	21,21,21,21	0
57	MG	2a	3142	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3525	1/1	0.96	0.11	36,36,36,36	0
57	MG	2A	3807	1/1	0.96	0.06	21,21,21,21	0
57	MG	2a	3148	1/1	0.96	0.08	75,75,75,75	0
57	MG	1A	3434	1/1	0.96	0.16	46,46,46,46	0
57	MG	1a	1683	1/1	0.96	0.21	47,47,47,47	0
57	MG	2A	3059	1/1	0.96	0.13	64,64,64,64	0
57	MG	2a	3153	1/1	0.96	0.08	69,69,69,69	0
57	MG	1A	3723	1/1	0.96	0.05	37,37,37,37	0
57	MG	1A	4006	1/1	0.96	0.04	36,36,36,36	0
57	MG	1F	306	1/1	0.96	0.14	28,28,28,28	0
57	MG	2A	3532	1/1	0.96	0.08	58,58,58,58	0
57	MG	1A	3597	1/1	0.96	0.08	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3534	1/1	0.96	0.08	56,56,56,56	0
57	MG	1A	3063	1/1	0.96	0.20	52,52,52,52	0
57	MG	1A	3436	1/1	0.96	0.26	32,32,32,32	0
57	MG	2A	3538	1/1	0.96	0.08	46,46,46,46	0
57	MG	2A	3068	1/1	0.96	0.08	48,48,48,48	0
57	MG	2A	3825	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3291	1/1	0.96	0.20	73,73,73,73	0
57	MG	1A	3505	1/1	0.96	0.25	30,30,30,30	0
57	MG	1A	3437	1/1	0.96	0.11	40,40,40,40	0
57	MG	1A	3732	1/1	0.96	0.05	41,41,41,41	0
57	MG	1A	4014	1/1	0.96	0.09	50,50,50,50	0
57	MG	1a	1694	1/1	0.96	0.15	55,55,55,55	0
57	MG	1A	3733	1/1	0.96	0.06	47,47,47,47	0
57	MG	2A	3547	1/1	0.96	0.10	31,31,31,31	0
57	MG	1A	3438	1/1	0.96	0.16	34,34,34,34	0
57	MG	2A	3299	1/1	0.96	0.18	67,67,67,67	0
57	MG	2a	3175	1/1	0.96	0.10	68,68,68,68	0
57	MG	2a	3176	1/1	0.96	0.13	58,58,58,58	0
57	MG	1A	3603	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3867	1/1	0.96	0.20	33,33,33,33	0
57	MG	1A	3605	1/1	0.96	0.10	39,39,39,39	0
57	MG	2A	3553	1/1	0.96	0.13	55,55,55,55	0
57	MG	1N	205	1/1	0.96	0.16	45,45,45,45	0
57	MG	1A	3272	1/1	0.96	0.10	50,50,50,50	0
57	MG	2A	3556	1/1	0.96	0.11	60,60,60,60	0
57	MG	1N	207	1/1	0.96	0.13	50,50,50,50	0
57	MG	1A	3510	1/1	0.96	0.10	29,29,29,29	0
57	MG	1O	203	1/1	0.96	0.06	46,46,46,46	0
57	MG	1A	3742	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3326	1/1	0.96	0.15	42,42,42,42	0
57	MG	2A	3566	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3874	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3183	1/1	0.96	0.15	46,46,46,46	0
57	MG	1A	3381	1/1	0.96	0.07	26,26,26,26	0
57	MG	1Q	205	1/1	0.96	0.11	48,48,48,48	0
57	MG	1Q	206	1/1	0.96	0.14	43,43,43,43	0
57	MG	1A	3123	1/1	0.96	0.18	29,29,29,29	0
57	MG	1a	1716	1/1	0.96	0.07	50,50,50,50	0
57	MG	2a	3198	1/1	0.96	0.07	54,54,54,54	0
57	MG	2A	3099	1/1	0.96	0.05	26,26,26,26	0
57	MG	1A	3878	1/1	0.96	0.09	27,27,27,27	0
57	MG	1A	3282	1/1	0.96	0.18	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3187	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3387	1/1	0.96	0.21	48,48,48,48	0
57	MG	1A	3617	1/1	0.96	0.07	47,47,47,47	0
57	MG	2A	3580	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	3518	1/1	0.96	0.07	62,62,62,62	0
57	MG	2A	3324	1/1	0.96	0.11	50,50,50,50	0
57	MG	1U	203	1/1	0.96	0.17	31,31,31,31	0
57	MG	2A	3107	1/1	0.96	0.18	37,37,37,37	0
57	MG	2A	3585	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	4038	1/1	0.96	0.05	34,34,34,34	0
57	MG	2a	3212	1/1	0.96	0.20	54,54,54,54	0
57	MG	1U	206	1/1	0.96	0.26	34,34,34,34	0
57	MG	1U	207	1/1	0.96	0.27	32,32,32,32	0
57	MG	1A	3622	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	3284	1/1	0.96	0.11	40,40,40,40	0
57	MG	1V	206	1/1	0.96	0.06	29,29,29,29	0
57	MG	1A	4042	1/1	0.96	0.08	28,28,28,28	0
57	MG	2a	3219	1/1	0.96	0.11	57,57,57,57	0
57	MG	1A	3520	1/1	0.96	0.08	44,44,44,44	0
57	MG	2A	3335	1/1	0.96	0.21	48,48,48,48	0
57	MG	1W	201	1/1	0.96	0.17	45,45,45,45	0
57	MG	1A	3888	1/1	0.96	0.11	66,66,66,66	0
57	MG	1A	3889	1/1	0.96	0.04	33,33,33,33	0
57	MG	2D	302	1/1	0.96	0.21	55,55,55,55	0
57	MG	2A	3600	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3758	1/1	0.96	0.07	35,35,35,35	0
57	MG	1X	103	1/1	0.96	0.09	39,39,39,39	0
57	MG	1X	105	1/1	0.96	0.15	38,38,38,38	0
57	MG	2a	3230	1/1	0.96	0.07	68,68,68,68	0
57	MG	2a	3231	1/1	0.96	0.07	62,62,62,62	0
57	MG	2A	3606	1/1	0.96	0.06	35,35,35,35	0
57	MG	1A	3036	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	3629	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	3066	1/1	0.96	0.10	35,35,35,35	0
57	MG	2E	307	1/1	0.96	0.13	37,37,37,37	0
57	MG	2F	301	1/1	0.96	0.11	38,38,38,38	0
57	MG	1a	1754	1/1	0.96	0.11	48,48,48,48	0
57	MG	1A	3192	1/1	0.96	0.17	33,33,33,33	0
57	MG	1A	4052	1/1	0.96	0.04	31,31,31,31	0
57	MG	1a	1757	1/1	0.96	0.08	72,72,72,72	0
57	MG	2F	306	1/1	0.96	0.17	42,42,42,42	0
57	MG	2A	3131	1/1	0.96	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3526	1/1	0.96	0.21	43,43,43,43	0
57	MG	1A	3898	1/1	0.96	0.18	17,17,17,17	0
57	MG	1A	4057	1/1	0.96	0.10	45,45,45,45	0
57	MG	1A	3238	1/1	0.96	0.27	38,38,38,38	0
57	MG	2Q	201	1/1	0.96	0.10	51,51,51,51	0
57	MG	10	103	1/1	0.96	0.13	40,40,40,40	0
57	MG	2A	3139	1/1	0.96	0.08	40,40,40,40	0
57	MG	1A	3193	1/1	0.96	0.10	45,45,45,45	0
57	MG	1A	3341	1/1	0.96	0.10	40,40,40,40	0
57	MG	1a	1766	1/1	0.96	0.07	63,63,63,63	0
57	MG	1A	3903	1/1	0.96	0.06	38,38,38,38	0
57	MG	2T	203	1/1	0.96	0.14	48,48,48,48	0
57	MG	2T	204	1/1	0.96	0.07	65,65,65,65	0
57	MG	2A	3144	1/1	0.96	0.15	38,38,38,38	0
57	MG	1A	4063	1/1	0.96	0.05	38,38,38,38	0
57	MG	2A	3629	1/1	0.96	0.15	56,56,56,56	0
57	MG	1A	3769	1/1	0.96	0.10	54,54,54,54	0
57	MG	1A	3241	1/1	0.96	0.24	50,50,50,50	0
57	MG	1A	3771	1/1	0.96	0.06	27,27,27,27	0
57	MG	1A	3194	1/1	0.96	0.14	34,34,34,34	0
57	MG	11	104	1/1	0.96	0.07	34,34,34,34	0
57	MG	1A	3640	1/1	0.96	0.08	29,29,29,29	0
57	MG	12	102	1/1	0.96	0.06	41,41,41,41	0
57	MG	13	102	1/1	0.96	0.12	39,39,39,39	0
57	MG	2A	3154	1/1	0.96	0.12	60,60,60,60	0
57	MG	1A	3458	1/1	0.96	0.13	33,33,33,33	0
57	MG	1A	4070	1/1	0.96	0.05	31,31,31,31	0
57	MG	2A	3159	1/1	0.96	0.09	40,40,40,40	0
57	MG	1a	1793	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	3460	1/1	0.96	0.07	46,46,46,46	0
60	ZN	24	501	1/1	0.96	0.08	110,110,110,110	0
62	PHE	1w	109	11/12	0.96	0.09	17,21,26,26	0
57	MG	1A	3085	1/1	0.96	0.25	31,31,31,31	0
63	FME	2x	107	10/11	0.96	0.10	37,44,50,51	0
57	MG	1R	203	1/1	0.97	0.19	37,37,37,37	0
57	MG	1A	3213	1/1	0.97	0.12	31,31,31,31	0
57	MG	2A	3712	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	3466	1/1	0.97	0.08	54,54,54,54	0
57	MG	1A	4047	1/1	0.97	0.08	50,50,50,50	0
57	MG	2A	3057	1/1	0.97	0.09	49,49,49,49	0
57	MG	1A	3641	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3892	1/1	0.97	0.08	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3762	1/1	0.97	0.12	24,24,24,24	0
57	MG	1A	3052	1/1	0.97	0.13	23,23,23,23	0
57	MG	1A	3134	1/1	0.97	0.07	44,44,44,44	0
57	MG	1U	205	1/1	0.97	0.18	37,37,37,37	0
57	MG	1A	4053	1/1	0.97	0.03	19,19,19,19	0
57	MG	2A	3483	1/1	0.97	0.08	39,39,39,39	0
57	MG	2A	3270	1/1	0.97	0.15	56,56,56,56	0
57	MG	1a	1712	1/1	0.97	0.10	55,55,55,55	0
57	MG	2A	3486	1/1	0.97	0.11	40,40,40,40	0
57	MG	1A	3644	1/1	0.97	0.06	33,33,33,33	0
57	MG	1V	201	1/1	0.97	0.11	26,26,26,26	0
57	MG	1A	3332	1/1	0.97	0.06	34,34,34,34	0
57	MG	1V	203	1/1	0.97	0.25	35,35,35,35	0
57	MG	2A	3492	1/1	0.97	0.08	31,31,31,31	0
57	MG	2A	3074	1/1	0.97	0.13	28,28,28,28	0
57	MG	1V	204	1/1	0.97	0.11	25,25,25,25	0
57	MG	1A	3542	1/1	0.97	0.14	25,25,25,25	0
57	MG	2A	3496	1/1	0.97	0.07	37,37,37,37	0
57	MG	2A	3077	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3172	1/1	0.97	0.13	32,32,32,32	0
57	MG	2A	3499	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3544	1/1	0.97	0.18	31,31,31,31	0
57	MG	1A	3650	1/1	0.97	0.10	46,46,46,46	0
57	MG	2A	3742	1/1	0.97	0.12	67,67,67,67	0
57	MG	1A	3651	1/1	0.97	0.06	26,26,26,26	0
57	MG	2A	3082	1/1	0.97	0.08	48,48,48,48	0
57	MG	2A	3745	1/1	0.97	0.05	54,54,54,54	0
57	MG	1A	3775	1/1	0.97	0.09	55,55,55,55	0
57	MG	2A	3748	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3545	1/1	0.97	0.10	27,27,27,27	0
57	MG	1A	3779	1/1	0.97	0.06	36,36,36,36	0
57	MG	1a	1728	1/1	0.97	0.04	39,39,39,39	0
57	MG	1a	1729	1/1	0.97	0.07	39,39,39,39	0
57	MG	2a	3062	1/1	0.97	0.15	46,46,46,46	0
57	MG	2a	3063	1/1	0.97	0.14	44,44,44,44	0
57	MG	1W	206	1/1	0.97	0.06	45,45,45,45	0
57	MG	2a	3065	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3173	1/1	0.97	0.05	35,35,35,35	0
57	MG	1X	104	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3911	1/1	0.97	0.21	56,56,56,56	0
57	MG	1a	1734	1/1	0.97	0.07	42,42,42,42	0
57	MG	1a	1735	1/1	0.97	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3760	1/1	0.97	0.14	50,50,50,50	0
57	MG	1A	3271	1/1	0.97	0.06	37,37,37,37	0
57	MG	1a	1738	1/1	0.97	0.08	47,47,47,47	0
57	MG	1X	107	1/1	0.97	0.06	31,31,31,31	0
57	MG	2A	3518	1/1	0.97	0.08	40,40,40,40	0
57	MG	2A	3519	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3782	1/1	0.97	0.07	18,18,18,18	0
57	MG	1A	3218	1/1	0.97	0.04	39,39,39,39	0
57	MG	1a	1742	1/1	0.97	0.07	63,63,63,63	0
57	MG	1A	3273	1/1	0.97	0.07	33,33,33,33	0
57	MG	2a	3081	1/1	0.97	0.13	47,47,47,47	0
57	MG	1A	3917	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3275	1/1	0.97	0.11	28,28,28,28	0
57	MG	1A	3090	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3921	1/1	0.97	0.05	42,42,42,42	0
57	MG	1A	3660	1/1	0.97	0.05	26,26,26,26	0
57	MG	1A	3277	1/1	0.97	0.10	31,31,31,31	0
57	MG	1A	3927	1/1	0.97	0.04	28,28,28,28	0
57	MG	1A	3280	1/1	0.97	0.19	39,39,39,39	0
57	MG	1A	3665	1/1	0.97	0.09	18,18,18,18	0
57	MG	2A	3780	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3666	1/1	0.97	0.09	24,24,24,24	0
57	MG	2A	3782	1/1	0.97	0.08	40,40,40,40	0
57	MG	2A	3783	1/1	0.97	0.07	34,34,34,34	0
57	MG	2a	3095	1/1	0.97	0.06	55,55,55,55	0
57	MG	2A	3536	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3558	1/1	0.97	0.07	20,20,20,20	0
57	MG	1A	3796	1/1	0.97	0.06	19,19,19,19	0
57	MG	1A	3136	1/1	0.97	0.07	29,29,29,29	0
57	MG	2A	3115	1/1	0.97	0.08	30,30,30,30	0
57	MG	1A	4085	1/1	0.97	0.11	40,40,40,40	0
57	MG	1A	3798	1/1	0.97	0.04	41,41,41,41	0
57	MG	1A	3799	1/1	0.97	0.05	26,26,26,26	0
57	MG	1A	3942	1/1	0.97	0.05	56,56,56,56	0
57	MG	1A	3800	1/1	0.97	0.27	23,23,23,23	0
57	MG	1A	4093	1/1	0.97	0.05	53,53,53,53	0
57	MG	1A	3177	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3414	1/1	0.97	0.07	48,48,48,48	0
57	MG	1a	1770	1/1	0.97	0.07	61,61,61,61	0
57	MG	1A	3673	1/1	0.97	0.08	50,50,50,50	0
57	MG	1A	3804	1/1	0.97	0.08	44,44,44,44	0
57	MG	2a	3112	1/1	0.97	0.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3948	1/1	0.97	0.05	47,47,47,47	0
57	MG	1A	3137	1/1	0.97	0.07	14,14,14,14	0
57	MG	1a	1779	1/1	0.97	0.06	41,41,41,41	0
57	MG	2A	3806	1/1	0.97	0.06	62,62,62,62	0
57	MG	1A	3565	1/1	0.97	0.09	40,40,40,40	0
57	MG	1a	1783	1/1	0.97	0.08	71,71,71,71	0
57	MG	1a	1785	1/1	0.97	0.08	81,81,81,81	0
57	MG	2A	3134	1/1	0.97	0.14	37,37,37,37	0
57	MG	1A	3676	1/1	0.97	0.06	20,20,20,20	0
57	MG	2A	3136	1/1	0.97	0.21	38,38,38,38	0
57	MG	1A	3111	1/1	0.97	0.05	32,32,32,32	0
57	MG	2A	3815	1/1	0.97	0.11	39,39,39,39	0
57	MG	1a	1788	1/1	0.97	0.06	64,64,64,64	0
57	MG	1A	3678	1/1	0.97	0.06	22,22,22,22	0
57	MG	2A	3818	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3180	1/1	0.97	0.07	48,48,48,48	0
57	MG	2a	3129	1/1	0.97	0.06	51,51,51,51	0
57	MG	2A	3820	1/1	0.97	0.04	57,57,57,57	0
57	MG	1A	3680	1/1	0.97	0.06	21,21,21,21	0
57	MG	17	103	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3681	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3958	1/1	0.97	0.08	23,23,23,23	0
57	MG	1A	3091	1/1	0.97	0.07	23,23,23,23	0
57	MG	1A	3814	1/1	0.97	0.03	30,30,30,30	0
57	MG	1A	3573	1/1	0.97	0.08	39,39,39,39	0
57	MG	1A	3420	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3817	1/1	0.97	0.06	33,33,33,33	0
57	MG	2a	3143	1/1	0.97	0.15	52,52,52,52	0
57	MG	2a	3145	1/1	0.97	0.07	61,61,61,61	0
57	MG	1B	204	1/1	0.97	0.17	49,49,49,49	0
57	MG	1A	3576	1/1	0.97	0.05	47,47,47,47	0
57	MG	1A	3488	1/1	0.97	0.22	28,28,28,28	0
57	MG	1a	1606	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3489	1/1	0.97	0.11	28,28,28,28	0
57	MG	1A	3688	1/1	0.97	0.05	35,35,35,35	0
57	MG	2A	3156	1/1	0.97	0.06	48,48,48,48	0
57	MG	2A	3837	1/1	0.97	0.13	54,54,54,54	0
57	MG	1A	3113	1/1	0.97	0.11	40,40,40,40	0
57	MG	2A	3158	1/1	0.97	0.12	53,53,53,53	0
57	MG	1a	1610	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3288	1/1	0.97	0.18	23,23,23,23	0
57	MG	1A	3141	1/1	0.97	0.14	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1613	1/1	0.97	0.09	28,28,28,28	0
57	MG	1A	3583	1/1	0.97	0.21	30,30,30,30	0
57	MG	1A	3142	1/1	0.97	0.11	31,31,31,31	0
57	MG	2A	3593	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3233	1/1	0.97	0.10	30,30,30,30	0
57	MG	1A	3234	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3696	1/1	0.97	0.06	12,12,12,12	0
57	MG	1A	3697	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3356	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3235	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3700	1/1	0.97	0.05	30,30,30,30	0
57	MG	2A	3172	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3981	1/1	0.97	0.08	28,28,28,28	0
57	MG	2A	3605	1/1	0.97	0.14	43,43,43,43	0
57	MG	1A	3236	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3359	1/1	0.97	0.18	40,40,40,40	0
57	MG	2A	3608	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3186	1/1	0.97	0.14	36,36,36,36	0
57	MG	2A	3610	1/1	0.97	0.06	50,50,50,50	0
57	MG	1m	3001	1/1	0.97	0.09	45,45,45,45	0
57	MG	2A	3178	1/1	0.97	0.08	44,44,44,44	0
57	MG	1A	3239	1/1	0.97	0.12	43,43,43,43	0
57	MG	1A	3028	1/1	0.97	0.22	26,26,26,26	0
57	MG	1A	3045	1/1	0.97	0.08	32,32,32,32	0
57	MG	2A	3385	1/1	0.97	0.09	55,55,55,55	0
57	MG	1A	3242	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3506	1/1	0.97	0.22	37,37,37,37	0
57	MG	1A	3843	1/1	0.97	0.15	40,40,40,40	0
57	MG	1A	3146	1/1	0.97	0.17	31,31,31,31	0
57	MG	1A	3845	1/1	0.97	0.12	37,37,37,37	0
57	MG	1a	1636	1/1	0.97	0.09	43,43,43,43	0
57	MG	1A	3994	1/1	0.97	0.22	25,25,25,25	0
57	MG	1D	301	1/1	0.97	0.10	27,27,27,27	0
57	MG	1A	3147	1/1	0.97	0.14	32,32,32,32	0
57	MG	2a	3194	1/1	0.97	0.20	51,51,51,51	0
57	MG	1A	3712	1/1	0.97	0.16	42,42,42,42	0
57	MG	1D	304	1/1	0.97	0.07	19,19,19,19	0
57	MG	1A	3046	1/1	0.97	0.04	24,24,24,24	0
57	MG	1A	3007	1/1	0.97	0.04	33,33,33,33	0
57	MG	2A	3630	1/1	0.97	0.09	48,48,48,48	0
57	MG	1A	3069	1/1	0.97	0.09	21,21,21,21	0
57	MG	1A	3717	1/1	0.97	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3852	1/1	0.97	0.25	33,33,33,33	0
57	MG	1A	3197	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3030	1/1	0.97	0.13	26,26,26,26	0
57	MG	1A	3121	1/1	0.97	0.25	33,33,33,33	0
57	MG	2A	3201	1/1	0.97	0.08	51,51,51,51	0
57	MG	1A	3722	1/1	0.97	0.07	38,38,38,38	0
57	MG	2A	3639	1/1	0.97	0.08	44,44,44,44	0
57	MG	2A	3641	1/1	0.97	0.09	39,39,39,39	0
57	MG	1A	3155	1/1	0.97	0.11	26,26,26,26	0
57	MG	1A	3201	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3314	1/1	0.97	0.07	39,39,39,39	0
57	MG	2A	3206	1/1	0.97	0.06	53,53,53,53	0
57	MG	1A	3005	1/1	0.97	0.07	45,45,45,45	0
57	MG	1x	114	1/1	0.97	0.12	45,45,45,45	0
57	MG	1F	301	1/1	0.97	0.10	32,32,32,32	0
57	MG	2A	3415	1/1	0.97	0.15	42,42,42,42	0
57	MG	1A	3254	1/1	0.97	0.05	34,34,34,34	0
57	MG	2A	3651	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3730	1/1	0.97	0.04	38,38,38,38	0
57	MG	1A	4015	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3158	1/1	0.97	0.24	31,31,31,31	0
57	MG	2A	3005	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3006	1/1	0.97	0.11	52,52,52,52	0
57	MG	1A	3101	1/1	0.97	0.05	26,26,26,26	0
57	MG	1F	310	1/1	0.97	0.14	26,26,26,26	0
57	MG	2A	3010	1/1	0.97	0.12	38,38,38,38	0
57	MG	2A	3011	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3522	1/1	0.97	0.24	39,39,39,39	0
57	MG	1A	3616	1/1	0.97	0.09	30,30,30,30	0
57	MG	1A	3736	1/1	0.97	0.08	31,31,31,31	0
57	MG	2A	3664	1/1	0.97	0.05	56,56,56,56	0
57	MG	1G	201	1/1	0.97	0.15	44,44,44,44	0
57	MG	1A	3523	1/1	0.97	0.20	32,32,32,32	0
57	MG	1A	3102	1/1	0.97	0.14	36,36,36,36	0
57	MG	2A	3433	1/1	0.97	0.19	45,45,45,45	0
57	MG	1A	3619	1/1	0.97	0.08	22,22,22,22	0
57	MG	1A	3871	1/1	0.97	0.13	32,32,32,32	0
57	MG	1A	3074	1/1	0.97	0.04	31,31,31,31	0
57	MG	2A	3672	1/1	0.97	0.05	56,56,56,56	0
57	MG	1A	3321	1/1	0.97	0.06	31,31,31,31	0
57	MG	2f	201	1/1	0.97	0.13	39,39,39,39	0
57	MG	1A	3389	1/1	0.97	0.04	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	23	101	1/1	0.97	0.11	50,50,50,50	0
57	MG	23	102	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3456	1/1	0.97	0.16	40,40,40,40	0
57	MG	2A	3026	1/1	0.97	0.16	42,42,42,42	0
57	MG	2A	3442	1/1	0.97	0.12	68,68,68,68	0
57	MG	1a	1676	1/1	0.97	0.07	60,60,60,60	0
57	MG	1N	204	1/1	0.97	0.05	27,27,27,27	0
57	MG	1a	1678	1/1	0.97	0.08	59,59,59,59	0
57	MG	1A	3745	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3627	1/1	0.97	0.09	32,32,32,32	0
57	MG	27	101	1/1	0.97	0.12	38,38,38,38	0
57	MG	1A	3628	1/1	0.97	0.06	19,19,19,19	0
57	MG	1A	3163	1/1	0.97	0.05	25,25,25,25	0
57	MG	1O	202	1/1	0.97	0.09	43,43,43,43	0
57	MG	1A	4035	1/1	0.97	0.11	32,32,32,32	0
57	MG	1A	3530	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	3105	1/1	0.97	0.29	41,41,41,41	0
57	MG	1A	3017	1/1	0.97	0.06	44,44,44,44	0
57	MG	2A	3692	1/1	0.97	0.11	43,43,43,43	0
57	MG	2A	3041	1/1	0.97	0.12	67,67,67,67	0
57	MG	2A	3694	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3262	1/1	0.97	0.10	38,38,38,38	0
57	MG	1P	204	1/1	0.97	0.30	29,29,29,29	0
57	MG	2A	3698	1/1	0.97	0.08	52,52,52,52	0
57	MG	1P	205	1/1	0.97	0.22	23,23,23,23	0
57	MG	1P	206	1/1	0.97	0.08	39,39,39,39	0
57	MG	1Q	201	1/1	0.97	0.06	29,29,29,29	0
57	MG	2A	3461	1/1	0.97	0.13	40,40,40,40	0
57	MG	1Q	202	1/1	0.97	0.04	37,37,37,37	0
58	K	2A	3432	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3129	1/1	0.97	0.04	35,35,35,35	0
57	MG	1Q	204	1/1	0.97	0.04	49,49,49,49	0
57	MG	1A	3061	1/1	0.97	0.08	25,25,25,25	0
57	MG	1A	3328	1/1	0.97	0.11	41,41,41,41	0
57	MG	1A	3638	1/1	0.97	0.05	26,26,26,26	0
63	FME	1x	115	10/11	0.97	0.13	16,19,24,30	10
57	MG	2A	3468	1/1	0.97	0.14	40,40,40,40	0
57	MG	1A	3734	1/1	0.98	0.04	47,47,47,47	0
57	MG	2O	201	1/1	0.98	0.08	55,55,55,55	0
57	MG	1A	3662	1/1	0.98	0.05	28,28,28,28	0
57	MG	1a	1743	1/1	0.98	0.06	52,52,52,52	0
57	MG	1a	1744	1/1	0.98	0.05	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3104	1/1	0.98	0.04	27,27,27,27	0
57	MG	2A	3747	1/1	0.98	0.05	50,50,50,50	0
57	MG	1A	4087	1/1	0.98	0.05	44,44,44,44	0
57	MG	1a	1747	1/1	0.98	0.05	50,50,50,50	0
57	MG	1A	3896	1/1	0.98	0.05	41,41,41,41	0
57	MG	1A	3269	1/1	0.98	0.08	30,30,30,30	0
57	MG	2A	3599	1/1	0.98	0.08	56,56,56,56	0
57	MG	2A	3031	1/1	0.98	0.13	33,33,33,33	0
57	MG	1A	3174	1/1	0.98	0.06	28,28,28,28	0
57	MG	2a	3130	1/1	0.98	0.04	72,72,72,72	0
57	MG	1A	4092	1/1	0.98	0.04	31,31,31,31	0
57	MG	2A	3603	1/1	0.98	0.09	32,32,32,32	0
57	MG	1A	3667	1/1	0.98	0.05	20,20,20,20	0
57	MG	1A	3740	1/1	0.98	0.07	50,50,50,50	0
57	MG	1P	202	1/1	0.98	0.13	28,28,28,28	0
57	MG	1A	3039	1/1	0.98	0.28	32,32,32,32	0
57	MG	1A	3022	1/1	0.98	0.06	40,40,40,40	0
57	MG	2X	102	1/1	0.98	0.12	42,42,42,42	0
57	MG	1A	3670	1/1	0.98	0.03	18,18,18,18	0
57	MG	1A	3107	1/1	0.98	0.32	30,30,30,30	0
57	MG	1A	3311	1/1	0.98	0.15	26,26,26,26	0
57	MG	1A	3051	1/1	0.98	0.11	22,22,22,22	0
57	MG	1A	3604	1/1	0.98	0.05	26,26,26,26	0
57	MG	1A	3151	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3064	1/1	0.98	0.13	37,37,37,37	0
57	MG	1A	3278	1/1	0.98	0.17	25,25,25,25	0
57	MG	2a	3150	1/1	0.98	0.08	60,60,60,60	0
57	MG	1R	201	1/1	0.98	0.11	28,28,28,28	0
57	MG	1A	3279	1/1	0.98	0.15	32,32,32,32	0
57	MG	1A	3008	1/1	0.98	0.11	18,18,18,18	0
57	MG	2A	3774	1/1	0.98	0.09	48,48,48,48	0
57	MG	1R	204	1/1	0.98	0.26	38,38,38,38	0
57	MG	1A	3835	1/1	0.98	0.08	29,29,29,29	0
57	MG	1S	201	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3130	1/1	0.98	0.06	31,31,31,31	0
57	MG	1a	1774	1/1	0.98	0.05	68,68,68,68	0
57	MG	1a	1775	1/1	0.98	0.05	54,54,54,54	0
57	MG	1a	1776	1/1	0.98	0.05	52,52,52,52	0
57	MG	1A	3032	1/1	0.98	0.18	21,21,21,21	0
57	MG	28	102	1/1	0.98	0.06	42,42,42,42	0
57	MG	1A	3920	1/1	0.98	0.06	35,35,35,35	0
57	MG	1a	1649	1/1	0.98	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1782	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3184	1/1	0.98	0.20	38,38,38,38	0
57	MG	1U	201	1/1	0.98	0.13	27,27,27,27	0
57	MG	1A	3095	1/1	0.98	0.04	34,34,34,34	0
57	MG	2A	3065	1/1	0.98	0.06	28,28,28,28	0
57	MG	2A	3066	1/1	0.98	0.08	50,50,50,50	0
57	MG	1A	3923	1/1	0.98	0.05	12,12,12,12	0
57	MG	2A	3792	1/1	0.98	0.04	41,41,41,41	0
57	MG	2A	3793	1/1	0.98	0.04	56,56,56,56	0
57	MG	1B	205	1/1	0.98	0.05	40,40,40,40	0
57	MG	2A	3343	1/1	0.98	0.07	53,53,53,53	0
57	MG	1B	206	1/1	0.98	0.04	46,46,46,46	0
57	MG	2A	3640	1/1	0.98	0.06	58,58,58,58	0
57	MG	1a	1790	1/1	0.98	0.04	58,58,58,58	0
57	MG	1A	3451	1/1	0.98	0.11	50,50,50,50	0
57	MG	2A	3072	1/1	0.98	0.10	37,37,37,37	0
57	MG	2A	3073	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3925	1/1	0.98	0.03	51,51,51,51	0
57	MG	1A	3404	1/1	0.98	0.10	31,31,31,31	0
57	MG	1A	3928	1/1	0.98	0.07	24,24,24,24	0
57	MG	1A	3929	1/1	0.98	0.09	51,51,51,51	0
57	MG	1A	3930	1/1	0.98	0.06	29,29,29,29	0
57	MG	1A	3931	1/1	0.98	0.03	46,46,46,46	0
57	MG	1A	3502	1/1	0.98	0.23	44,44,44,44	0
57	MG	1B	215	1/1	0.98	0.05	46,46,46,46	0
57	MG	1A	3933	1/1	0.98	0.05	43,43,43,43	0
57	MG	2A	3812	1/1	0.98	0.04	48,48,48,48	0
57	MG	1A	4027	1/1	0.98	0.05	37,37,37,37	0
57	MG	1A	3360	1/1	0.98	0.14	48,48,48,48	0
57	MG	1A	3556	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3620	1/1	0.98	0.04	50,50,50,50	0
57	MG	1A	3621	1/1	0.98	0.03	25,25,25,25	0
57	MG	2A	3088	1/1	0.98	0.20	43,43,43,43	0
57	MG	1X	102	1/1	0.98	0.28	37,37,37,37	0
57	MG	1A	3557	1/1	0.98	0.09	31,31,31,31	0
57	MG	1A	3939	1/1	0.98	0.04	43,43,43,43	0
57	MG	1A	3406	1/1	0.98	0.13	37,37,37,37	0
57	MG	1A	3157	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3133	1/1	0.98	0.25	34,34,34,34	0
57	MG	1A	3096	1/1	0.98	0.15	21,21,21,21	0
57	MG	1A	3190	1/1	0.98	0.27	38,38,38,38	0
57	MG	1a	1815	1/1	0.98	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3774	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	4040	1/1	0.98	0.06	36,36,36,36	0
57	MG	2A	3521	1/1	0.98	0.10	28,28,28,28	0
57	MG	2A	3522	1/1	0.98	0.07	35,35,35,35	0
57	MG	1A	3564	1/1	0.98	0.10	42,42,42,42	0
57	MG	1A	3459	1/1	0.98	0.09	37,37,37,37	0
57	MG	1A	3566	1/1	0.98	0.16	31,31,31,31	0
57	MG	1A	3567	1/1	0.98	0.29	34,34,34,34	0
57	MG	1A	3568	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3016	1/1	0.98	0.17	45,45,45,45	0
57	MG	1A	3115	1/1	0.98	0.08	35,35,35,35	0
57	MG	10	106	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3784	1/1	0.98	0.07	44,44,44,44	0
57	MG	1A	3571	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3955	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3225	1/1	0.98	0.08	27,27,27,27	0
57	MG	1D	306	1/1	0.98	0.05	29,29,29,29	0
57	MG	1D	307	1/1	0.98	0.13	33,33,33,33	0
57	MG	1D	308	1/1	0.98	0.17	46,46,46,46	0
57	MG	1A	3787	1/1	0.98	0.04	18,18,18,18	0
57	MG	1A	3083	1/1	0.98	0.10	25,25,25,25	0
57	MG	2A	3253	1/1	0.98	0.05	47,47,47,47	0
57	MG	1D	311	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3574	1/1	0.98	0.12	37,37,37,37	0
57	MG	1a	1700	1/1	0.98	0.13	36,36,36,36	0
57	MG	1A	3293	1/1	0.98	0.13	35,35,35,35	0
57	MG	1E	304	1/1	0.98	0.13	30,30,30,30	0
57	MG	1A	4056	1/1	0.98	0.05	40,40,40,40	0
57	MG	2A	3123	1/1	0.98	0.12	50,50,50,50	0
57	MG	2A	3401	1/1	0.98	0.28	59,59,59,59	0
57	MG	1E	306	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	3044	1/1	0.98	0.06	35,35,35,35	0
57	MG	1a	1706	1/1	0.98	0.08	32,32,32,32	0
57	MG	1A	3710	1/1	0.98	0.09	30,30,30,30	0
57	MG	1A	3295	1/1	0.98	0.10	30,30,30,30	0
57	MG	1E	310	1/1	0.98	0.08	19,19,19,19	0
57	MG	1A	3009	1/1	0.98	0.04	18,18,18,18	0
57	MG	1A	3373	1/1	0.98	0.14	24,24,24,24	0
57	MG	16	103	1/1	0.98	0.09	38,38,38,38	0
57	MG	2A	3559	1/1	0.98	0.07	62,62,62,62	0
57	MG	1A	3196	1/1	0.98	0.15	22,22,22,22	0
57	MG	1A	3715	1/1	0.98	0.05	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3166	1/1	0.98	0.07	14,14,14,14	0
57	MG	2A	3564	1/1	0.98	0.04	33,33,33,33	0
57	MG	1A	3376	1/1	0.98	0.05	44,44,44,44	0
57	MG	2A	3274	1/1	0.98	0.10	53,53,53,53	0
57	MG	1A	3649	1/1	0.98	0.07	38,38,38,38	0
57	MG	1A	3472	1/1	0.98	0.09	41,41,41,41	0
57	MG	1F	305	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3010	1/1	0.98	0.07	25,25,25,25	0
57	MG	19	102	1/1	0.98	0.18	33,33,33,33	0
57	MG	1F	307	1/1	0.98	0.09	28,28,28,28	0
57	MG	1F	308	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3973	1/1	0.98	0.04	33,33,33,33	0
57	MG	2D	303	1/1	0.98	0.07	28,28,28,28	0
57	MG	2D	304	1/1	0.98	0.15	36,36,36,36	0
57	MG	1A	3721	1/1	0.98	0.07	42,42,42,42	0
57	MG	1A	3337	1/1	0.98	0.24	33,33,33,33	0
57	MG	1A	3379	1/1	0.98	0.08	31,31,31,31	0
57	MG	1A	3724	1/1	0.98	0.04	20,20,20,20	0
57	MG	1A	3011	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3038	1/1	0.98	0.15	27,27,27,27	0
57	MG	1A	3340	1/1	0.98	0.16	31,31,31,31	0
57	MG	1A	3383	1/1	0.98	0.29	38,38,38,38	0
57	MG	1A	3658	1/1	0.98	0.08	37,37,37,37	0
58	K	1A	3553	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3434	1/1	0.98	0.10	21,21,21,21	0
57	MG	1A	3983	1/1	0.98	0.04	22,22,22,22	0
57	MG	2A	3017	1/1	0.98	0.09	24,24,24,24	0
60	ZN	1n	103	1/1	0.98	0.03	56,56,56,56	0
60	ZN	2Y	202	1/1	0.98	0.04	83,83,83,83	0
57	MG	1A	3143	1/1	0.98	0.06	31,31,31,31	0
60	ZN	29	102	1/1	0.98	0.05	64,64,64,64	0
60	ZN	2n	501	1/1	0.98	0.05	85,85,85,85	0
61	SF4	1d	302	8/8	0.98	0.05	59,62,66,68	0
57	MG	1A	3122	1/1	0.98	0.14	34,34,34,34	0
57	MG	2A	3740	1/1	0.98	0.07	46,46,46,46	0
57	MG	2F	307	1/1	0.98	0.13	45,45,45,45	0
57	MG	1A	3386	1/1	0.98	0.07	52,52,52,52	0
57	MG	1E	301	1/1	0.99	0.13	30,30,30,30	0
57	MG	1A	3219	1/1	0.99	0.06	34,34,34,34	0
57	MG	2A	3487	1/1	0.99	0.06	39,39,39,39	0
57	MG	1E	303	1/1	0.99	0.15	31,31,31,31	0
57	MG	1A	3559	1/1	0.99	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1633	1/1	0.99	0.15	24,24,24,24	0
57	MG	1A	4009	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	4059	1/1	0.99	0.08	29,29,29,29	0
57	MG	13	101	1/1	0.99	0.07	27,27,27,27	0
57	MG	1A	3018	1/1	0.99	0.08	20,20,20,20	0
57	MG	1A	3014	1/1	0.99	0.03	21,21,21,21	0
57	MG	1a	1765	1/1	0.99	0.05	50,50,50,50	0
57	MG	1A	3003	1/1	0.99	0.05	23,23,23,23	0
57	MG	1A	3171	1/1	0.99	0.21	31,31,31,31	0
57	MG	15	3201	1/1	0.99	0.12	25,25,25,25	0
57	MG	1A	3592	1/1	0.99	0.11	37,37,37,37	0
57	MG	1A	3623	1/1	0.99	0.04	17,17,17,17	0
57	MG	15	3204	1/1	0.99	0.19	25,25,25,25	0
57	MG	1A	3224	1/1	0.99	0.08	24,24,24,24	0
57	MG	1A	3188	1/1	0.99	0.17	27,27,27,27	0
57	MG	1A	3226	1/1	0.99	0.08	33,33,33,33	0
57	MG	1a	1648	1/1	0.99	0.10	39,39,39,39	0
57	MG	2a	3135	1/1	0.99	0.03	57,57,57,57	0
57	MG	1A	3926	1/1	0.99	0.04	32,32,32,32	0
57	MG	1a	1777	1/1	0.99	0.09	51,51,51,51	0
57	MG	2a	3138	1/1	0.99	0.05	55,55,55,55	0
57	MG	1A	3881	1/1	0.99	0.05	48,48,48,48	0
57	MG	2A	3358	1/1	0.99	0.04	42,42,42,42	0
57	MG	1A	3725	1/1	0.99	0.03	23,23,23,23	0
57	MG	1A	3021	1/1	0.99	0.09	21,21,21,21	0
57	MG	1a	1781	1/1	0.99	0.04	62,62,62,62	0
57	MG	2a	3144	1/1	0.99	0.02	51,51,51,51	0
57	MG	1A	3037	1/1	0.99	0.13	20,20,20,20	0
57	MG	1A	4024	1/1	0.99	0.03	25,25,25,25	0
57	MG	2A	3756	1/1	0.99	0.03	47,47,47,47	0
57	MG	1a	1784	1/1	0.99	0.04	55,55,55,55	0
57	MG	1A	3416	1/1	0.99	0.13	37,37,37,37	0
57	MG	1A	3296	1/1	0.99	0.04	22,22,22,22	0
57	MG	1A	3208	1/1	0.99	0.13	30,30,30,30	0
57	MG	1a	1719	1/1	0.99	0.04	35,35,35,35	0
57	MG	1A	3664	1/1	0.99	0.05	37,37,37,37	0
57	MG	1a	1721	1/1	0.99	0.07	40,40,40,40	0
57	MG	1a	1791	1/1	0.99	0.04	63,63,63,63	0
57	MG	1A	3768	1/1	0.99	0.03	30,30,30,30	0
57	MG	1A	3274	1/1	0.99	0.09	20,20,20,20	0
57	MG	1A	3056	1/1	0.99	0.03	27,27,27,27	0
57	MG	2A	3009	1/1	0.99	0.08	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3634	1/1	0.99	0.04	12,12,12,12	0
57	MG	2A	3688	1/1	0.99	0.03	48,48,48,48	0
57	MG	1A	3772	1/1	0.99	0.03	20,20,20,20	0
57	MG	2A	3855	1/1	0.99	0.03	59,59,59,59	0
57	MG	1W	203	1/1	0.99	0.10	31,31,31,31	0
57	MG	2A	3857	1/1	0.99	0.05	41,41,41,41	0
57	MG	1A	3159	1/1	0.99	0.17	47,47,47,47	0
57	MG	1A	3067	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	3548	1/1	0.99	0.06	40,40,40,40	0
57	MG	1X	101	1/1	0.99	0.03	29,29,29,29	0
57	MG	1A	3012	1/1	0.99	0.03	27,27,27,27	0
57	MG	1A	4088	1/1	0.99	0.06	40,40,40,40	0
57	MG	2A	3697	1/1	0.99	0.07	38,38,38,38	0
57	MG	1A	3777	1/1	0.99	0.03	58,58,58,58	0
57	MG	1A	3778	1/1	0.99	0.05	39,39,39,39	0
57	MG	1A	3023	1/1	0.99	0.04	12,12,12,12	0
57	MG	1a	1737	1/1	0.99	0.17	42,42,42,42	0
57	MG	2A	3023	1/1	0.99	0.12	32,32,32,32	0
57	MG	1A	3579	1/1	0.99	0.04	37,37,37,37	0
57	MG	1A	3070	1/1	0.99	0.08	13,13,13,13	0
57	MG	1A	3610	1/1	0.99	0.04	29,29,29,29	0
57	MG	1A	3995	1/1	0.99	0.07	17,17,17,17	0
57	MG	1A	3996	1/1	0.99	0.03	32,32,32,32	0
57	MG	2A	3470	1/1	0.99	0.04	61,61,61,61	0
57	MG	1A	3031	1/1	0.99	0.09	31,31,31,31	0
57	MG	2A	3472	1/1	0.99	0.10	56,56,56,56	0
57	MG	1A	3906	1/1	0.99	0.04	31,31,31,31	0
57	MG	1A	3907	1/1	0.99	0.04	28,28,28,28	0
57	MG	1A	3237	1/1	0.99	0.18	28,28,28,28	0
57	MG	1A	3150	1/1	0.99	0.10	33,33,33,33	0
60	ZN	1Y	203	1/1	0.99	0.02	62,62,62,62	0
60	ZN	14	102	1/1	0.99	0.04	83,83,83,83	0
60	ZN	16	104	1/1	0.99	0.07	51,51,51,51	0
57	MG	2A	3034	1/1	0.99	0.07	21,21,21,21	0
57	MG	1A	3072	1/1	0.99	0.04	13,13,13,13	0
57	MG	1A	3747	1/1	0.99	0.05	13,13,13,13	0
60	ZN	25	108	1/1	0.99	0.03	61,61,61,61	0
60	ZN	26	102	1/1	0.99	0.04	60,60,60,60	0
57	MG	2A	3557	1/1	0.99	0.06	33,33,33,33	0
57	MG	1A	3788	1/1	0.99	0.04	16,16,16,16	0
57	MG	1A	3013	1/1	0.99	0.07	22,22,22,22	0
61	SF4	2d	303	8/8	0.99	0.04	62,66,72,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1752	1/1	0.99	0.05	47,47,47,47	0
57	MG	1A	3914	1/1	0.99	0.07	37,37,37,37	0
57	MG	1D	313	1/1	0.99	0.16	29,29,29,29	0
57	MG	2A	3563	1/1	0.99	0.06	33,33,33,33	0
57	MG	2A	3680	1/1	1.00	0.03	27,27,27,27	0
57	MG	1A	3754	1/1	1.00	0.08	35,35,35,35	0
60	ZN	15	3209	1/1	1.00	0.02	45,45,45,45	0
57	MG	2A	3802	1/1	1.00	0.05	28,28,28,28	0
60	ZN	19	103	1/1	1.00	0.06	41,41,41,41	0
57	MG	1A	3901	1/1	1.00	0.04	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.