



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 10:11 AM EDT

PDB ID : 9D7R / pdb_00009d7r
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with Fva1 antimicrobial peptide, mRNA, A-site release factor 1, and deacylated P-site and E-site tRNA^{phe} at 2.70Å resolution
Authors : Aleksandrova, E.V.; Huang, W.; Baliga, C.; Atkinson, G.C.; Vazquez-Laslop, N.; Mankin, A.S.; Polikanov, Y.S.
Deposited on : 2024-08-17
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

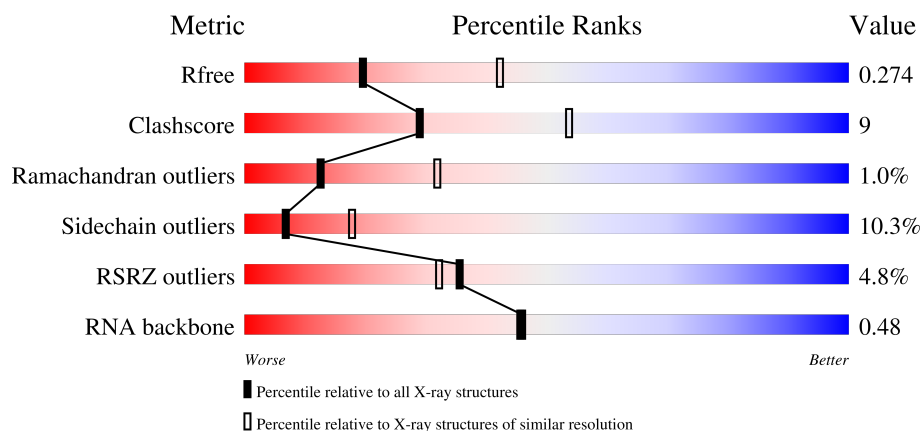
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
2	1B	121	

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Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	

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Mol	Chain	Length	Quality of chain
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	
27	15	60	

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Mol	Chain	Length	Quality of chain
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	
39	2h	138	

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Mol	Chain	Length	Quality of chain
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	
52	1u	27	

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Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	354	
54	2w	354	
55	1x	76	
55	1y	76	
55	2x	76	
55	2y	76	
56	1z	20	
56	2z	20	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	2a	1666	-	-	-	X
59	SF4	1d	302	-	-	X	-
59	SF4	2d	303	-	-	X	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 299076 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
			2576	1146	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	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
			1425	914	256	251	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	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
			1085	693	189	202	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	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
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			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
			746	485	134	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
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	183	Total	C	N	O	S	0	0	0
			1437	919	256	260	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1451	928	256	265	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			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
			548	347	99	97	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	68	Total	C	N	O	S	0	0	0
			517	330	92	90	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
			511	328	99	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
			1554	977	302	274	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
			1659	1040	326	286	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
			1130	714	214	199	3			

- 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	513	143	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			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	123	Total	C	N	O	0	0	0
			940	593	185	162			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	98	Total	C	N	O	0	0	0
			721	449	140	132			
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	118	Total	C	N	O	S	0	0	0
			923	569	191	161	2			
44	2m	115	Total	C	N	O	S	0	0	0
			889	546	183	158	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
			486	309	101	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
			551	353	108	90				

- 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 PHE-Stop mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			274	124	48	89	13			
53	2v	13	Total	C	N	O	P	0	0	0
			274	124	48	89	13			

- Molecule 54 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	249	Total	C	N	O	S	0	0	0
			1939	1199	360	371	9			
54	2w	253	Total	C	N	O	S	0	0	0
			1954	1208	361	377	8			

- Molecule 55 is a RNA chain called P-site and E-site Deacylated tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	75	Total	C	N	O	P	S	0	0	0
			1612	722	288	525	75	2			
55	1y	74	Total	C	N	O	P	S	0	0	0
			1590	712	285	517	74	2			
55	2x	75	Total	C	N	O	P	S	0	0	0
			1612	722	288	525	75	2			
55	2y	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			

- Molecule 56 is a protein called Fva1 Antimicrobial Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	1z	14	Total	C	N	O	0	0	0
			121	79	25	17			
56	2z	14	Total	C	N	O	0	0	0
			121	79	25	17			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	795	Total	Mg	0	0
			795	795		
57	1B	20	Total	Mg	0	0
			20	20		
57	1D	8	Total	Mg	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1E	9	Total 9	Mg 9	0	0
57	1F	11	Total 11	Mg 11	0	0
57	1G	3	Total 3	Mg 3	0	0
57	1N	4	Total 4	Mg 4	0	0
57	1O	1	Total 1	Mg 1	0	0
57	1P	4	Total 4	Mg 4	0	0
57	1Q	6	Total 6	Mg 6	0	0
57	1R	3	Total 3	Mg 3	0	0
57	1U	7	Total 7	Mg 7	0	0
57	1V	5	Total 5	Mg 5	0	0
57	1W	5	Total 5	Mg 5	0	0
57	1X	2	Total 2	Mg 2	0	0
57	1Z	1	Total 1	Mg 1	0	0
57	10	5	Total 5	Mg 5	0	0
57	11	4	Total 4	Mg 4	0	0
57	12	2	Total 2	Mg 2	0	0
57	13	2	Total 2	Mg 2	0	0
57	14	1	Total 1	Mg 1	0	0
57	15	4	Total 4	Mg 4	0	0
57	16	1	Total 1	Mg 1	0	0
57	17	7	Total 7	Mg 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	18	2	Total 2	Mg 2	0	0
57	19	2	Total 2	Mg 2	0	0
57	1a	189	Total 189	Mg 189	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1f	1	Total 1	Mg 1	0	0
57	1k	1	Total 1	Mg 1	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	1	Total 1	Mg 1	0	0
57	1v	2	Total 2	Mg 2	0	0
57	1w	3	Total 3	Mg 3	0	0
57	1x	9	Total 9	Mg 9	0	0
57	1y	1	Total 1	Mg 1	0	0
57	2A	640	Total 640	Mg 640	0	0
57	2B	11	Total 11	Mg 11	0	0
57	2D	8	Total 8	Mg 8	0	0
57	2E	5	Total 5	Mg 5	0	0
57	2F	7	Total 7	Mg 7	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2P	2	Total 2	Mg 2	0	0
57	2Q	3	Total 3	Mg 3	0	0

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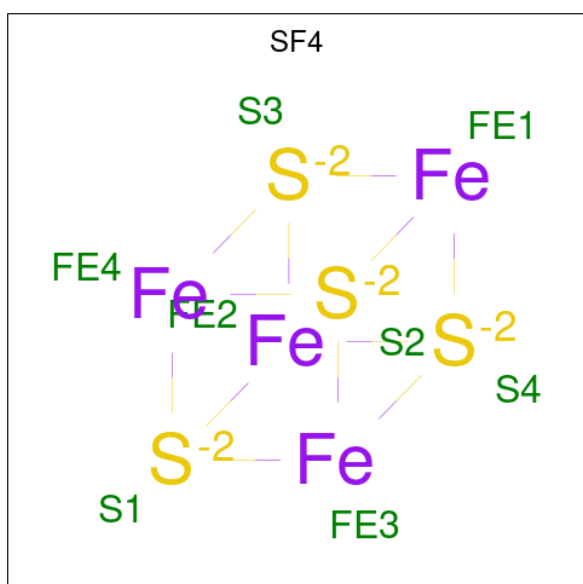
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2R	3	Total 3	Mg 3	0	0
57	2U	1	Total 1	Mg 1	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	1	Total 1	Mg 1	0	0
57	2X	3	Total 3	Mg 3	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	20	2	Total 2	Mg 2	0	0
57	23	1	Total 1	Mg 1	0	0
57	25	1	Total 1	Mg 1	0	0
57	26	1	Total 1	Mg 1	0	0
57	28	1	Total 1	Mg 1	0	0
57	29	1	Total 1	Mg 1	0	0
57	2a	168	Total 168	Mg 168	0	0
57	2d	2	Total 2	Mg 2	0	0
57	2e	3	Total 3	Mg 3	0	0
57	2f	1	Total 1	Mg 1	0	0
57	2j	2	Total 2	Mg 2	0	0
57	2k	2	Total 2	Mg 2	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2v	1	Total 1	Mg 1	0	0
57	2x	9	Total 9	Mg 9	0	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1395	Total	O	0	0
			1395	1395		
60	1B	27	Total	O	0	0
			27	27		
60	1D	15	Total	O	0	0
			15	15		
60	1E	13	Total	O	0	0
			13	13		
60	1F	8	Total	O	0	0
			8	8		
60	1G	1	Total	O	0	0
			1	1		
60	1N	3	Total	O	0	0
			3	3		
60	1O	3	Total	O	0	0
			3	3		
60	1P	15	Total	O	0	0
			15	15		
60	1Q	6	Total	O	0	0
			6	6		
60	1R	3	Total	O	0	0
			3	3		
60	1T	1	Total	O	0	0
			1	1		
60	1U	4	Total	O	0	0
			4	4		
60	1V	1	Total	O	0	0
			1	1		
60	1W	3	Total	O	0	0
			3	3		
60	1X	3	Total	O	0	0
			3	3		
60	1Z	1	Total	O	0	0
			1	1		
60	10	2	Total	O	0	0
			2	2		

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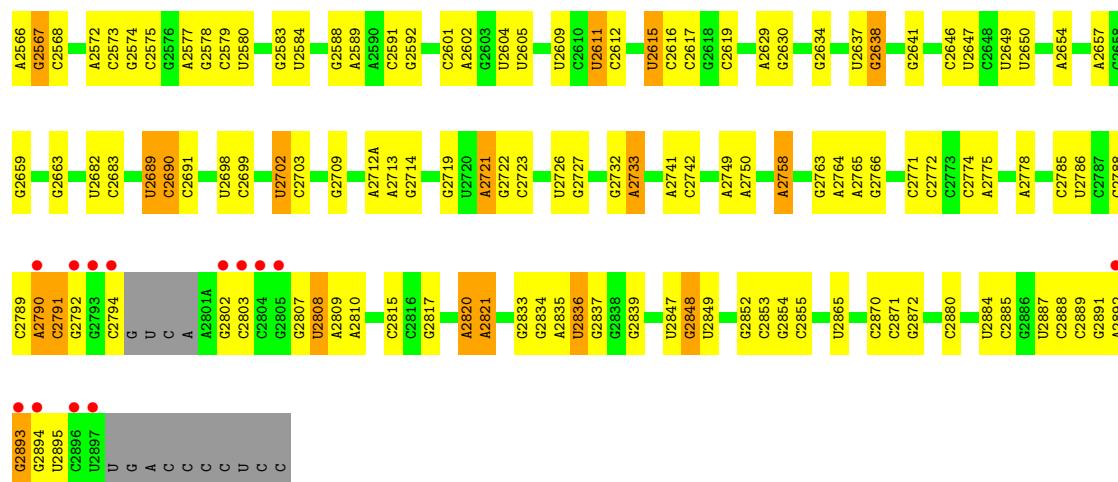
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	11	3	Total 3	O 3	0	0
60	13	2	Total 2	O 2	0	0
60	15	3	Total 3	O 3	0	0
60	16	1	Total 1	O 1	0	0
60	17	2	Total 2	O 2	0	0
60	18	7	Total 7	O 7	0	0
60	1a	180	Total 180	O 180	0	0
60	1d	1	Total 1	O 1	0	0
60	1l	1	Total 1	O 1	0	0
60	1v	4	Total 4	O 4	0	0
60	1w	2	Total 2	O 2	0	0
60	1x	24	Total 24	O 24	0	0
60	2A	946	Total 946	O 946	0	0
60	2B	6	Total 6	O 6	0	0
60	2D	18	Total 18	O 18	0	0
60	2E	7	Total 7	O 7	0	0
60	2F	5	Total 5	O 5	0	0
60	2N	1	Total 1	O 1	0	0
60	2O	2	Total 2	O 2	0	0
60	2P	16	Total 16	O 16	0	0
60	2Q	3	Total 3	O 3	0	0

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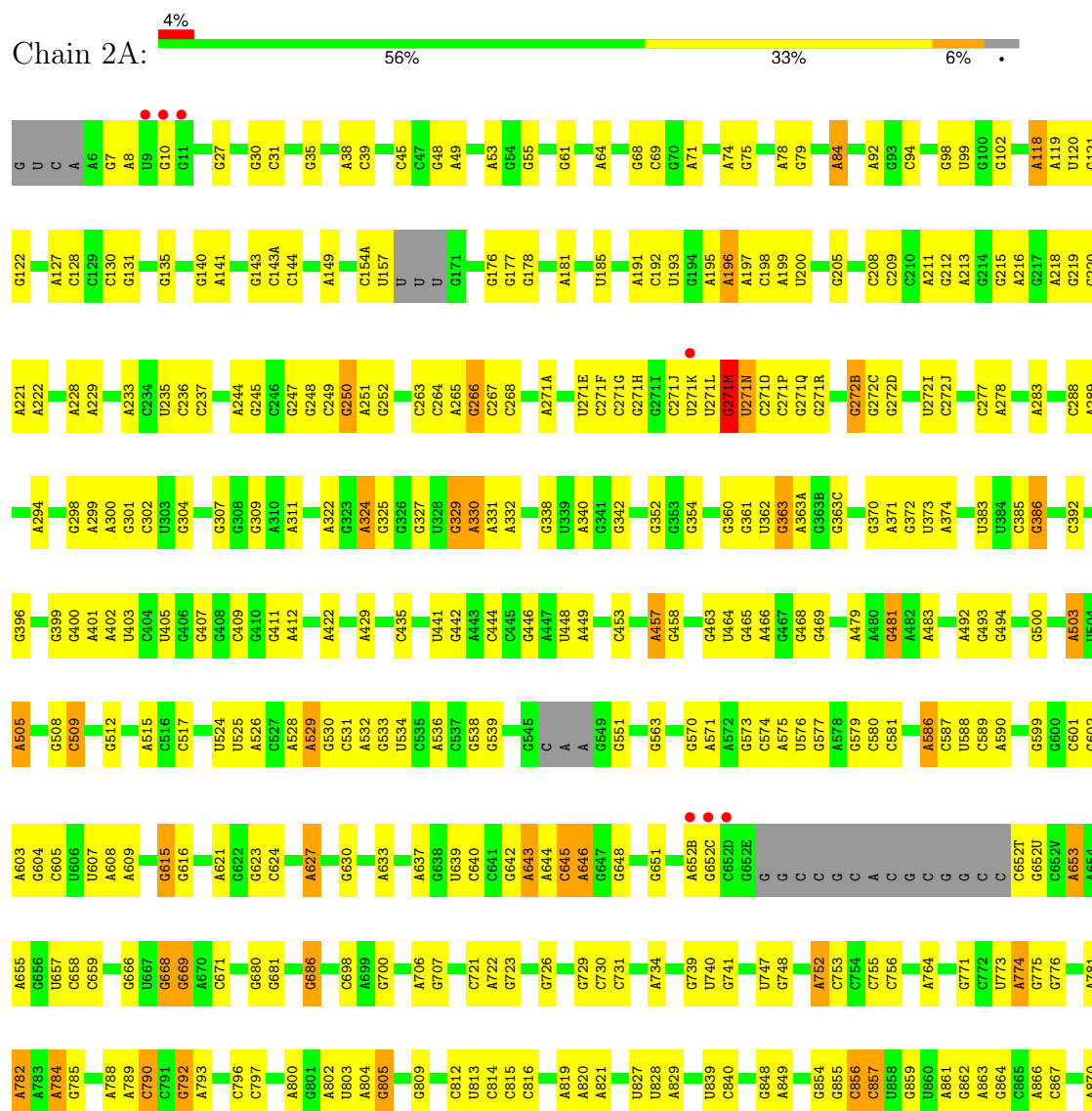
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2R	2	Total	O	0	0
			2	2		
60	2U	1	Total	O	0	0
			1	1		
60	2X	3	Total	O	0	0
			3	3		
60	2Y	2	Total	O	0	0
			2	2		
60	20	4	Total	O	0	0
			4	4		
60	21	2	Total	O	0	0
			2	2		
60	23	2	Total	O	0	0
			2	2		
60	25	2	Total	O	0	0
			2	2		
60	27	4	Total	O	0	0
			4	4		
60	28	4	Total	O	0	0
			4	4		
60	2a	152	Total	O	0	0
			152	152		
60	2d	1	Total	O	0	0
			1	1		
60	2j	1	Total	O	0	0
			1	1		
60	2q	1	Total	O	0	0
			1	1		
60	2t	1	Total	O	0	0
			1	1		
60	2w	1	Total	O	0	0
			1	1		
60	2x	13	Total	O	0	0
			13	13		
60	2z	2	Total	O	0	0
			2	2		

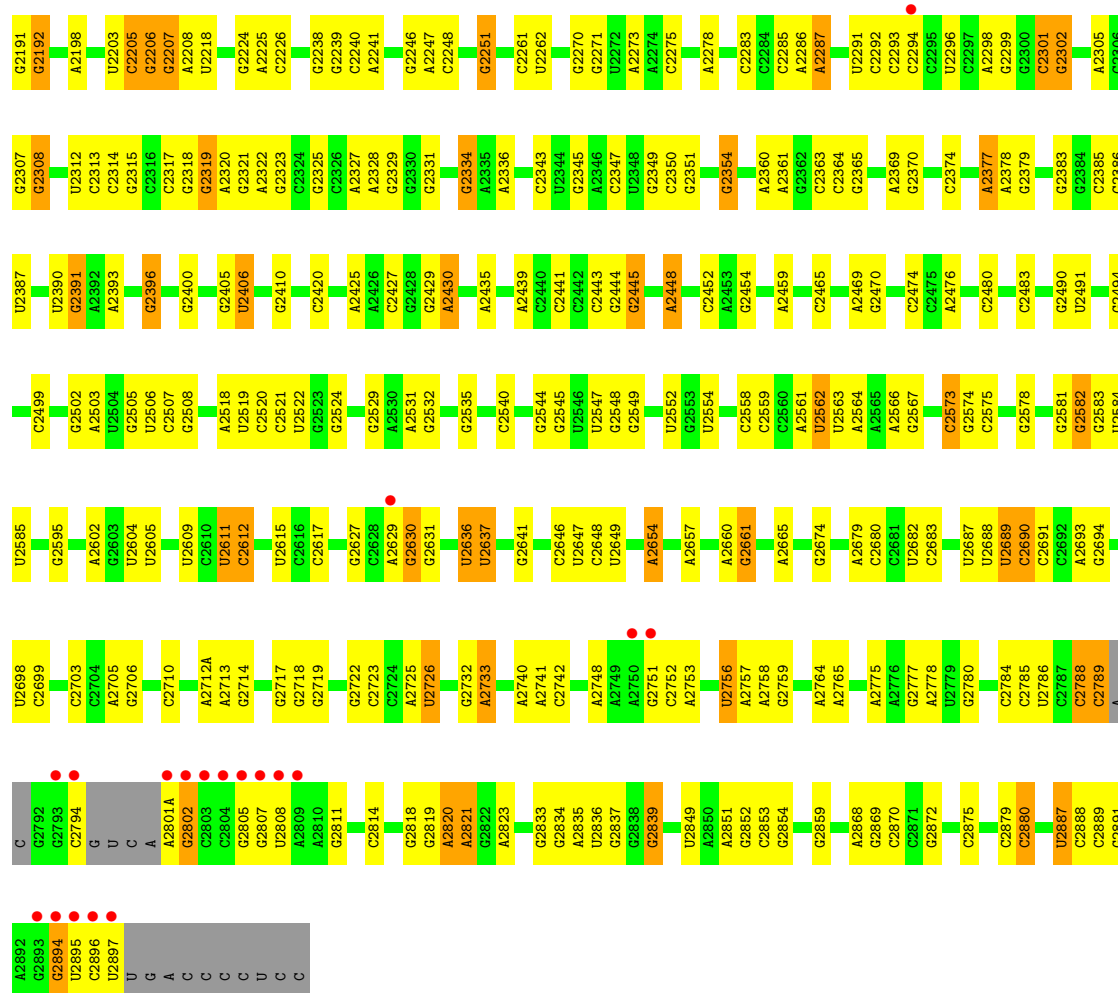
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G2445	G2341	G2234	U2144	A2060	G1929	C1793	A1654	G	G1426	U1300	A1174	U1083	
G2447	G2342	G2235	C2145	G2061	G1930	C1794	A1655	U	A1427	A1301	G1176	A1084	G1003
A2448	A2346	G2238	C2146	A2062	A1938	C1795	C1657	A	C1428	G1309	A1177	A1085	
	G2347	G2239	U2149	G2063	U1939	U1796	G1657	C	G1429	G1309	C1178	A1086	U1012
G2454	U2348	U2243	U2150	C2064	C1942	U1798	A1664	G1537	G1429	G1309	C1179	G1087	C1013
G2455	G2349	U2244	G2151	G2065	G1942	G1799	A1664	G1538	C1430	U1313	C1180	A1088	
	C2350	U2244	G2152				A1668	G1539	G1435	C1314		U1089	G1022
G2458	G2354		G2153	G2069	G1945	G1801	A1669		G1436		C1185	G1091	U1023
U2462	G2355	A2247	G2155		U1946	A1802		A1542	U1437	A1321	G1186	G1092	G1025
G2468	C2359	G2251	G2156	G2080	A1952	U1808	G1674	C1543	U1438	G1328	G1187	G1093	U1026
A2469	A2360	G2255	A2158	U2086	A1953	A1809	C1683	C1546	A1439	G1328	A1188	A1094	A1027
	G2265	G2087	G2159	G2087	U1955	A1811	C1685	C1550	G1442	A1331	G1190	A1095	A1028
A2364	G2365	A2268	C2161	C2095	U1956	A1812	C1686	C1551		C1333	G1191	U1097	U1033
		A2269	G2162	U2096		G1813	U1687	C1557		G1332		A1098	
A2369		A2273	C2163	U2096	C1962	G1814	U1688	A1558	G1448	U1335	U1198	G1099	G1039
		A2274	G2164	C2097	U1963	A1815	A1689	A1558	A1449	A1336	U1199	C1100	C1040
C2483			G2165	U2098	U1963	G1816	A1690		G1450	G1337	C1201	G1102	G1041
	G2373		C2166	U2099	C1967			A1566		G1338	C1202	A1103	C1043
G2489	C2381	G2277	U2167			A1825	U1693		A1452		G1203	A1103	G1044
G2490	G2382	A2278	G2168	U2102	A1970	G1826		A1569	U1453	A1342		G1107	A1045
U2491	G2383	G2280	A2170	C2108	A1971	G1826	G1696	A1570	G1455	U1352	C1207	U1108	A1046
G2494	C2384	G2281	A2171	U2109	A1972	A1829	A1700	A1571		U1352	C1208	G1109	G1047
C2385		C2283	U2172	G2110	C1979	G1839	U1709	U1578	A1460	A1353	A1220	A1111	A1048
U2390	G2284	G2284	A2173	C2111	G1980		C1710	A1579	G1461	A1354	G1225	G1112	A1050
G2391	C2285	A2286	C2174	G2112	A1981	A1847		A1580	G1466	G1355	G1225	U1113	G1051
A2287	A2287		C2175	U2113			G1719	G1581	C1467	U1357	A1226	G1114	C1052
G2396			A2176	A2114	U1993	G1857	G1719	C1584	C1468	G1358	C1230	G1115	A1053
U2291			C2177	G2115	C1996	G1858	A1722	U1584	A1469	A1359	G1230	C1116	A1054
C2292			C2178	G2116	G1997	A1859	U1739	A1587			G1236	G1125	G1055
			C2179	A2117				C1588	G1473	A1365		U1125	A1056
A2298			G2182	U2118	A2001	A1876	G1746	U1588		U1372	G1244	A1129	A1057
G2299			A2119	G2120	G2002	G1877	G1746	U1602	G1482	U1372	G1244	U1129	G1058
			G2180	G2121	G2002	C1879	G1753	A1603	U1489	G1377	G1252	G1130	G1059
A2305			G2184	U2122	A2013		G1753	C1604	A1490	A1378	A1253	G1131	U1060
				G2123		G1883	G1756			A1379	A1253	U	
G2308			G2187	G2123	U2022			C1607	C1493	G1380	G1256	C1135	G1062
G2421			C2188	G2124	G2023	A1889	G1763	A1608	A1494	G1337	G1256	G1136	C1063
A2422			U2189	G2125	G2023		G1764	A1609	A1495	A1384	U1263	G1138	C1064
U2423			G2190	A2126	G2024			A1610	A1496	G1385	U1263	U1065	U1066
C2424			G2127	G2127	C2025	G1899	A1773	A1610		G1385	G1264	U1066	U1066
A2425			U2197	C2128		A1900	A1773			A1265	A1265	A1067	A1067
			A2198	C2129	G2029		G1774	G1628	U1503	A1393	G1266	A1142A	G1068
G2428			C2130	U2130	A2030	G1906	U1775	U1629	C1504	U1394	U1267	A1143	A1069
G2429			C2200	G2131	A2031		U1778	A1632	A1507	A1395	A1268	A1070	A1070
C2324			G2032	U2132	G2032	U1911	U1779			U1396		C1153	G1071
A2430			G2032	U2132	G2032		U1779	U1639	A1508	U1405	G1271	A1508	C1072
U2431			G2206	G2033	A2033	C1914	U1780	C1640	C1509	U1405	A1272	A1155	A1073
A2432			A2134	G2133			G1781	U1639	A1509A	U1406	U1273	A1156	
			A2208	A2135	G2037	U1915	G1781	C1640	A1509B	C1407			G1074
			G2218	C2136		A1916	G1782	A1641					C1075
A2435			G2219	C2137	C2043	U1917	A1783	G1642	U1514	U1415	U1288	U1165	C1076
				C2138	C2043		A1784		G1515	U1415		C1166	U1077
A2439			A2225	C2139	A2051	A1919	A1785	G1645	U1514	U1415	C1291	U1167	U1078
C2440			C2226	C2139		A1919	A1785	C1646	G1416	C1417	U1292	C1079	C1079
A2442			A2227	C2140	C2055	G1920	A1786	C1647			C1292		C1080

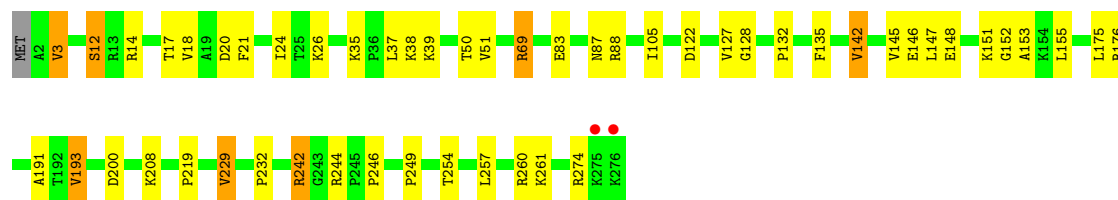


Molecule 1: 23S Ribosomal RNA

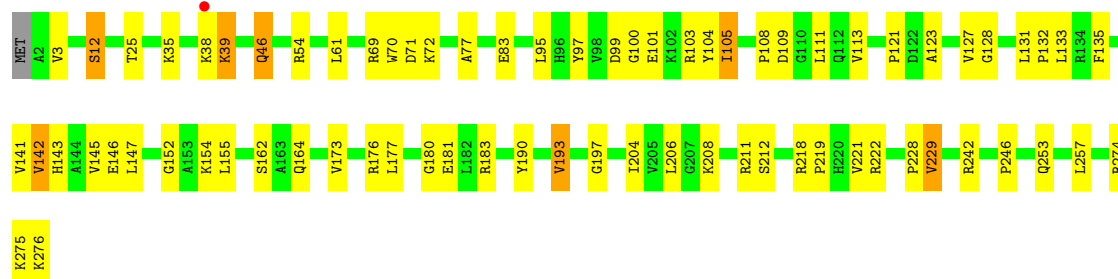


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G2131	A2051	U1956	A1848	G1740	C1607	A1495	C1402	C1297	G1187	C	G1040	G948	A872
G2132	G2052	C1957	A1849	A1741	A1608	A1496	A1405	U1300	U1188	U	G1041	G949	G873
G2133	C1958	C1958	A1853	G1746	A1609	C1498	U1406	A1301	C1200	C	G1042	A953	G874
A2134	C2055	G1959	A1854	G1756	A1610	C1499	U1406	A1301	C1200	A	G1043	G956	G875
A2135	G2056	A1960	A1854	G1757	G1628	G1500	U1406	C1314	A1204	A	G	U877	U877
C2136	C2061	C1961	G1858	U1757	U1629	G1501	G1413	C1315	U1205	A	A	A959	A878
C2137	A2060	C1962	A1859	G1758	G1630	C1502	G1414	C1316	A960	G	A	A960	G879
C2138	G2061	U1963	G1859	G1758	C1631	U1503	U1415	A1317	G1209	G	A	C961	G880
C2139	C2064	G1964	A1865	A1762	C1631	C1504	G1416	U1211	U1211	C	C	G962	G881
C2140	C2065	C1965	U1864	G1763	A1631A	C1505	C1417	A1321	A	A	A	U963	G882
C2066	C2066	C1966	G1865	G1764	A1632	C1506	C1418	G1324	A1220	G	A	G	G883
C2067	C2067	C1967	C1866	G1765	G1633	A1507	A1419	G1324	A1220	C	C	C970	C884
U2068	U2068	G1968	A1876	U1766	A1634	A1508	U1420	C1327	G1221	U	A	C971	C885
G2069	G2147	A1969	A1877	G1767	G1635	C1509	G1421	C1327	C1221A	A	A	A	C886
G2148	G2148	A1970	G1878	U1768	G1636	A1509A	G1422	G1332	G1115	G	G	G974	A887
G2149	A2071	A1971	G1883	G1770	C1638	U1514	G1423	G1332	C1116	G	A	C975	C888
U2150	U2079	A1972	G1883	G1771	U1639	G1515	C1428	C1333	G1117	A	A	A981	C889
G2151	G2080	A1978	A1890	C1772	C1648	A1528A	U1434	U1335	G1125	G	G	C982	A890
G2152	U2086	G1984	G1899	A1773	A1652	G1529	A1434	U1336	A1126	G	A	A983	C892
G2153	G2087	U1993	A1900	C1774	G1653	C1530	G1436	G1337	U1130	U	U	A	C894
G2154	U2096	G1992	G1906	A1780	A1654	G1531	U1445	U1340	A1129	G	G	G987	U895
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G2156	U2098	G1997	C1908	A1782	A1656	U	C1445A	G1342	G1335	U	A	G993	A899
G2157	U2099	G1998	A1785	A1785	A1657	A	G1447	G1343	U1249	U	U	C994	A900
G2160	G2100	C2000	U1911	A1786	C1658	C1536	G1448	A1349	G1139	G	A	C995	A901
C2161	G2101	A2001	A1912	A1786	C1658	C1536	A1449	U1352	G1140	A	A	A996	C902
G2162	G2102	G2002	A1913	C1790	G1663	G1539	G1450	U1352	U1141	A	A	C997	C903
C2163	C2103	G2002	A1914	A1791	A1664	U1540	C1450A	U1357	U1142	G	G	C998	C904
G2164	G2104	C2006	U1915	U1796	A1665	G1541	U1453	G1358	A1142A	C	C	U999	C908
G2165	C2105	C2006	A1916	C1797	G1666	A1542	G1455	A1359	G1149	G	A	C1005	A909
G2166	C2106	G2010	U1917	U1798	G1667	A1543	G1455	A1360	G1150	C	C	C1006	A910
U2167	C2107	G2010	A1918	G1799	A1669	G1547	A1460	G1361	G1151	C	C	A1010	A911
G2168	C2108	A2014	U1923	C1800	C1670	A1554	G1461	G1364	C1152	A	A	U1019	C912
A2169	U2109	C2021	C1924	G1801	G1674	A1558	C1462	A1365	C1153	U	U	A1020	U922
A2170	C2110	C2021	U1925	A1815	G1686	A1568	C1463	A1366	G1154	C	A	A1021	U923
A2171	C2111	G2022	U1926	A1816	C1687	G1568	C1464	A1367	C1155	C	C	U1012	C914
A2172	C2112	G2023	A1927	G1817	U1688	A1569	G1465	A1368	A1156	C	U	C1013	C915
A2173	G2113	G2024	A1928	G1817	A1689	U1578	G1466	G1369	A1156	U	U	G1024	G916
A2174	U2113	C2025	G1929	U1818	U1689	A1579	C1467	G1270	U1165	U	U	U1019	A917
C2175	A2114	C2026	G1930	U1818	A1689	U1578	A1471	G1271	C1166	A	A	A1020	C922
A2176	G2115	C2026	U1931	G1823	G1696	A1579	A1471	U1273	U1167	A	A	U1022	C924
A2177	G2116	G2027	A1932	G1823	G1697	A1580	C1474	A1274	G1171	G	G	G1025	C925
C2178	A2117	C2027	G1933	G1826	A1698	A1581	G1475	G1277	G	A	A	U1026	C932
C2179	U2118	A2030	C1934	C1827	G1699	C1582	C1476	A1278	U	A	G	A1027	G938
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G2181	G2120	G2032	A1936	A1827	A1700	C1584	G1478	G1283	A	U	C	A1029	G942
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G2183	U2122	U2034	A1938	U1834	U1709	C1588	G1482	A1287	C1179	G	U	G1031	G942
G2184	G2123	G2035	A1938	U1834	U1709	C1588	G1482	A1287	C1179	G	U	A1032	U943
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G2187	A2126	G2038	C1946	G1839	A1722	A1603	C1493	C1293	C1185	G	A	C1038	G946
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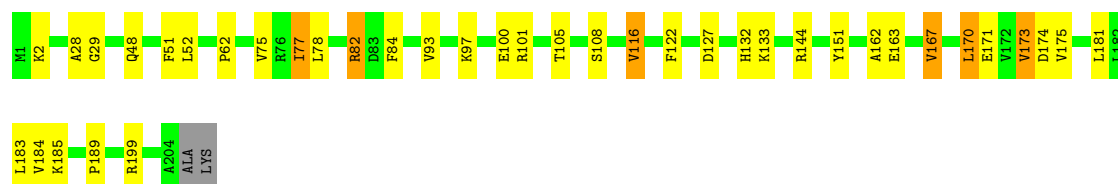
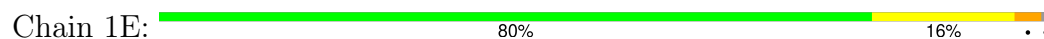




• Molecule 3: 50S ribosomal protein L2



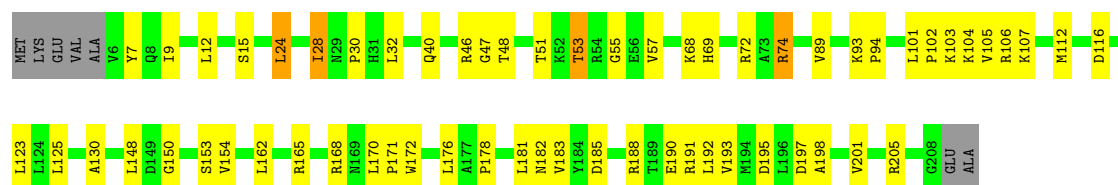
• Molecule 4: 50S ribosomal protein L3



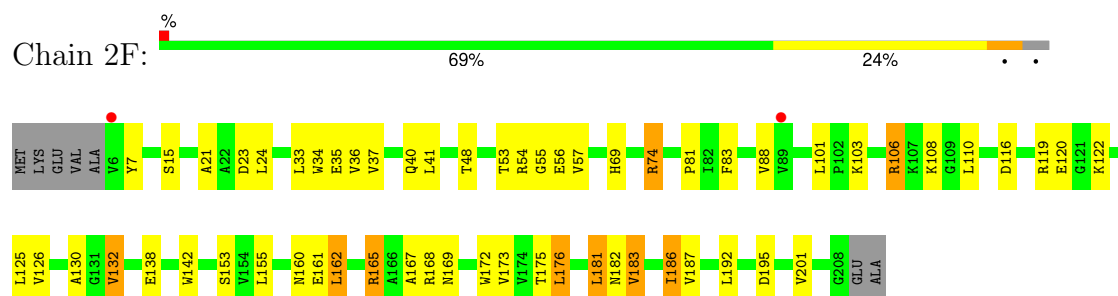
• Molecule 4: 50S ribosomal protein L3



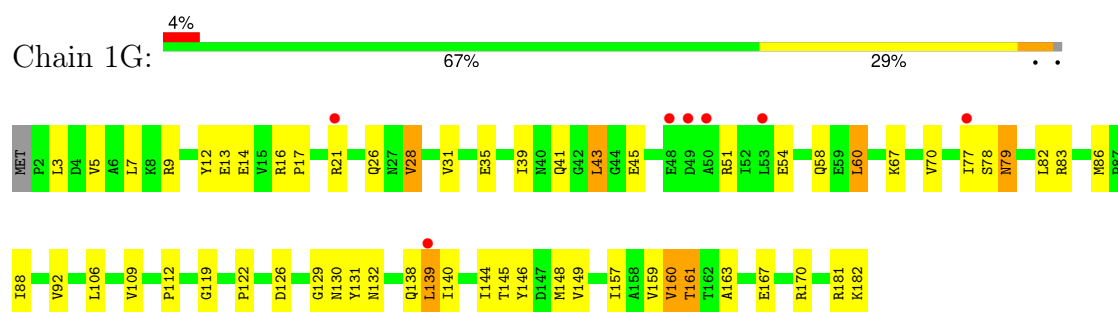
• Molecule 5: 50S ribosomal protein L4



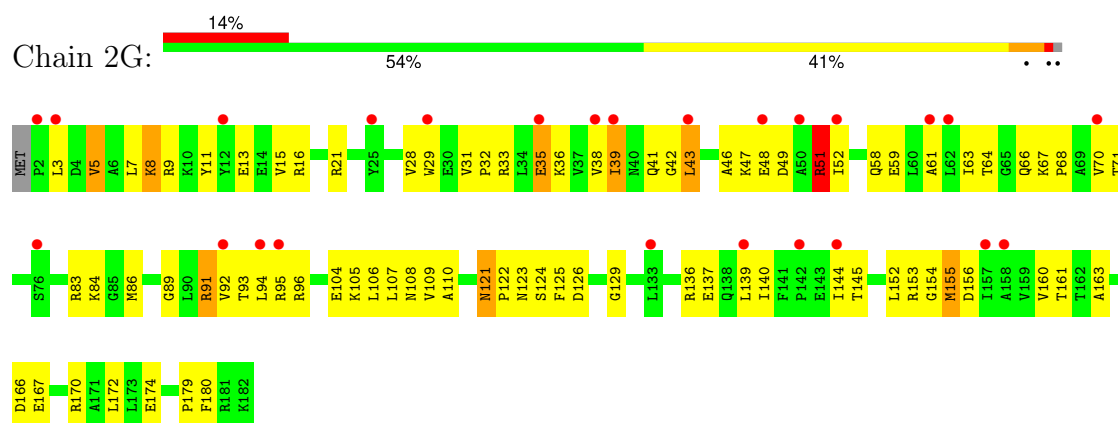
- Molecule 5: 50S ribosomal protein L4



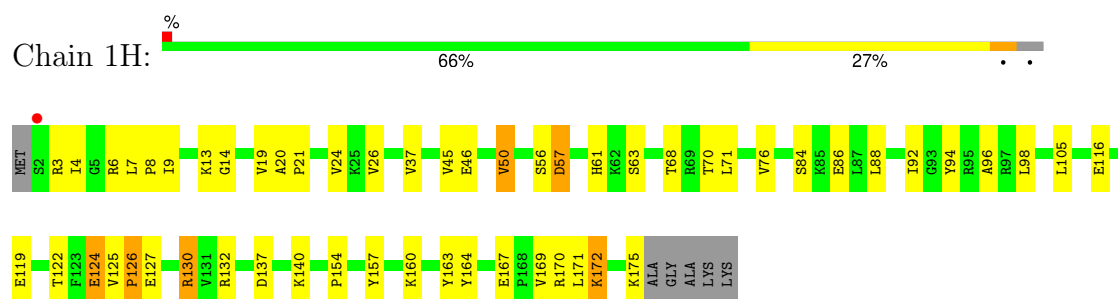
- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5

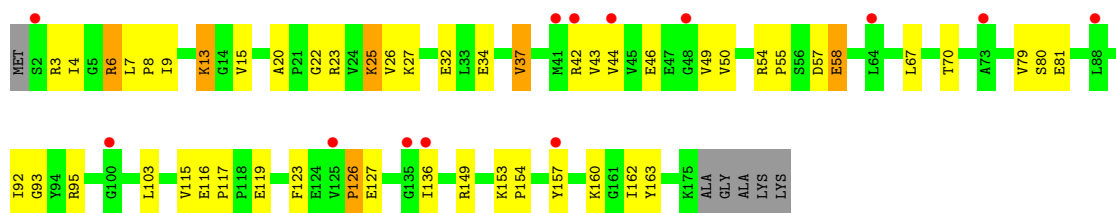


- Molecule 7: 50S ribosomal protein L6



- Molecule 7: 50S ribosomal protein L6

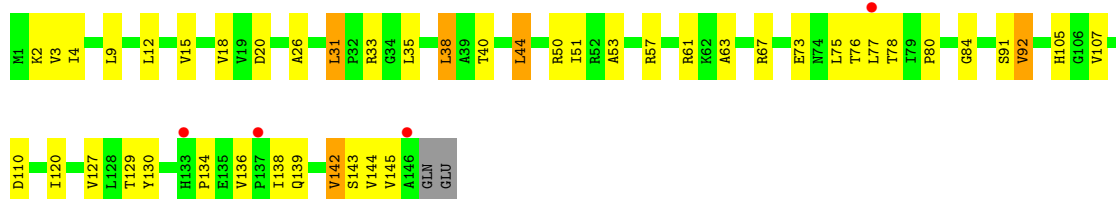




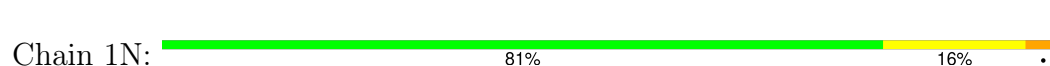
• Molecule 8: 50S ribosomal protein L9



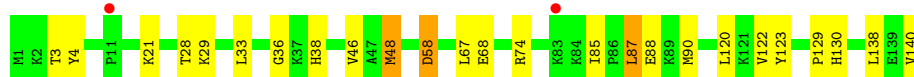
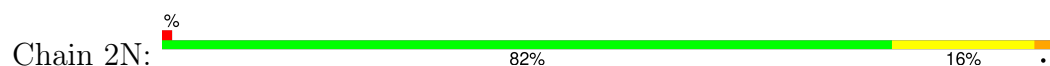
• Molecule 8: 50S ribosomal protein L9



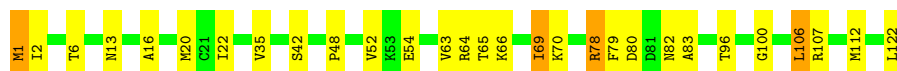
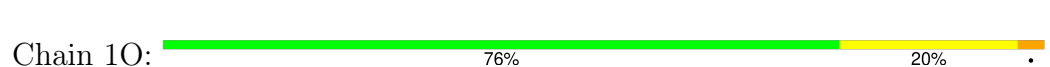
• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  82% 17%



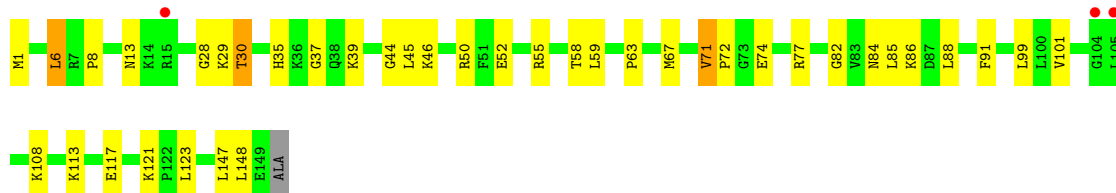
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  81% 16%



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  73% 24%



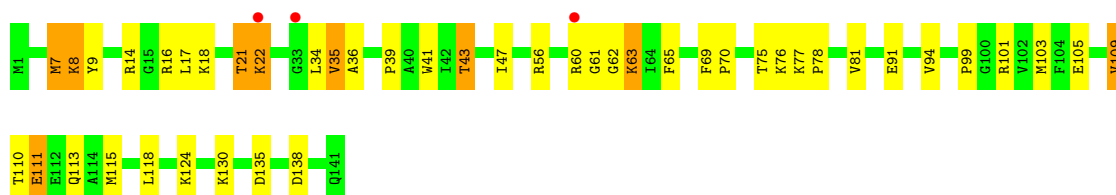
- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  79% 18%



- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  68% 26% 6%



- Molecule 13: 50S ribosomal protein L17

Chain 1R:  80% 19%



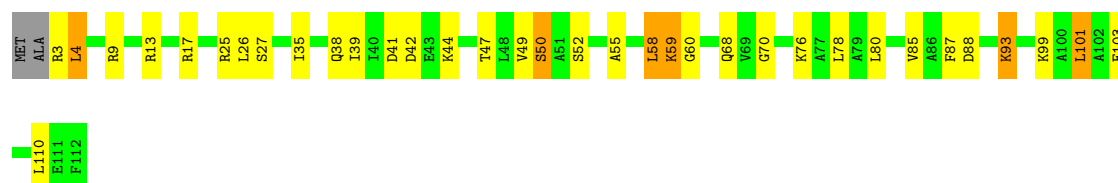
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  73% 25% .



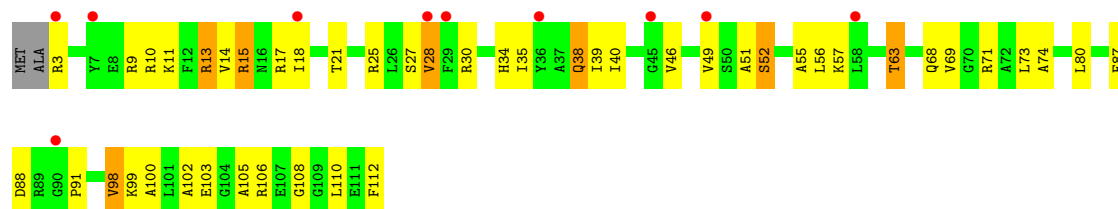
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  67% 26% 5% .



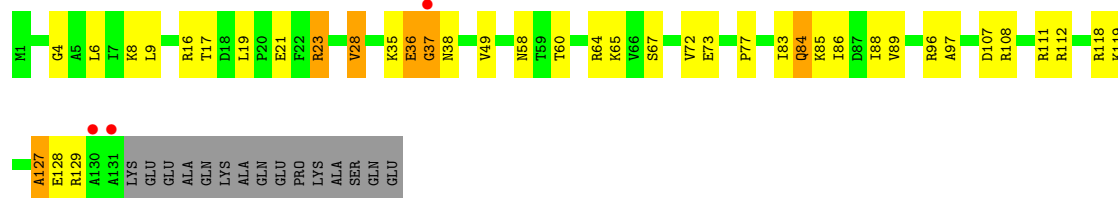
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  9% 57% 35% 6% .



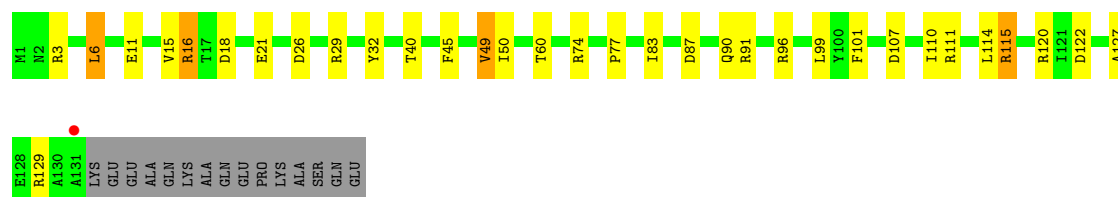
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  2% 62% 23% 10% .



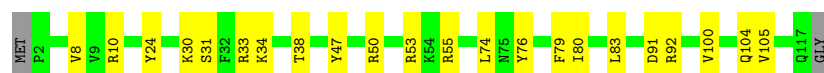
- Molecule 15: 50S ribosomal protein L19

Chain 2T:  67% 20% 10% .



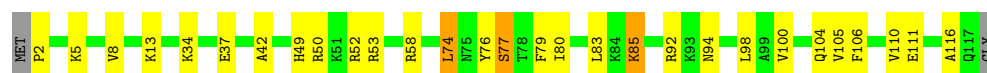
- Molecule 16: 50S ribosomal protein L20

Chain 1U:  80% 19%



- Molecule 16: 50S ribosomal protein L20

Chain 2U:  74% 22%



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  80% 19%



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  80% 18%



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  81% 18%



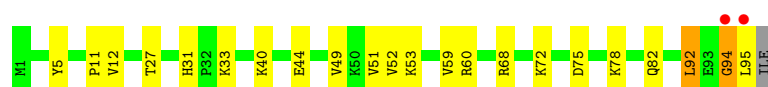
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  82% 16%



- Molecule 19: 50S ribosomal protein L23

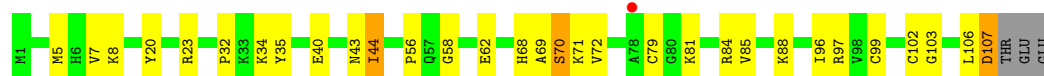
Chain 1X:  76% 21%



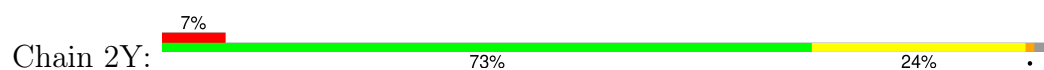
- Molecule 19: 50S ribosomal protein L23



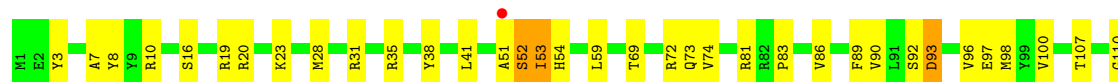
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

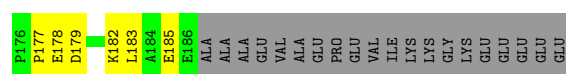
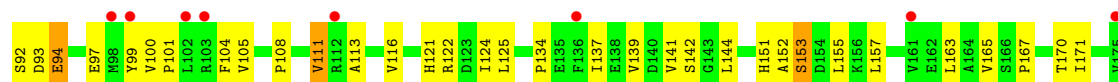
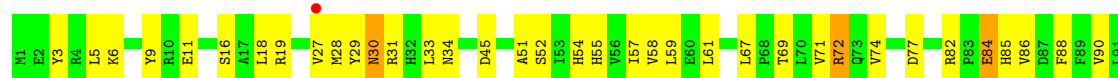


- Molecule 21: 50S ribosomal protein L25

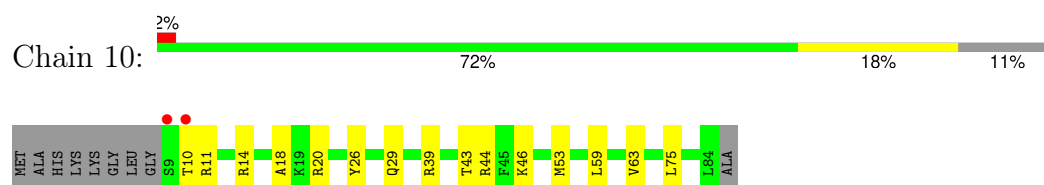


LYS
LYS
GLY
LYS
GLU
GLU
GLU

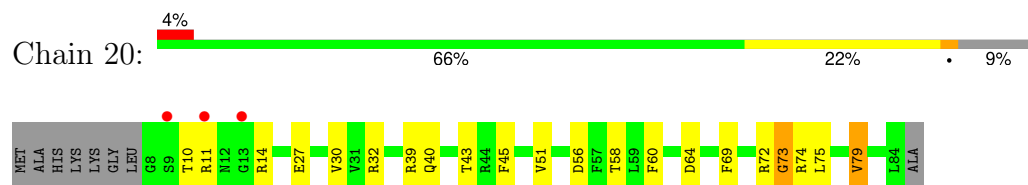
- Molecule 21: 50S ribosomal protein L25



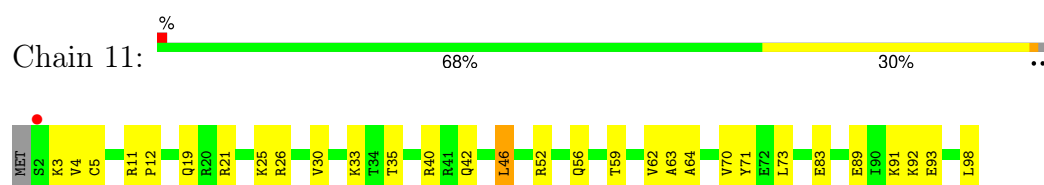
- Molecule 22: 50S ribosomal protein L27



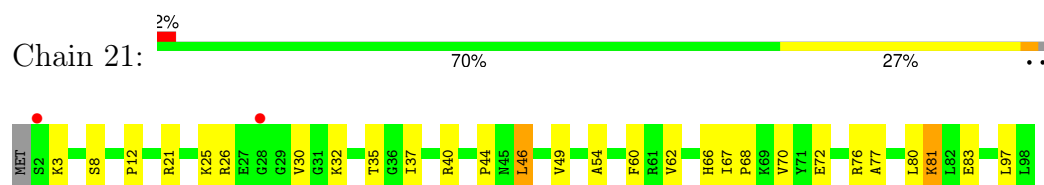
- Molecule 22: 50S ribosomal protein L27



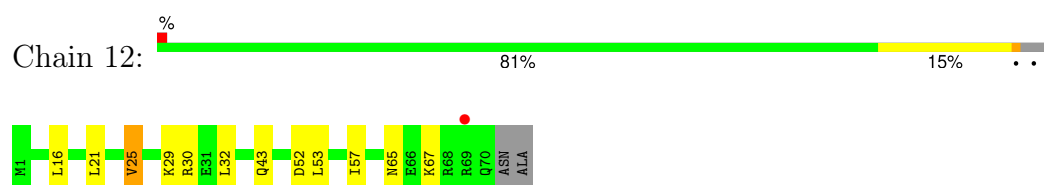
- Molecule 23: 50S ribosomal protein L28



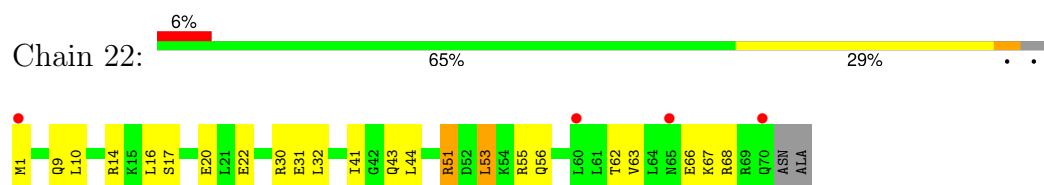
- Molecule 23: 50S ribosomal protein L28



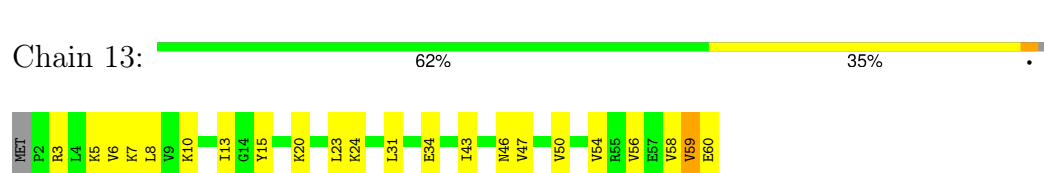
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



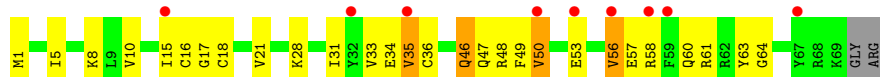
- Molecule 25: 50S ribosomal protein L30

Chain 23:  63% 32% ..



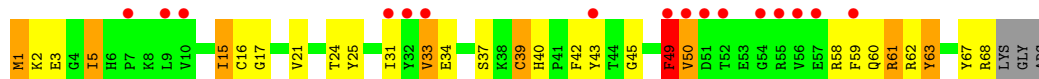
- Molecule 26: 50S ribosomal protein L31

Chain 14:  13% 58% 34% 6% .



- Molecule 26: 50S ribosomal protein L31

Chain 24:  23% 55% 28% 11% ..



- Molecule 27: 50S ribosomal protein L32

Chain 15:  75% 22% ..



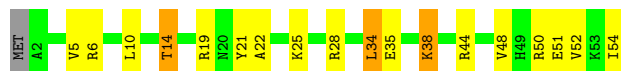
- Molecule 27: 50S ribosomal protein L32

Chain 25:  3% 70% 28% .



- Molecule 28: 50S ribosomal protein L33

Chain 16:  65% 28% 6% .

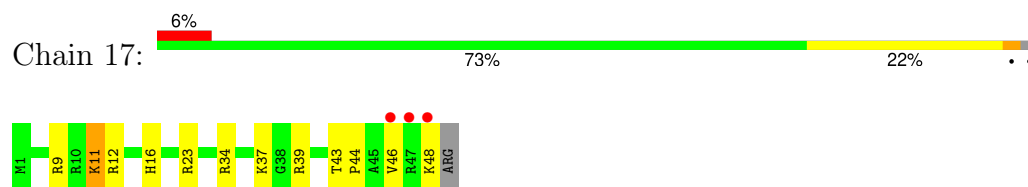


- Molecule 28: 50S ribosomal protein L33

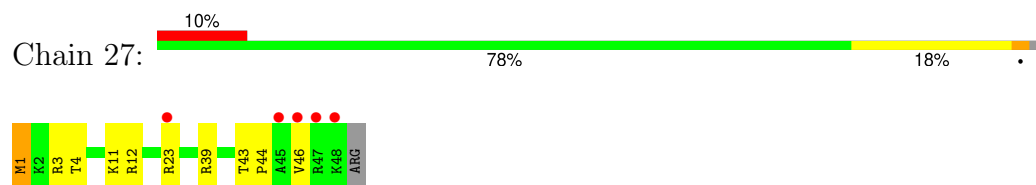
Chain 26:  2% 63% 31% ..



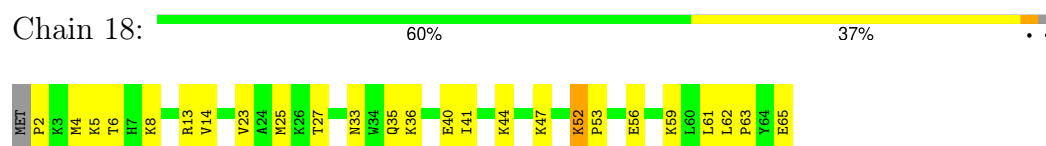
- Molecule 29: 50S ribosomal protein L34



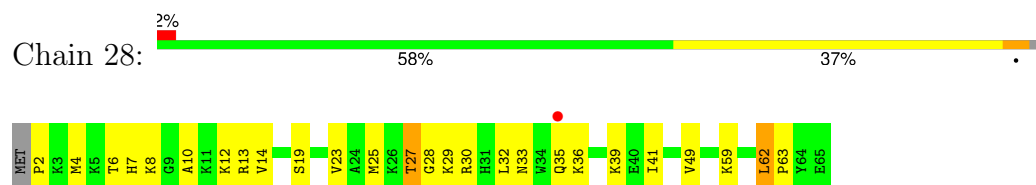
- Molecule 29: 50S ribosomal protein L34



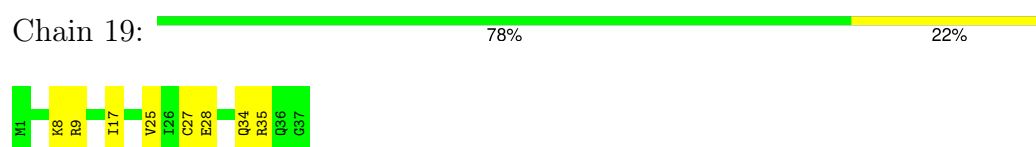
- Molecule 30: 50S ribosomal protein L35



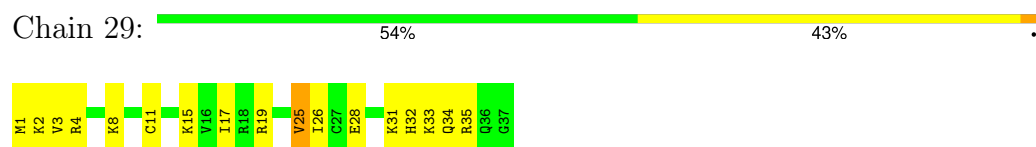
- Molecule 30: 50S ribosomal protein L35



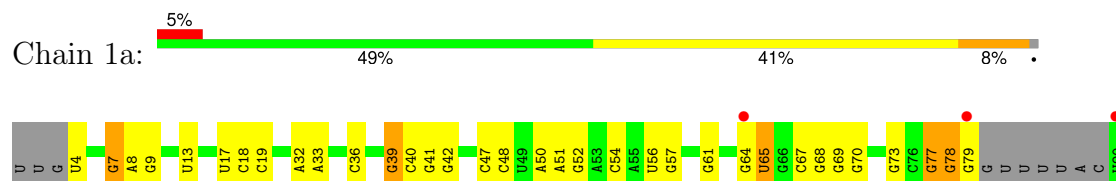
- Molecule 31: 50S ribosomal protein L36

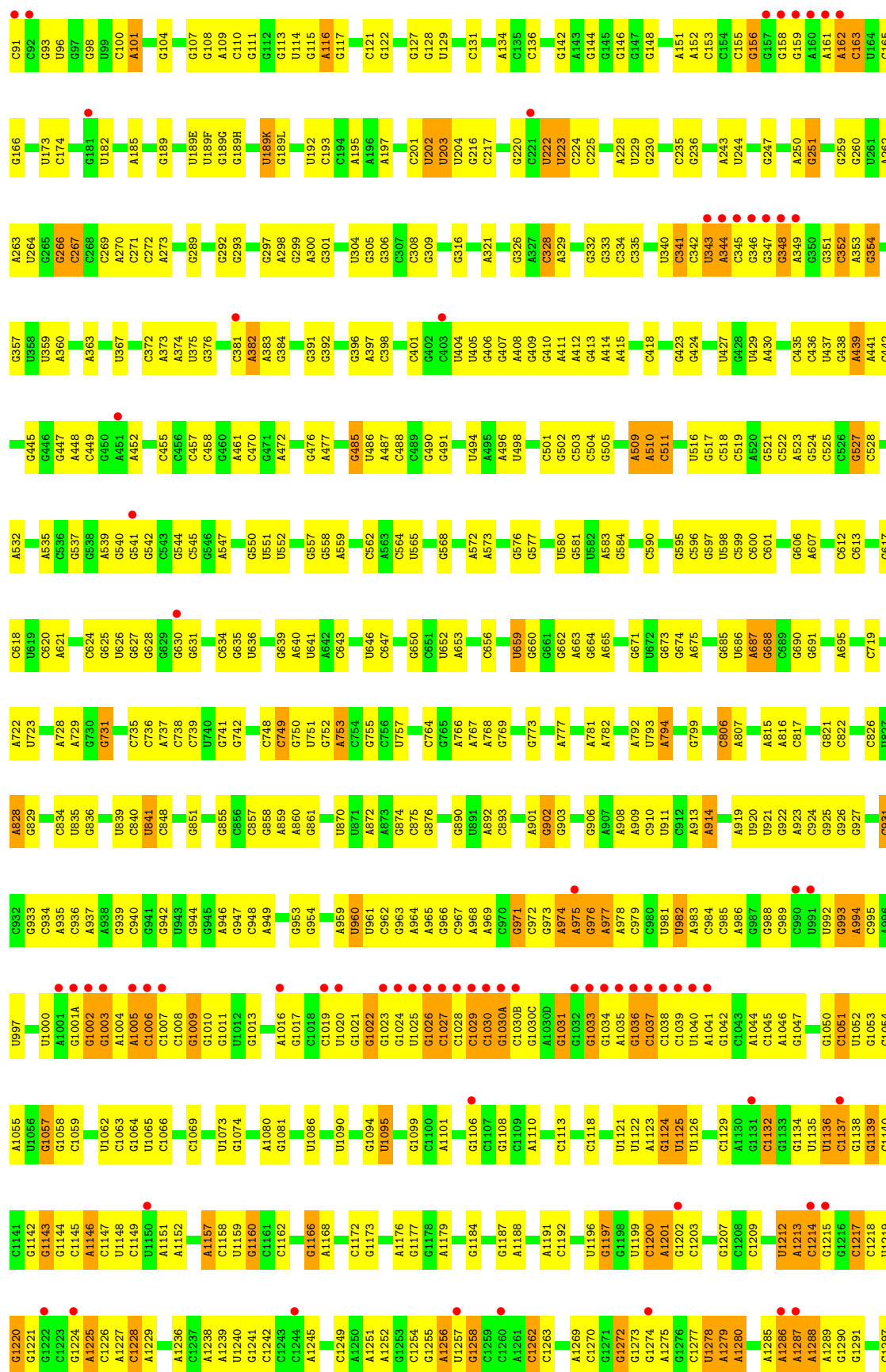


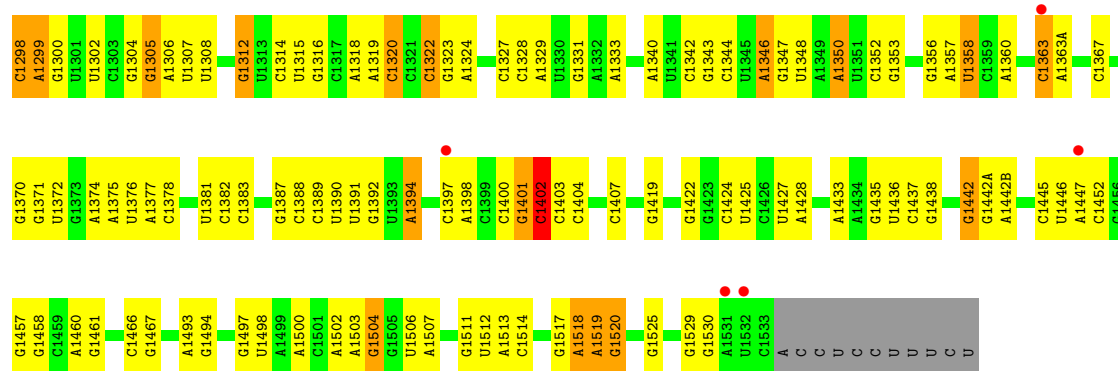
- Molecule 31: 50S ribosomal protein L36



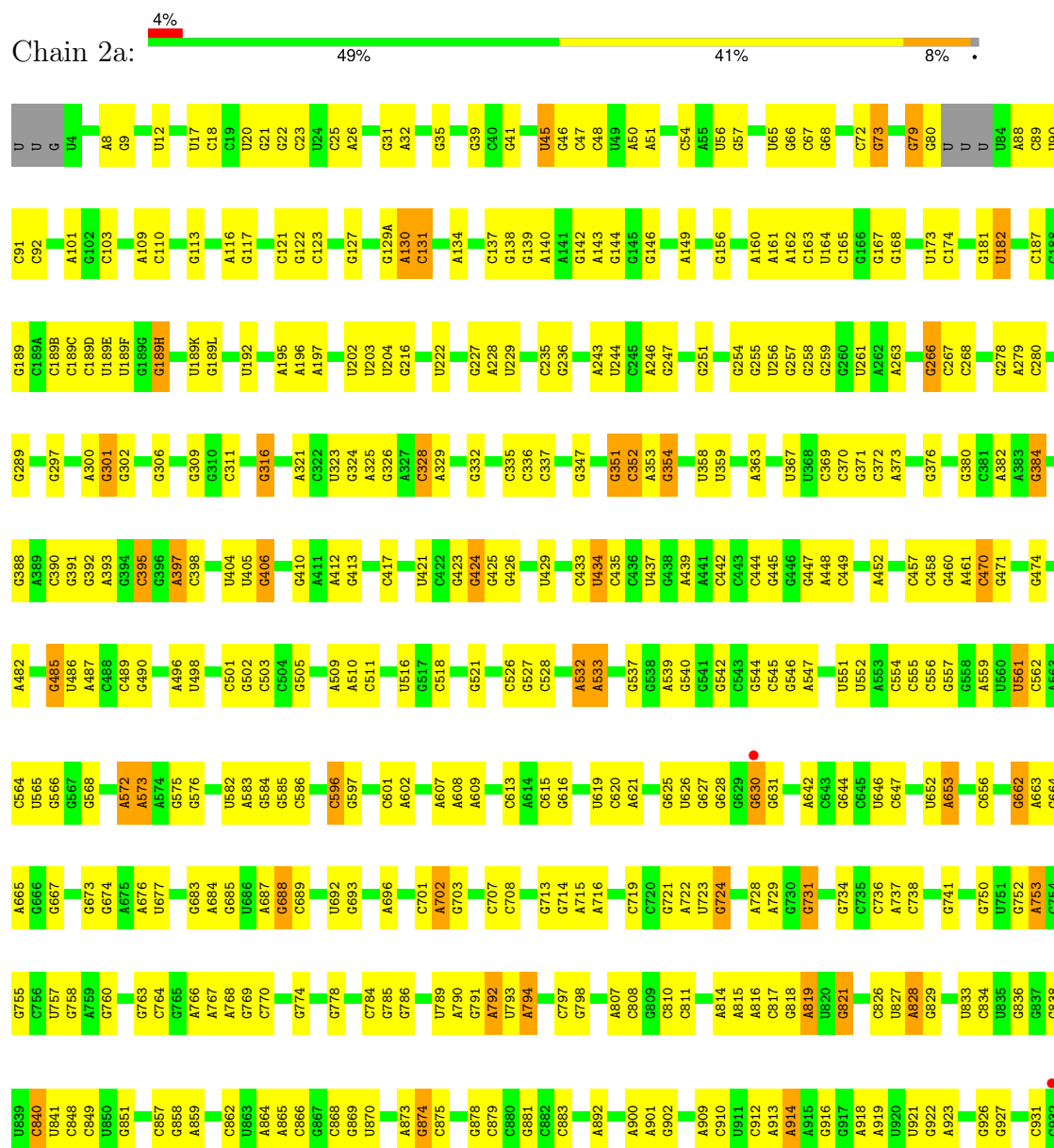
- Molecule 32: 16S Ribosomal RNA

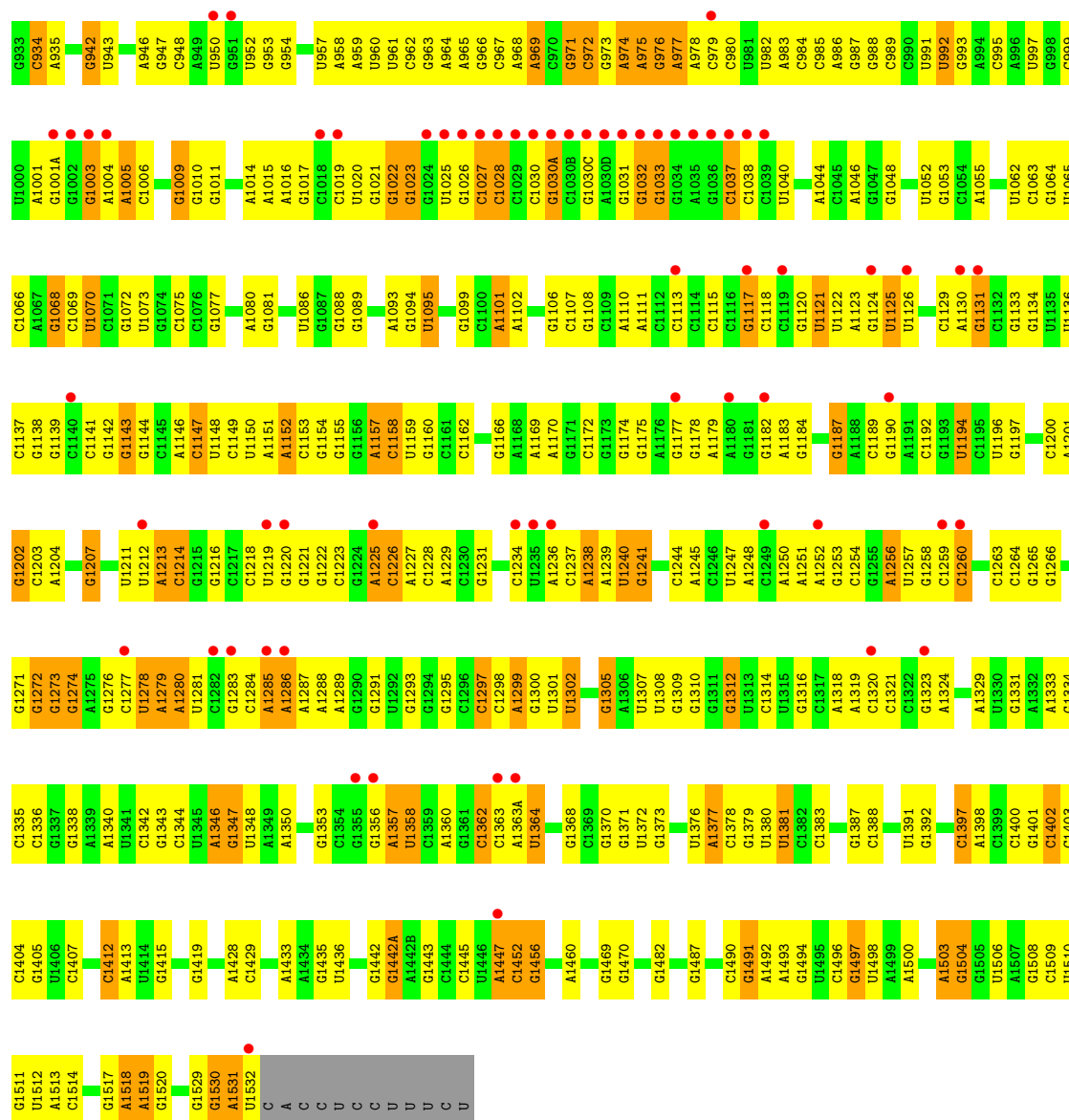




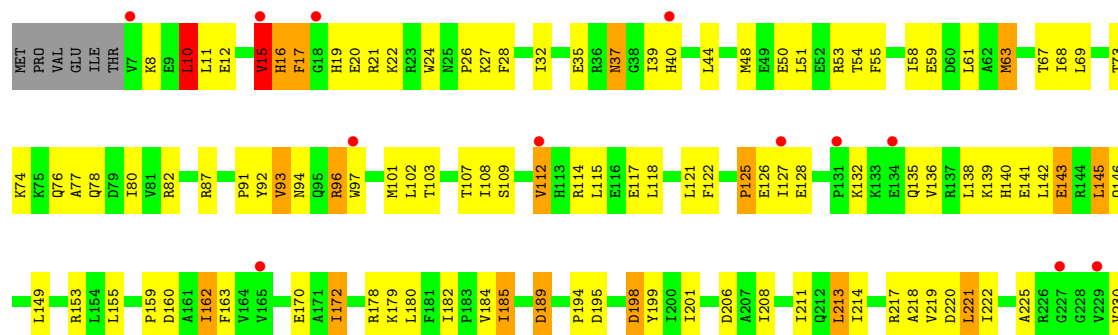


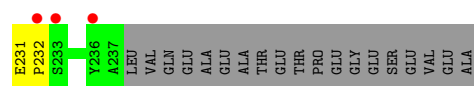
• Molecule 32: 16S Ribosomal RNA



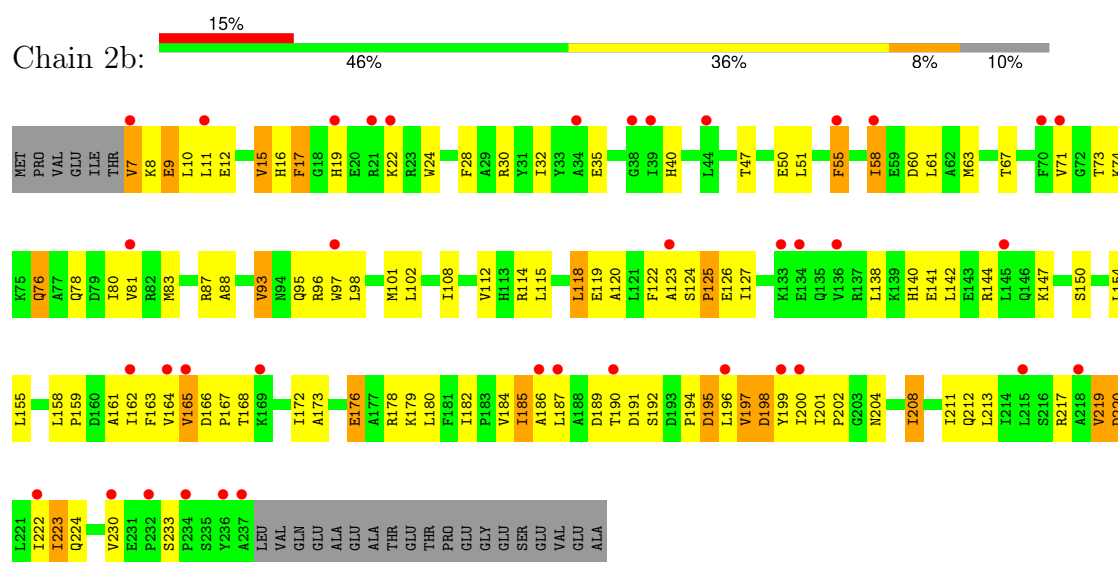


• Molecule 33: 30S ribosomal protein S2

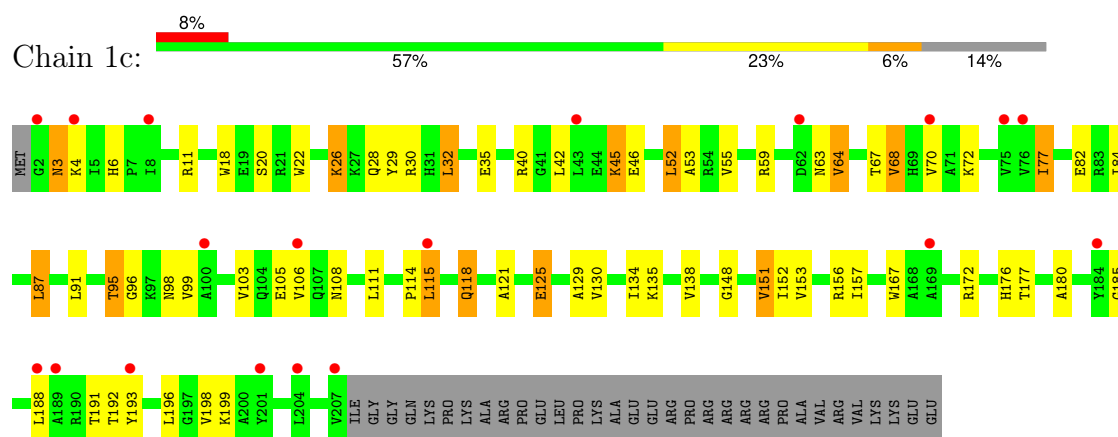




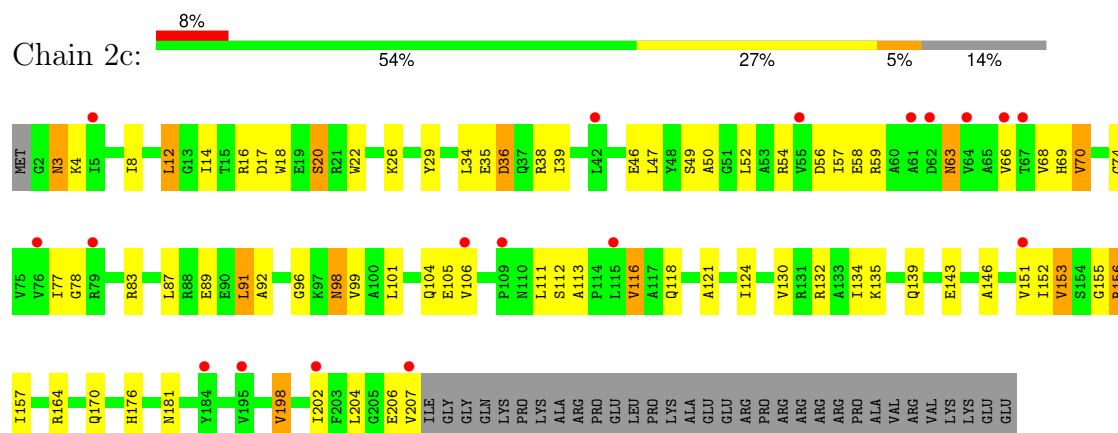
• Molecule 33: 30S ribosomal protein S2



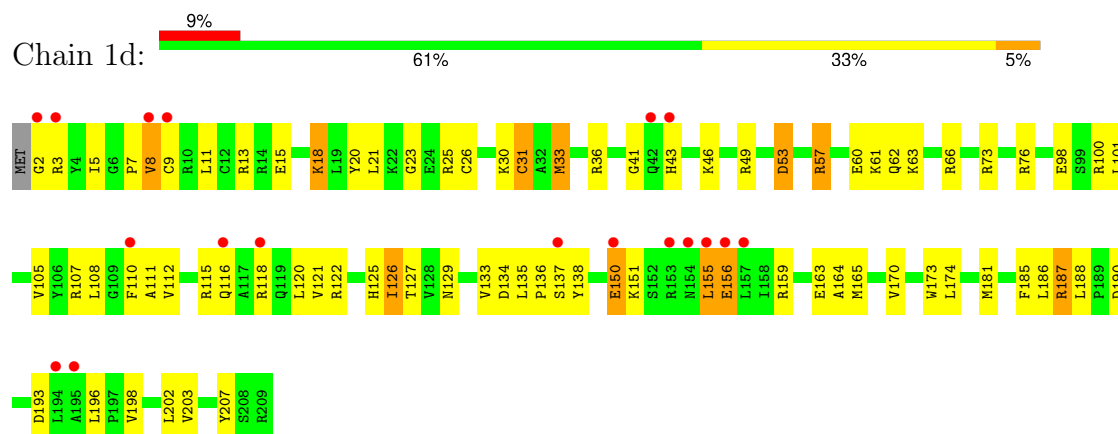
• Molecule 34: 30S ribosomal protein S3



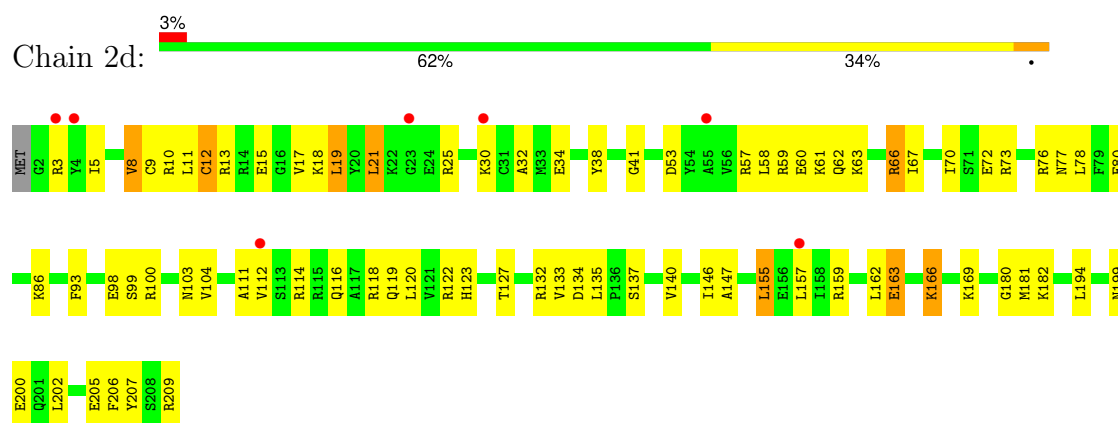
• Molecule 34: 30S ribosomal protein S3



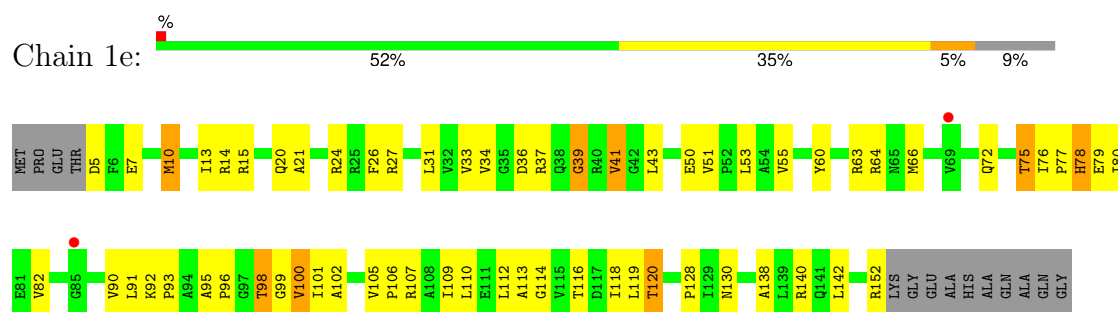
- Molecule 35: 30S ribosomal protein S4



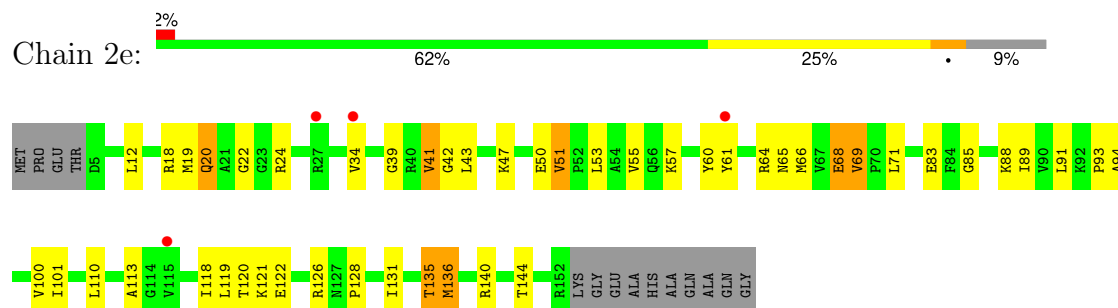
- Molecule 35: 30S ribosomal protein S4



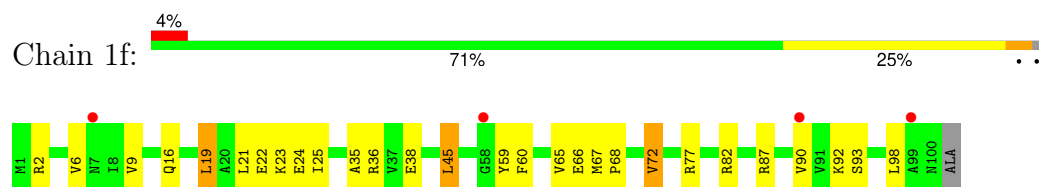
- Molecule 36: 30S ribosomal protein S5



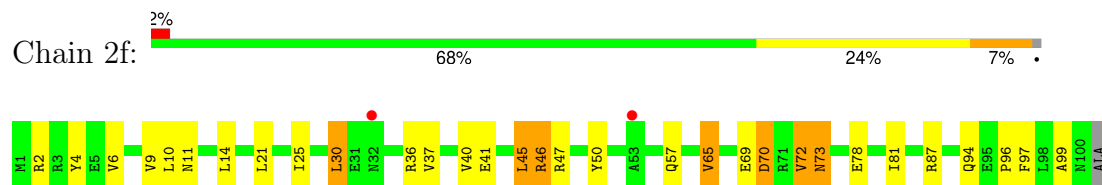
- Molecule 36: 30S ribosomal protein S5



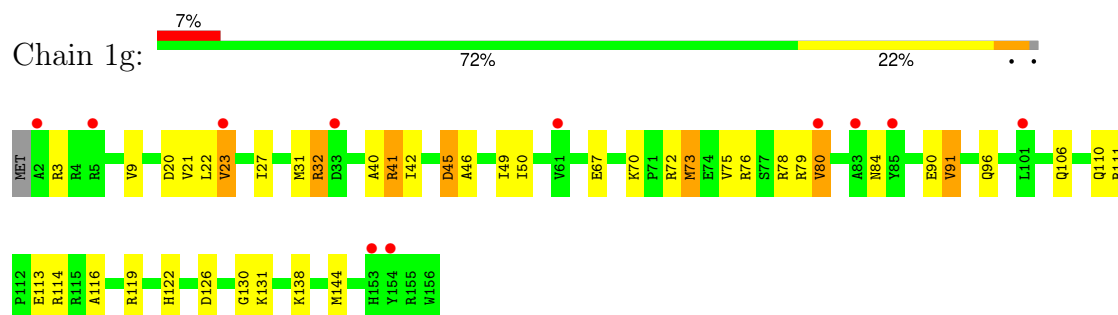
- Molecule 37: 30S ribosomal protein S6



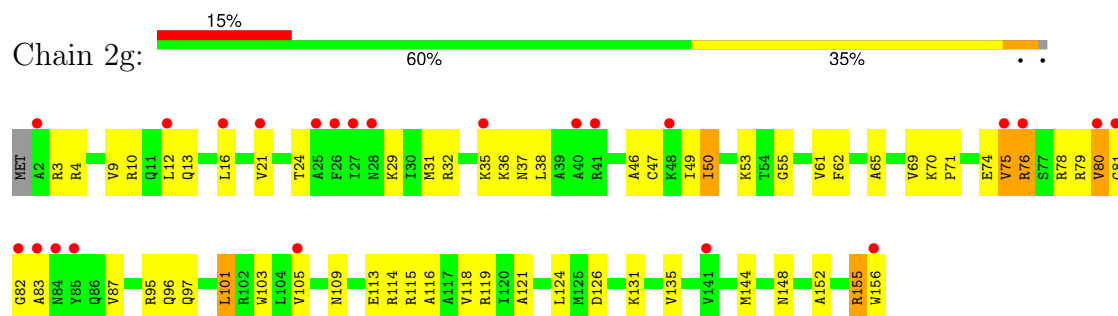
- Molecule 37: 30S ribosomal protein S6



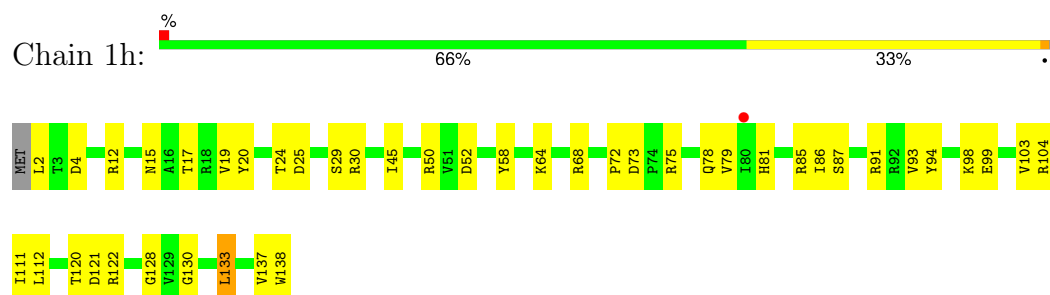
- Molecule 38: 30S ribosomal protein S7



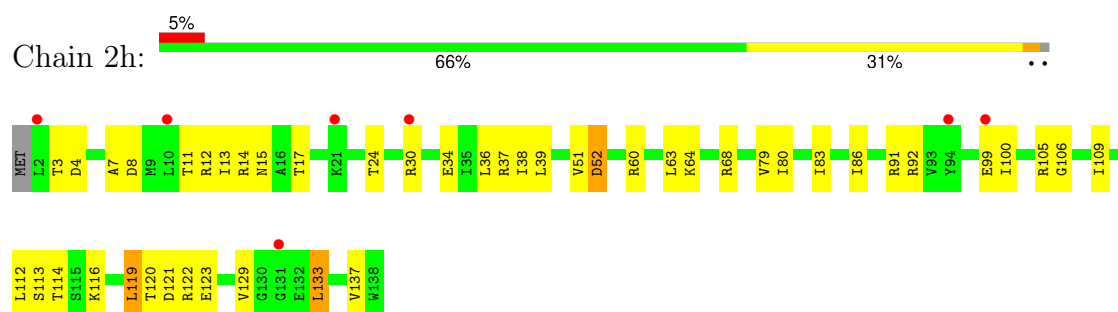
- Molecule 38: 30S ribosomal protein S7



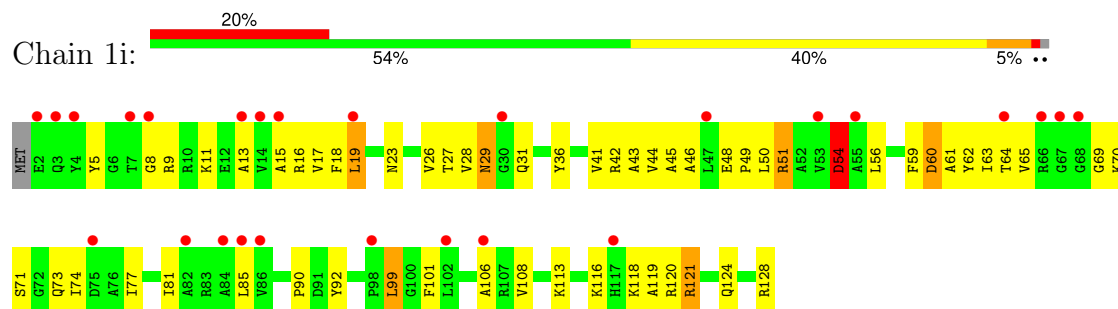
- Molecule 39: 30S ribosomal protein S8



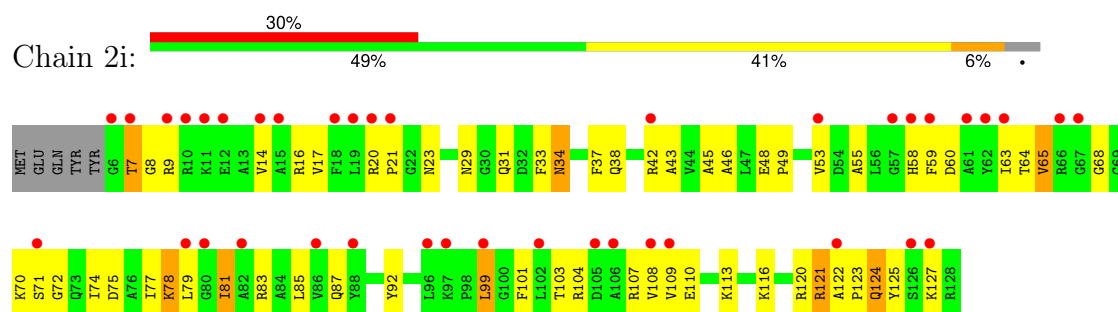
- Molecule 39: 30S ribosomal protein S8



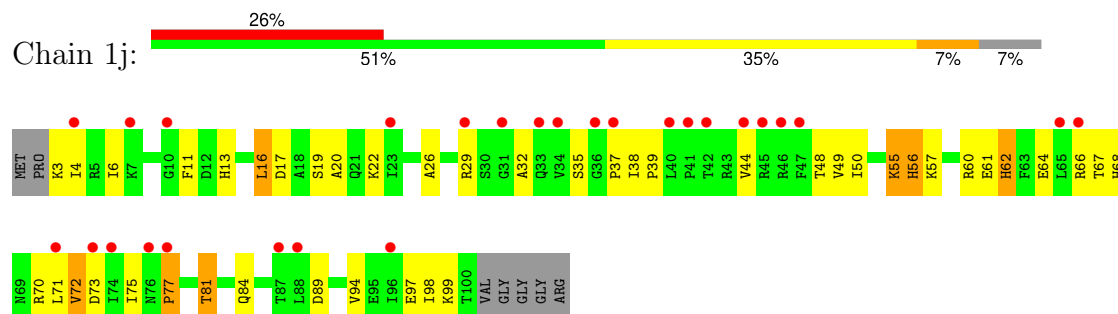
- Molecule 40: 30S ribosomal protein S9



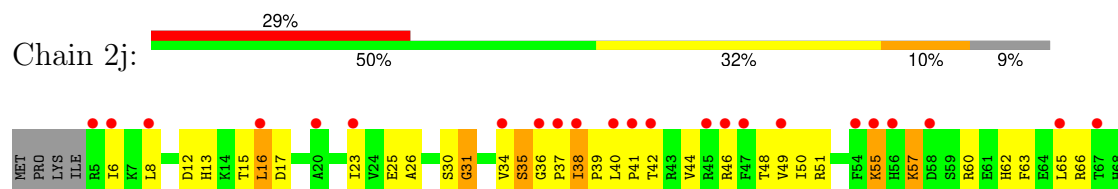
- Molecule 40: 30S ribosomal protein S9

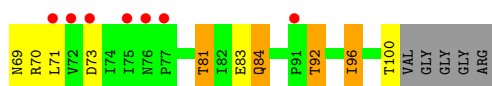


- Molecule 41: 30S ribosomal protein S10

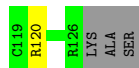
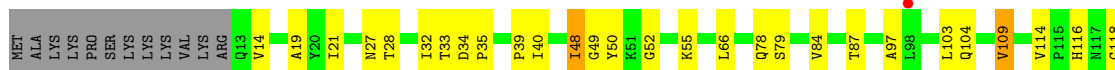


- Molecule 41: 30S ribosomal protein S10





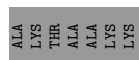
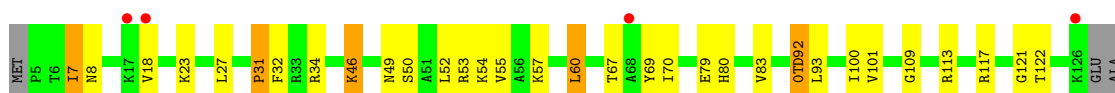
- Molecule 42: 30S ribosomal protein S11



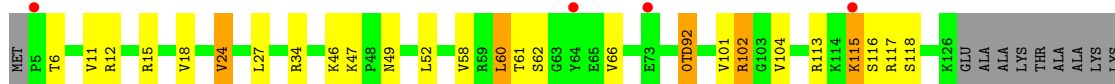
- Molecule 42: 30S ribosomal protein S11



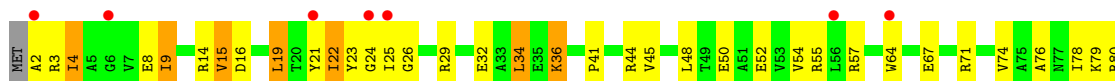
- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12

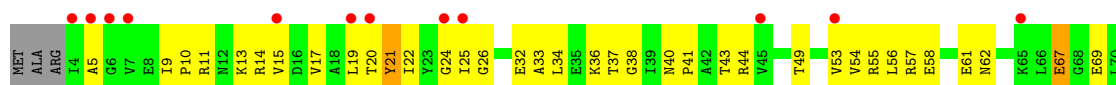


- Molecule 44: 30S ribosomal protein S13





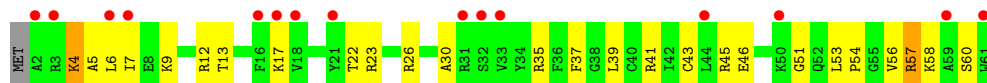
- Molecule 44: 30S ribosomal protein S13



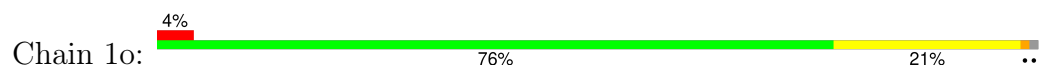
- Molecule 45: 30S ribosomal protein S14 type Z



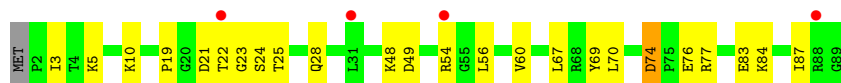
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

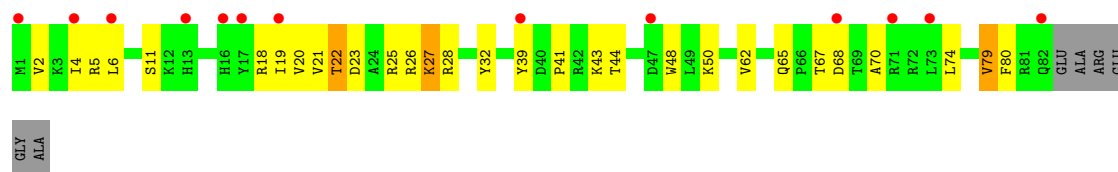


- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

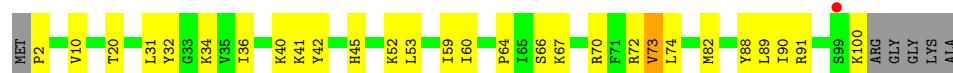




- Molecule 47: 30S ribosomal protein S16



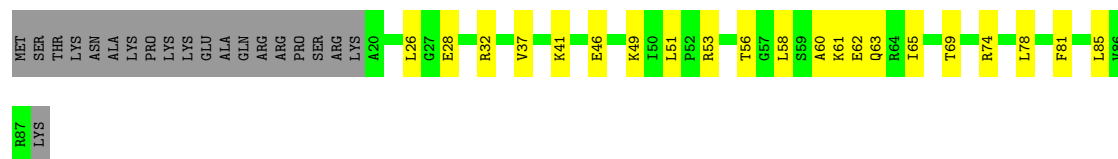
- Molecule 48: 30S ribosomal protein S17



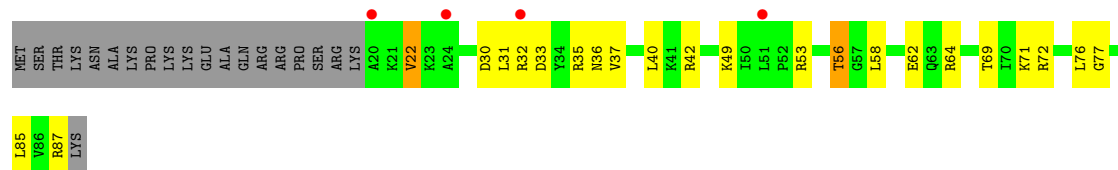
- Molecule 48: 30S ribosomal protein S17



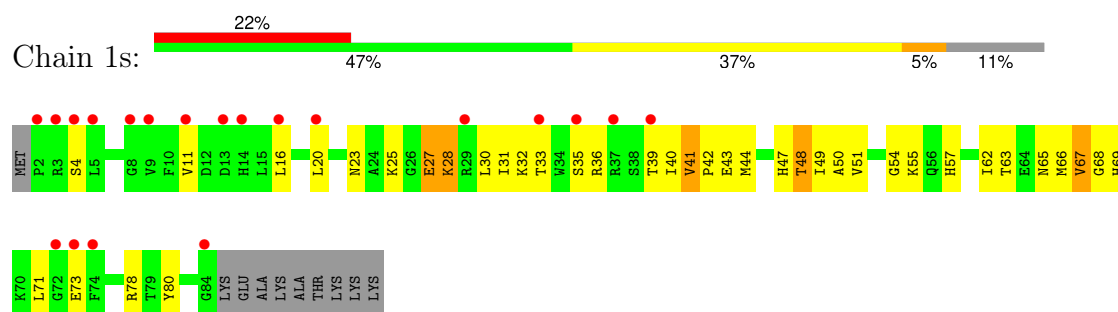
- Molecule 49: 30S ribosomal protein S18



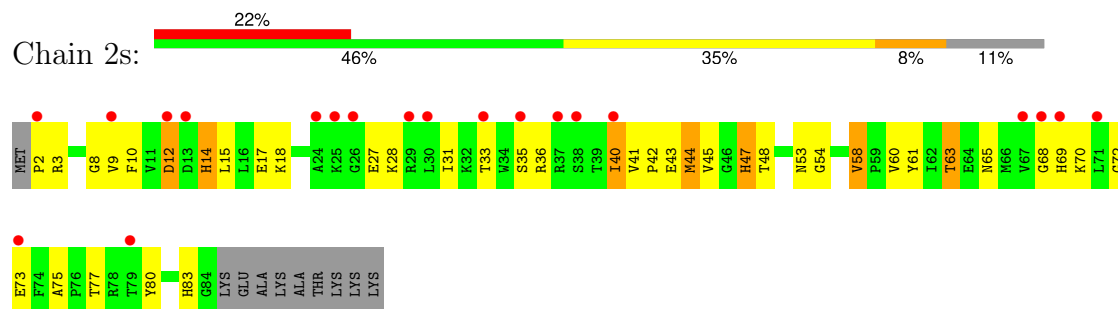
- Molecule 49: 30S ribosomal protein S18



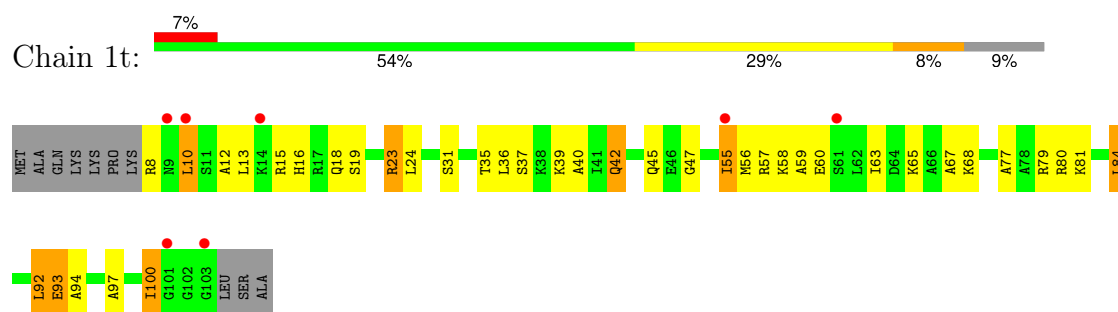
- Molecule 50: 30S ribosomal protein S19



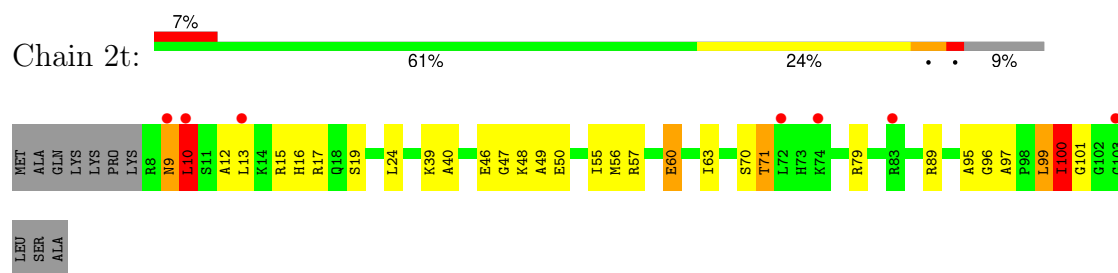
- Molecule 50: 30S ribosomal protein S19



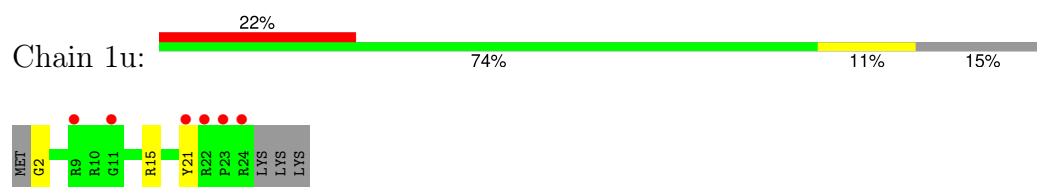
- Molecule 51: 30S ribosomal protein S20



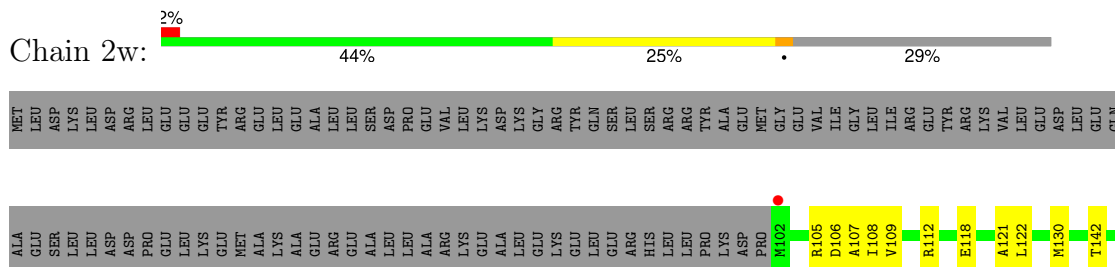
- Molecule 51: 30S ribosomal protein S20

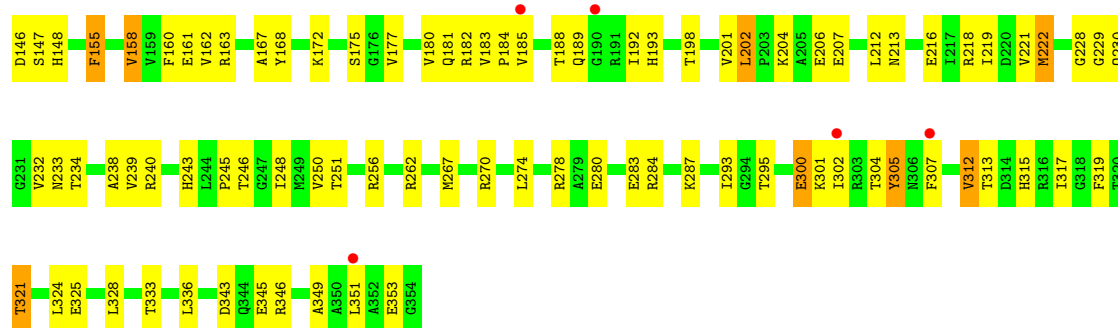


- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx





• Molecule 55: P-site and E-site Deacylated tRNAphe



• Molecule 55: P-site and E-site Deacylated tRNAphe



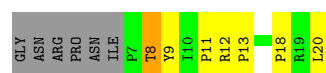
• Molecule 55: P-site and E-site Deacylated tRNAphe



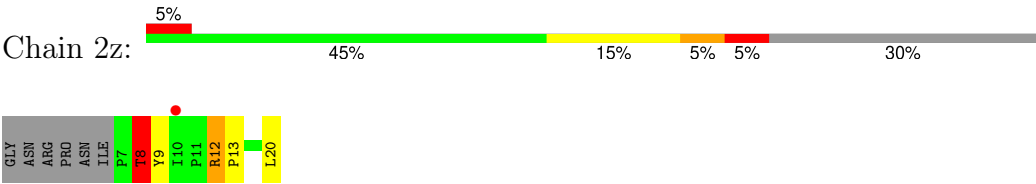
• Molecule 55: P-site and E-site Deacylated tRNAphe



• Molecule 56: Fva1 Antimicrobial Peptide



● Molecule 56: Fva1 Antimicrobial Peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.39Å 451.41Å 623.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.02 – 2.70 37.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (37.02-2.70) 96.7 (37.02-2.70)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.226 , 0.275 0.226 , 0.274	Depositor DCC
R_{free} test set	77897 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299076	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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: ZN, 2MA, PSU, MG, 5MC, OMU, 4SU, UR3, MEQ, 4OC, SF4, G7M, 5MU, M2G, MIA, OMG, 2MG, 0TD, MA6, OMC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.28	0/69011	0.46	1/107720 (0.0%)
1	2A	0.21	1/67295 (0.0%)	0.39	2/105042 (0.0%)
2	1B	0.21	0/2881	0.38	0/4494
2	2B	0.18	0/2881	0.34	0/4494
3	1D	0.26	0/2186	0.49	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.27	0/1592	0.48	0/2149
4	2E	0.21	0/1592	0.43	0/2149
5	1F	0.26	0/1619	0.49	0/2193
5	2F	0.20	0/1615	0.43	0/2188
6	1G	0.21	0/1450	0.42	0/1959
6	2G	0.21	0/1449	0.45	0/1958
7	1H	0.23	0/1356	0.46	0/1834
7	2H	0.19	0/1356	0.38	0/1834
8	1I	0.21	0/1100	0.42	0/1501
8	2I	0.18	0/1076	0.40	0/1471
9	1N	0.26	0/1144	0.44	0/1543
9	2N	0.20	0/1144	0.41	0/1543
10	1O	0.26	0/943	0.44	0/1269
10	2O	0.21	0/943	0.40	0/1269
11	1P	0.26	0/1152	0.52	0/1533
11	2P	0.20	0/1152	0.47	0/1533
12	1Q	0.26	0/1143	0.48	0/1527
12	2Q	0.20	0/1143	0.42	0/1527
13	1R	0.26	0/982	0.51	0/1312
13	2R	0.21	0/982	0.44	0/1312
14	1S	0.21	0/887	0.45	0/1180
14	2S	0.20	0/880	0.44	0/1172
15	1T	0.24	0/1105	0.47	0/1477
15	2T	0.21	0/1097	0.45	0/1468
16	1U	0.31	0/977	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.40	0/1301
17	1V	0.28	0/782	0.49	0/1049
17	2V	0.18	0/782	0.41	0/1049
18	1W	0.31	0/897	0.46	0/1205
18	2W	0.21	0/897	0.43	0/1205
19	1X	0.25	0/764	0.45	0/1025
19	2X	0.21	0/760	0.37	0/1021
20	1Y	0.25	0/819	0.59	0/1095
20	2Y	0.21	0/823	0.43	0/1100
21	1Z	0.23	0/1469	0.47	0/1998
21	2Z	0.20	0/1483	0.42	0/2018
22	10	0.27	0/612	0.54	0/816
22	20	0.21	0/616	0.50	0/821
23	11	0.24	0/762	0.47	0/1014
23	21	0.21	0/762	0.39	0/1014
24	12	0.26	0/590	0.45	0/781
24	22	0.21	0/590	0.40	0/781
25	13	0.27	0/474	0.51	0/635
25	23	0.21	0/469	0.43	0/630
26	14	0.22	0/561	0.49	0/756
26	24	0.28	0/530	0.61	0/719
27	15	0.29	0/469	0.51	0/635
27	25	0.23	0/469	0.44	0/635
28	16	0.24	0/460	0.47	0/613
28	26	0.20	0/456	0.43	0/608
29	17	0.31	0/426	0.48	0/561
29	27	0.24	0/426	0.52	0/561
30	18	0.28	0/519	0.44	0/684
30	28	0.19	0/525	0.39	0/691
31	19	0.27	0/310	0.48	0/407
31	29	0.24	0/310	0.47	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.20	1/35886 (0.0%)	0.38	0/56005
33	1b	0.23	0/1881	0.49	0/2542
33	2b	0.25	0/1860	0.51	0/2518
34	1c	0.21	0/1578	0.44	0/2133
34	2c	0.20	0/1566	0.44	1/2119 (0.0%)
35	1d	0.20	0/1689	0.43	0/2267
35	2d	0.19	0/1704	0.46	0/2284
36	1e	0.21	0/1145	0.49	1/1543 (0.1%)
36	2e	0.21	0/1146	0.46	0/1545
37	1f	0.21	0/823	0.41	0/1116
37	2f	0.20	0/829	0.43	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.20	0/1250	0.40	0/1679
38	2g	0.21	0/1254	0.41	0/1683
39	1h	0.20	0/1108	0.42	0/1494
39	2h	0.19	0/1108	0.43	0/1494
40	1i	0.23	0/1002	0.52	1/1346 (0.1%)
40	2i	0.24	0/957	0.46	0/1288
41	1j	0.22	0/734	0.48	0/997
41	2j	0.23	0/727	0.45	0/988
42	1k	0.19	0/844	0.45	1/1145 (0.1%)
42	2k	0.20	0/848	0.44	0/1149
43	1l	0.21	0/937	0.43	0/1260
43	2l	0.20	0/937	0.41	0/1260
44	1m	0.21	0/933	0.49	0/1254
44	2m	0.22	0/899	0.51	0/1212
45	1n	0.21	0/501	0.50	0/664
45	2n	0.20	0/495	0.45	0/657
46	1o	0.19	0/739	0.41	0/985
46	2o	0.18	0/739	0.40	0/985
47	1p	0.20	0/697	0.45	0/939
47	2p	0.20	0/693	0.45	0/935
48	1q	0.19	0/836	0.41	0/1117
48	2q	0.19	0/836	0.40	0/1117
49	1r	0.21	0/560	0.42	0/746
49	2r	0.18	0/556	0.44	0/741
50	1s	0.21	0/667	0.42	0/900
50	2s	0.18	0/661	0.46	0/893
51	1t	0.21	0/730	0.44	0/965
51	2t	0.19	0/729	0.43	0/965
52	1u	0.20	0/203	0.42	0/266
52	2u	0.19	0/203	0.47	0/266
53	1v	0.24	0/306	0.43	0/473
53	2v	0.21	0/306	0.43	0/473
54	1w	0.21	0/1956	0.42	0/2634
54	2w	0.19	0/1971	0.41	0/2654
55	1x	0.27	0/1629	0.42	0/2535
55	1y	0.27	1/1602 (0.1%)	0.40	0/2488
55	2x	0.26	1/1629 (0.1%)	0.35	0/2535
55	2y	0.30	1/1606 (0.1%)	0.39	0/2497
56	1z	0.28	0/128	0.51	0/175
56	2z	0.20	0/128	0.42	0/175
All	All	0.23	5/317654 (0.0%)	0.42	7/474763 (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
11	1P	0	1
11	2P	0	1
14	1S	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2y	46	G7M	O3'-P	5.57	1.61	1.56
55	1y	46	G7M	O3'-P	5.28	1.61	1.56
32	2a	527	G7M	O3'-P	5.20	1.61	1.56
55	2x	46	G7M	O3'-P	5.20	1.61	1.56
1	2A	2552	OMU	O3'-P	5.06	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1k	118	GLY	N-CA-C	6.50	116.13	110.21
34	2c	116	VAL	N-CA-C	-5.86	105.66	112.98
40	1i	51	ARG	N-CA-C	-5.68	108.14	114.62
36	1e	113	ALA	N-CA-C	-5.48	106.57	113.20
1	1A	1653	G	C2'-C3'-O3'	5.09	117.14	109.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
14	1S	58	LEU	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31196	580	0
1	2A	60322	0	30426	658	0
2	1B	2576	0	1305	19	0
2	2B	2576	0	1305	31	0
3	1D	2136	0	2218	38	0
3	2D	2136	0	2218	56	0
4	1E	1559	0	1618	26	0
4	2E	1559	0	1618	40	0
5	1F	1584	0	1625	41	0
5	2F	1580	0	1619	39	0
6	1G	1425	0	1443	32	0
6	2G	1424	0	1434	51	0
7	1H	1330	0	1407	29	0
7	2H	1330	0	1407	28	0
8	1I	1085	0	1114	24	0
8	2I	1061	0	1080	27	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	15	0
10	1O	933	0	996	23	0
10	2O	933	0	996	14	0
11	1P	1135	0	1212	23	0
11	2P	1135	0	1212	31	0
12	1Q	1122	0	1178	18	0
12	2Q	1122	0	1179	30	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	23	0
14	1S	877	0	938	21	0
14	2S	870	0	923	28	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	21	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	25	0
17	1V	771	0	830	12	0
17	2V	771	0	829	9	0
18	1W	886	0	940	11	0
18	2W	886	0	940	10	0
19	1X	750	0	814	11	0
19	2X	746	0	803	17	0
20	1Y	806	0	881	17	0
20	2Y	810	0	887	17	0
21	1Z	1437	0	1446	45	0
21	2Z	1451	0	1450	44	0
22	10	604	0	619	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	608	0	622	15	0
23	11	755	0	825	19	0
23	21	755	0	826	16	0
24	12	588	0	643	4	0
24	22	588	0	643	11	0
25	13	469	0	518	11	0
25	23	464	0	514	14	0
26	14	548	0	529	14	0
26	24	517	0	479	24	0
27	15	455	0	465	11	0
27	25	455	0	465	10	0
28	16	453	0	473	14	0
28	26	449	0	469	11	0
29	17	418	0	466	10	0
29	27	418	0	467	7	0
30	18	511	0	571	21	0
30	28	517	0	582	20	0
31	19	307	0	335	5	0
31	29	307	0	335	11	0
32	1a	32246	0	16295	482	0
32	2a	32327	0	16338	520	0
33	1b	1846	0	1867	76	0
33	2b	1825	0	1828	81	0
34	1c	1554	0	1551	38	0
34	2c	1542	0	1517	56	0
35	1d	1659	0	1676	62	0
35	2d	1674	0	1714	59	0
36	1e	1129	0	1185	44	0
36	2e	1130	0	1184	25	0
37	1f	810	0	797	17	0
37	2f	816	0	808	19	0
38	1g	1231	0	1238	26	0
38	2g	1235	0	1249	36	0
39	1h	1088	0	1126	29	0
39	2h	1088	0	1126	31	0
40	1i	983	0	986	39	0
40	2i	940	0	938	51	0
41	1j	721	0	672	28	0
41	2j	714	0	672	34	0
42	1k	829	0	825	14	0
42	2k	833	0	836	27	0
43	1l	932	0	979	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	979	15	0
44	1m	923	0	962	40	0
44	2m	889	0	901	43	0
45	1n	492	0	529	24	0
45	2n	486	0	518	26	0
46	1o	728	0	760	13	0
46	2o	728	0	760	11	0
47	1p	681	0	697	20	0
47	2p	677	0	686	18	0
48	1q	823	0	891	18	0
48	2q	823	0	891	19	0
49	1r	555	0	618	12	0
49	2r	551	0	614	16	0
50	1s	652	0	662	28	0
50	2s	646	0	644	33	0
51	1t	728	0	798	30	0
51	2t	727	0	796	18	0
52	1u	199	0	208	3	0
52	2u	199	0	208	1	0
53	1v	274	0	139	4	0
53	2v	274	0	139	7	0
54	1w	1939	0	1927	47	0
54	2w	1954	0	1930	50	0
55	1x	1612	0	829	11	0
55	1y	1590	0	815	17	0
55	2x	1612	0	829	10	0
55	2y	1592	0	818	28	0
56	1z	121	0	126	7	0
56	2z	121	0	126	4	0
57	10	5	0	0	0	0
57	11	4	0	0	0	0
57	12	2	0	0	0	0
57	13	2	0	0	0	0
57	14	1	0	0	0	0
57	15	4	0	0	0	0
57	16	1	0	0	0	0
57	17	7	0	0	0	0
57	18	2	0	0	0	0
57	19	2	0	0	0	0
57	1A	795	0	0	0	0
57	1B	20	0	0	0	0
57	1D	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1E	9	0	0	0	0
57	1F	11	0	0	0	0
57	1G	3	0	0	0	0
57	1N	4	0	0	0	0
57	1O	1	0	0	0	0
57	1P	4	0	0	0	0
57	1Q	6	0	0	0	0
57	1R	3	0	0	0	0
57	1U	7	0	0	0	0
57	1V	5	0	0	0	0
57	1W	5	0	0	0	0
57	1X	2	0	0	0	0
57	1Z	1	0	0	0	0
57	1a	189	0	0	0	0
57	1d	1	0	0	0	0
57	1f	1	0	0	0	0
57	1k	1	0	0	0	0
57	1m	1	0	0	0	0
57	1n	1	0	0	0	0
57	1v	2	0	0	0	0
57	1w	3	0	0	0	0
57	1x	9	0	0	0	0
57	1y	1	0	0	0	0
57	20	2	0	0	0	0
57	23	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	28	1	0	0	0	0
57	29	1	0	0	0	0
57	2A	640	0	0	0	0
57	2B	11	0	0	0	0
57	2D	8	0	0	0	0
57	2E	5	0	0	0	0
57	2F	7	0	0	0	0
57	2N	1	0	0	0	0
57	2O	1	0	0	0	0
57	2P	2	0	0	0	0
57	2Q	3	0	0	0	0
57	2R	3	0	0	0	0
57	2U	1	0	0	0	0
57	2V	2	0	0	0	0
57	2W	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2X	3	0	0	0	0
57	2Y	1	0	0	0	0
57	2a	168	0	0	0	0
57	2d	2	0	0	0	0
57	2e	3	0	0	0	0
57	2f	1	0	0	0	0
57	2j	2	0	0	0	0
57	2k	2	0	0	0	0
57	2t	1	0	0	0	0
57	2v	1	0	0	0	0
57	2x	9	0	0	0	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	3	0
59	2d	8	0	0	2	0
60	10	2	0	0	0	0
60	11	3	0	0	0	0
60	13	2	0	0	1	0
60	15	3	0	0	0	0
60	16	1	0	0	1	0
60	17	2	0	0	1	0
60	18	7	0	0	0	0
60	1A	1395	0	0	83	0
60	1B	27	0	0	0	0
60	1D	15	0	0	1	0
60	1E	13	0	0	3	0
60	1F	8	0	0	2	0
60	1G	1	0	0	0	0
60	1N	3	0	0	0	0
60	1O	3	0	0	1	0
60	1P	15	0	0	1	0
60	1Q	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1R	3	0	0	0	0
60	1T	1	0	0	0	0
60	1U	4	0	0	0	0
60	1V	1	0	0	0	0
60	1W	3	0	0	0	0
60	1X	3	0	0	0	0
60	1Z	1	0	0	0	0
60	1a	180	0	0	15	0
60	1d	1	0	0	0	0
60	1l	1	0	0	0	0
60	1v	4	0	0	3	0
60	1w	2	0	0	0	0
60	1x	24	0	0	0	0
60	20	4	0	0	1	0
60	21	2	0	0	0	0
60	23	2	0	0	0	0
60	25	2	0	0	0	0
60	27	4	0	0	0	0
60	28	4	0	0	0	0
60	2A	946	0	0	81	0
60	2B	6	0	0	0	0
60	2D	18	0	0	1	0
60	2E	7	0	0	2	0
60	2F	5	0	0	0	0
60	2N	1	0	0	0	0
60	2O	2	0	0	0	0
60	2P	16	0	0	2	0
60	2Q	3	0	0	0	0
60	2R	2	0	0	0	0
60	2U	1	0	0	0	0
60	2X	3	0	0	0	0
60	2Y	2	0	0	0	0
60	2a	152	0	0	12	0
60	2d	1	0	0	0	0
60	2j	1	0	0	0	0
60	2q	1	0	0	0	0
60	2t	1	0	0	0	0
60	2w	1	0	0	0	0
60	2x	13	0	0	0	0
60	2z	2	0	0	0	0
All	All	299076	0	199299	4213	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 9.

The worst 5 of 4213 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)
32:2a:1006:C:H42	32:2a:1023:G:H1	1.12	0.98
1:1A:1057:A:N6	1:1A:1081:U:H3	1.62	0.96
1:2A:2129:C:N4	1:2A:2159:G:H1	1.65	0.95
1:1A:1057:A:H61	1:1A:1081:U:H3	1.07	0.93
1:1A:510:C:OP1	60:1A:3804:HOH:O	1.88	0.92

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%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24	48
4	2E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24	48
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	48
5	2F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	48
6	1G	179/182 (98%)	153 (86%)	26 (14%)	0	100	100
6	2G	179/182 (98%)	150 (84%)	23 (13%)	6 (3%)	3	7
7	1H	172/180 (96%)	157 (91%)	14 (8%)	1 (1%)	21	44
7	2H	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	7	19
8	1I	144/148 (97%)	125 (87%)	16 (11%)	3 (2%)	5	15
8	2I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9	23
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	2N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
11	1P	147/150 (98%)	136 (92%)	9 (6%)	2 (1%)	9	23
11	2P	147/150 (98%)	136 (92%)	9 (6%)	2 (1%)	9	23
12	1Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18	41
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	14	35
14	2S	108/112 (96%)	96 (89%)	9 (8%)	3 (3%)	4	9
15	1T	129/146 (88%)	122 (95%)	4 (3%)	3 (2%)	5	13
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	32
17	2V	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	3	8
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%)	4 (4%)	1 (1%)	11	29
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	92 (88%)	13 (12%)	0	100	100
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
21	1Z	181/206 (88%)	162 (90%)	17 (9%)	2 (1%)	11	29
21	2Z	184/206 (89%)	159 (86%)	24 (13%)	1 (0%)	24	48
22	10	74/85 (87%)	70 (95%)	3 (4%)	1 (1%)	9	23
22	20	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	9	25
23	11	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	11	29
23	21	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	11	29
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	13	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6	18
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	50 (75%)	11 (16%)	6 (9%)	0	0
26	24	66/71 (93%)	36 (54%)	27 (41%)	3 (4%)	2	4
27	15	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
27	25	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	190 (83%)	31 (14%)	8 (4%)	3	6
33	2b	229/256 (90%)	189 (82%)	35 (15%)	5 (2%)	5	14
34	1c	204/239 (85%)	166 (81%)	37 (18%)	1 (0%)	24	48
34	2c	204/239 (85%)	177 (87%)	24 (12%)	3 (2%)	8	22
35	1d	206/209 (99%)	180 (87%)	24 (12%)	2 (1%)	12	32
35	2d	206/209 (99%)	185 (90%)	19 (9%)	2 (1%)	12	32
36	1e	146/162 (90%)	126 (86%)	17 (12%)	3 (2%)	5	15
36	2e	146/162 (90%)	127 (87%)	16 (11%)	3 (2%)	5	15
37	1f	98/101 (97%)	90 (92%)	8 (8%)	0	100	100
37	2f	98/101 (97%)	86 (88%)	12 (12%)	0	100	100
38	1g	153/156 (98%)	135 (88%)	15 (10%)	3 (2%)	6	16
38	2g	153/156 (98%)	136 (89%)	14 (9%)	3 (2%)	6	16
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
40	1i	125/128 (98%)	108 (86%)	14 (11%)	3 (2%)	4	12
40	2i	121/128 (94%)	96 (79%)	25 (21%)	0	100	100
41	1j	96/105 (91%)	78 (81%)	13 (14%)	5 (5%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	2j	94/105 (90%)	81 (86%)	11 (12%)	2 (2%)	5	15
42	1k	112/129 (87%)	93 (83%)	18 (16%)	1 (1%)	14	35
42	2k	112/129 (87%)	95 (85%)	16 (14%)	1 (1%)	14	35
43	1l	119/132 (90%)	104 (87%)	14 (12%)	1 (1%)	16	37
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	116/126 (92%)	100 (86%)	15 (13%)	1 (1%)	14	35
44	2m	113/126 (90%)	93 (82%)	17 (15%)	3 (3%)	4	10
45	1n	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	7
45	2n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	27
47	1p	80/88 (91%)	68 (85%)	12 (15%)	0	100	100
47	2p	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
48	2q	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	58 (88%)	7 (11%)	1 (2%)	8	22
50	1s	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	4	11
50	2s	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	10	27
51	1t	94/106 (89%)	79 (84%)	12 (13%)	3 (3%)	3	7
51	2t	94/106 (89%)	78 (83%)	8 (8%)	8 (8%)	0	1
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	3
54	1w	246/354 (70%)	230 (94%)	15 (6%)	1 (0%)	30	54
54	2w	250/354 (71%)	231 (92%)	19 (8%)	0	100	100
56	1z	12/20 (60%)	9 (75%)	3 (25%)	0	100	100
56	2z	12/20 (60%)	10 (83%)	1 (8%)	1 (8%)	0	1
All	All	11922/12876 (93%)	10759 (90%)	1039 (9%)	124 (1%)	12	32

5 of 124 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1H	126	PRO

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Mol	Chain	Res	Type
8	1I	10	GLU
17	1V	79	VAL
21	1Z	53	ILE
26	14	18	CYS

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%)	15	37
3	2D	215/218 (99%)	205 (95%)	10 (5%)	23	51
4	1E	164/166 (99%)	155 (94%)	9 (6%)	19	45
4	2E	164/166 (99%)	148 (90%)	16 (10%)	7	19
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8	21
5	2F	159/166 (96%)	141 (89%)	18 (11%)	5	14
6	1G	143/156 (92%)	125 (87%)	18 (13%)	4	11
6	2G	142/156 (91%)	119 (84%)	23 (16%)	2	6
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	23
7	2H	144/148 (97%)	129 (90%)	15 (10%)	7	17
8	1I	110/124 (89%)	97 (88%)	13 (12%)	5	13
8	2I	104/124 (84%)	90 (86%)	14 (14%)	4	9
9	1N	118/119 (99%)	107 (91%)	11 (9%)	8	21
9	2N	118/119 (99%)	112 (95%)	6 (5%)	21	48
10	1O	100/100 (100%)	92 (92%)	8 (8%)	11	28
10	2O	100/100 (100%)	96 (96%)	4 (4%)	28	56
11	1P	115/116 (99%)	110 (96%)	5 (4%)	26	54
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11	29
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9	23
12	2Q	111/111 (100%)	99 (89%)	12 (11%)	6	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	23
13	2R	101/101 (100%)	96 (95%)	5 (5%)	22	48
14	1S	87/88 (99%)	78 (90%)	9 (10%)	7	18
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4	10
15	1T	115/127 (91%)	102 (89%)	13 (11%)	5	14
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16	39
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	64
16	2U	93/94 (99%)	86 (92%)	7 (8%)	12	31
17	1V	80/82 (98%)	74 (92%)	6 (8%)	12	31
17	2V	80/82 (98%)	74 (92%)	6 (8%)	12	31
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19	44
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25	53
19	1X	77/78 (99%)	71 (92%)	6 (8%)	11	29
19	2X	76/78 (97%)	68 (90%)	8 (10%)	6	17
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5	13
20	2Y	86/91 (94%)	79 (92%)	7 (8%)	11	27
21	1Z	155/179 (87%)	144 (93%)	11 (7%)	13	33
21	2Z	155/179 (87%)	136 (88%)	19 (12%)	4	12
22	10	61/67 (91%)	59 (97%)	2 (3%)	33	63
22	20	61/67 (91%)	57 (93%)	4 (7%)	15	36
23	11	80/83 (96%)	72 (90%)	8 (10%)	7	19
23	21	80/83 (96%)	73 (91%)	7 (9%)	9	23
24	12	65/67 (97%)	59 (91%)	6 (9%)	8	22
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	22
25	13	51/52 (98%)	46 (90%)	5 (10%)	7	19
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	28
26	14	58/63 (92%)	51 (88%)	7 (12%)	5	12
26	24	51/63 (81%)	40 (78%)	11 (22%)	1	3
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	41
27	25	50/52 (96%)	45 (90%)	5 (10%)	7	19
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	26	50/52 (96%)	40 (80%)	10 (20%)	1	4
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	32
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	32
30	18	53/55 (96%)	49 (92%)	4 (8%)	12	31
30	28	54/55 (98%)	48 (89%)	6 (11%)	6	15
31	19	34/34 (100%)	32 (94%)	2 (6%)	18	42
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	42
33	1b	192/220 (87%)	163 (85%)	29 (15%)	3	7
33	2b	187/220 (85%)	148 (79%)	39 (21%)	1	3
34	1c	144/188 (77%)	116 (81%)	28 (19%)	1	4
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4	10
35	1d	170/181 (94%)	149 (88%)	21 (12%)	4	11
35	2d	173/181 (96%)	153 (88%)	20 (12%)	5	13
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9	23
36	2e	113/123 (92%)	101 (89%)	12 (11%)	6	17
37	1f	84/90 (93%)	76 (90%)	8 (10%)	8	20
37	2f	85/90 (94%)	73 (86%)	12 (14%)	3	9
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7	18
38	2g	120/127 (94%)	104 (87%)	16 (13%)	4	10
39	1h	114/119 (96%)	100 (88%)	14 (12%)	4	12
39	2h	114/119 (96%)	107 (94%)	7 (6%)	17	40
40	1i	90/99 (91%)	79 (88%)	11 (12%)	5	12
40	2i	86/99 (87%)	70 (81%)	16 (19%)	1	4
41	1j	68/92 (74%)	61 (90%)	7 (10%)	7	18
41	2j	69/92 (75%)	56 (81%)	13 (19%)	1	4
42	1k	82/99 (83%)	77 (94%)	5 (6%)	17	40
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10	26
43	1l	96/108 (89%)	88 (92%)	8 (8%)	10	26
43	2l	96/108 (89%)	83 (86%)	13 (14%)	4	9
44	1m	90/101 (89%)	79 (88%)	11 (12%)	5	12
44	2m	85/101 (84%)	78 (92%)	7 (8%)	10	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	18
45	2n	48/50 (96%)	44 (92%)	4 (8%)	10	26
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16	38
46	2o	78/80 (98%)	67 (86%)	11 (14%)	3	9
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3	8
47	2p	68/74 (92%)	64 (94%)	4 (6%)	18	42
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8	20
48	2q	94/97 (97%)	84 (89%)	10 (11%)	6	17
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	18
49	2r	58/77 (75%)	50 (86%)	8 (14%)	3	9
50	1s	69/80 (86%)	60 (87%)	9 (13%)	4	10
50	2s	67/80 (84%)	55 (82%)	12 (18%)	2	5
51	1t	70/82 (85%)	58 (83%)	12 (17%)	2	6
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5	14
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	44
54	1w	203/298 (68%)	183 (90%)	20 (10%)	7	19
54	2w	202/298 (68%)	170 (84%)	32 (16%)	2	7
56	1z	14/19 (74%)	13 (93%)	1 (7%)	13	33
56	2z	14/19 (74%)	12 (86%)	2 (14%)	3	8
All	All	9747/10698 (91%)	8743 (90%)	1004 (10%)	7	18

5 of 1004 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	1w	209	ASP
42	2k	30	VAL
9	2N	68	GLU
41	2j	46	ARG
49	2r	76	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 158 such sidechains are listed below:

Mol	Chain	Res	Type
31	29	34	GLN
41	2j	68	HIS
33	2b	204	ASN
35	2d	77	ASN
50	2s	23	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	443 (15%)	28 (0%)
1	2A	2791/2915 (95%)	480 (17%)	22 (0%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	119/121 (98%)	15 (12%)	0
32	1a	1497/1521 (98%)	307 (20%)	0
32	2a	1501/1521 (98%)	297 (19%)	0
53	1v	10/24 (41%)	3 (30%)	0
53	2v	10/24 (41%)	2 (20%)	0
55	1x	73/76 (96%)	9 (12%)	0
55	1y	71/76 (93%)	21 (29%)	0
55	2x	73/76 (96%)	12 (16%)	0
55	2y	72/76 (94%)	26 (36%)	0
All	All	9200/9466 (97%)	1627 (17%)	50 (0%)

5 of 1627 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	63	U

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	196	A
1	2A	774	A
1	2A	2756	U
1	2A	228	A
1	2A	277	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	1a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.11	3 (11%)
55	G7M	2y	46	55	23,26,27	1.54	4 (17%)	34,39,42	1.79	5 (14%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.13	9 (27%)
55	MIA	1y	37	55	28,31,32	2.24	7 (25%)	38,44,47	2.82	13 (34%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.04	9 (27%)
1	5MU	1A	1939	1,57	19,22,23	1.39	5 (26%)	27,32,35	2.39	6 (22%)
32	G7M	1a	527	32	23,26,27	1.56	3 (13%)	34,39,42	1.81	5 (14%)
43	0TD	2l	92	43	8,9,10	4.48	2 (25%)	6,11,13	4.62	3 (50%)
55	PSU	2x	39	55	18,21,22	1.40	3 (16%)	21,30,33	1.82	4 (19%)
32	5MC	2a	1407	32	19,22,23	1.58	3 (15%)	26,32,35	1.07	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.42	3 (16%)	21,30,33	2.05	4 (19%)
1	PSU	1A	2605	1,57	18,21,22	1.41	3 (16%)	21,30,33	2.02	4 (19%)
55	MIA	2y	37	55	28,31,32	2.36	6 (21%)	38,44,47	2.91	14 (36%)
55	5MU	1x	54	55	19,22,23	1.44	3 (15%)	27,32,35	1.76	6 (22%)
1	OMG	2A	2251	55,1,57	23,26,27	1.22	3 (13%)	32,38,41	1.95	6 (18%)
1	5MC	1A	1962	1,57	19,22,23	1.62	3 (15%)	26,32,35	1.08	1 (3%)
55	G7M	2x	46	55	23,26,27	1.53	3 (13%)	34,39,42	1.70	5 (14%)
55	PSU	2y	39	55	18,21,22	1.36	2 (11%)	21,30,33	1.87	3 (14%)
32	2MG	2a	1207	32	23,26,27	1.25	3 (13%)	33,38,41	2.14	8 (24%)
1	5MU	1A	1915	1,57	19,22,23	1.44	5 (26%)	27,32,35	2.10	5 (18%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	0.96	1 (4%)
1	PSU	2A	2605	1	18,21,22	1.28	2 (11%)	21,30,33	2.08	4 (19%)
32	UR3	1a	1498	32	19,22,23	1.04	2 (10%)	26,32,35	1.70	5 (19%)
32	PSU	2a	516	32,57	18,21,22	1.38	2 (11%)	21,30,33	1.98	5 (23%)
55	G7M	1x	46	55	23,26,27	1.56	3 (13%)	34,39,42	1.75	5 (14%)
55	4SU	1y	8	55	18,21,22	1.79	4 (22%)	25,30,33	2.01	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PSU	1y	32	55	18,21,22	1.39	2 (11%)	21,30,33	1.95	3 (14%)
1	2MA	1A	2503	1,57	22,25,26	1.47	4 (18%)	32,37,40	2.32	9 (28%)
32	G7M	2a	527	32	23,26,27	1.50	3 (13%)	34,39,42	1.78	5 (14%)
55	PSU	1x	55	55	18,21,22	1.39	2 (11%)	21,30,33	2.01	4 (19%)
55	PSU	2y	55	55	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
55	5MU	1y	54	55	19,22,23	1.42	5 (26%)	27,32,35	1.77	6 (22%)
1	OMG	1A	2251	55,1,57	23,26,27	1.24	3 (13%)	32,38,41	2.07	7 (21%)
55	4SU	2y	8	55	18,21,22	1.74	4 (22%)	25,30,33	2.00	4 (16%)
43	0TD	1l	92	43	8,9,10	4.21	2 (25%)	6,11,13	9.98	3 (50%)
1	PSU	2A	1911	1	18,21,22	1.41	2 (11%)	21,30,33	2.11	6 (28%)
54	MEQ	1w	230	54	8,9,10	0.98	0	5,10,12	0.69	0
1	OMU	1A	2552	1,57	19,22,23	1.33	4 (21%)	25,31,34	2.01	5 (20%)
32	2MG	1a	1207	32,57	23,26,27	1.25	4 (17%)	33,38,41	2.17	8 (24%)
32	5MC	2a	967	32,57	19,22,23	1.67	3 (15%)	26,32,35	1.14	3 (11%)
54	MEQ	2w	230	54	8,9,10	0.92	0	5,10,12	0.46	0
32	M2G	2a	966	32	24,27,28	1.27	4 (16%)	33,40,43	1.92	5 (15%)
55	PSU	1x	32	55	18,21,22	1.36	2 (11%)	21,30,33	1.99	3 (14%)
55	PSU	1y	39	55	18,21,22	1.45	3 (16%)	21,30,33	1.73	3 (14%)
55	PSU	2x	32	55	18,21,22	1.36	2 (11%)	21,30,33	2.01	4 (19%)
1	2MA	2A	2503	1,57	22,25,26	1.47	4 (18%)	32,37,40	2.32	8 (25%)
32	5MC	1a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.21	3 (11%)
55	5MU	2x	54	55	19,22,23	1.38	5 (26%)	27,32,35	1.91	6 (22%)
55	MIA	2x	37	55	28,31,32	2.40	6 (21%)	38,44,47	2.80	14 (36%)
32	4OC	1a	1402	32,57	20,23,24	0.79	0	25,32,35	1.05	3 (12%)
32	5MC	2a	1404	32	19,22,23	1.68	3 (15%)	26,32,35	1.25	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.06	4 (19%)
55	5MU	2y	54	55	19,22,23	1.47	5 (26%)	27,32,35	2.41	8 (29%)
1	OMU	2A	2552	1,57	19,22,23	1.27	3 (15%)	25,31,34	1.86	5 (20%)
32	5MC	2a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.12	2 (7%)
32	4OC	2a	1402	32,57	20,23,24	0.78	0	25,32,35	0.96	1 (4%)
55	PSU	1x	39	55	18,21,22	1.39	2 (11%)	21,30,33	1.90	3 (14%)
32	5MC	1a	967	32	19,22,23	1.77	3 (15%)	26,32,35	1.17	2 (7%)
55	PSU	1y	55	55	18,21,22	1.36	2 (11%)	21,30,33	2.00	3 (14%)
1	5MU	2A	1939	1	19,22,23	1.48	6 (31%)	27,32,35	2.25	7 (25%)
55	PSU	2x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.03	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	4SU	2x	8	57,55	18,21,22	1.88	4 (22%)	25,30,33	1.69	4 (16%)
1	5MC	2A	1962	1,57	19,22,23	1.52	3 (15%)	26,32,35	1.03	2 (7%)
55	MIA	1x	37	55	28,31,32	2.48	7 (25%)	38,44,47	2.58	14 (36%)
1	5MU	2A	1915	1	19,22,23	1.45	5 (26%)	27,32,35	2.12	5 (18%)
32	UR3	2a	1498	32	19,22,23	0.94	1 (5%)	26,32,35	1.73	3 (11%)
55	4SU	1x	8	55	18,21,22	1.78	4 (22%)	25,30,33	1.91	4 (16%)
1	OMC	2A	1920	1,57	19,22,23	0.80	0	25,31,34	0.88	0
55	PSU	2y	32	55	18,21,22	1.35	2 (11%)	21,30,33	1.94	3 (14%)
32	M2G	1a	966	32	24,27,28	1.32	3 (12%)	33,40,43	1.94	6 (18%)
1	5MC	1A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.24	3 (11%)
32	PSU	1a	516	32,57	18,21,22	1.40	2 (11%)	21,30,33	2.03	5 (23%)
1	PSU	1A	1917	1	18,21,22	1.43	2 (11%)	21,30,33	1.99	3 (14%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.08	9 (27%)
32	5MC	1a	1407	32	19,22,23	1.44	3 (15%)	26,32,35	1.03	2 (7%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.07	8 (24%)
55	G7M	1y	46	55	23,26,27	1.53	4 (17%)	34,39,42	1.83	5 (14%)
1	5MC	2A	1942	1	19,22,23	1.66	3 (15%)	26,32,35	1.22	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
55	G7M	2y	46	55	-	3/7/25/26	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
55	MIA	1y	37	55	-	3/15/33/34	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	1/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	5/7/12/14	-
55	PSU	2x	39	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
55	MIA	2y	37	55	-	2/15/33/34	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	2A	2251	55,1,57	-	0/9/27/28	0/3/3/3
1	5MC	1A	1962	1,57	-	0/7/25/26	0/2/2/2
55	G7M	2x	46	55	-	3/7/25/26	0/3/3/3
55	PSU	2y	39	55	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	5MU	1A	1915	1,57	-	2/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,57	-	0/7/25/26	0/2/2/2
55	G7M	1x	46	55	-	3/7/25/26	0/3/3/3
55	4SU	1y	8	55	-	0/7/25/26	0/2/2/2
55	PSU	1y	32	55	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,57	-	2/7/25/26	0/3/3/3
32	G7M	2a	527	32	-	0/7/25/26	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
55	PSU	2y	55	55	-	0/7/25/26	0/2/2/2
55	5MU	1y	54	55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,1,57	-	1/9/27/28	0/3/3/3
55	4SU	2y	8	55	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	6/7/12/14	-
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	MEQ	1w	230	54	-	3/8/9/11	-
1	OMU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
32	2MG	1a	1207	32,57	-	0/9/27/28	0/3/3/3
32	5MC	2a	967	32,57	-	0/7/25/26	0/2/2/2
54	MEQ	2w	230	54	-	1/8/9/11	-
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
55	PSU	1x	32	55	-	0/7/25/26	0/2/2/2
55	PSU	1y	39	55	-	0/7/25/26	0/2/2/2
55	PSU	2x	32	55	-	1/7/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	3/7/25/26	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
55	MIA	2x	37	55	-	6/15/33/34	0/3/3/3
32	4OC	1a	1402	32,57	-	2/9/29/30	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
55	5MU	2y	54	55	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,57	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,57	-	2/9/29/30	0/2/2/2
55	PSU	1x	39	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
55	PSU	1y	55	55	-	2/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	57,55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
55	MIA	1x	37	55	-	7/15/33/34	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1,57	-	2/9/27/28	0/2/2/2
55	PSU	2y	32	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
55	G7M	1y	46	55	-	4/7/25/26	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2

The worst 5 of 223 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.03	1.70	1.82
43	1l	92	0TD	CB-SB	-11.42	1.70	1.82
55	1x	37	MIA	C2-S10	-7.91	1.69	1.75
55	2x	37	MIA	C2-S10	-7.23	1.69	1.75
55	1x	37	MIA	C13-C14	7.14	1.53	1.32

The worst 5 of 375 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	23.93	145.39	102.36
43	2l	92	0TD	CSB-SB-CB	10.13	120.57	102.36
55	2y	37	MIA	C12-C13-C14	-9.50	109.96	127.01
55	1y	37	MIA	C12-C13-C14	-9.26	110.38	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	37	MIA	C12-C13-C14	-8.67	111.45	127.01

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
55	1x	37	MIA	C12-C13-C14-C15

There are no ring outliers.

32 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1519	MA6	1	0
55	1y	37	MIA	3	0
32	1a	1518	MA6	1	0
1	1A	1939	5MU	1	0
32	1a	527	G7M	2	0
43	2l	92	0TD	1	0
1	2A	1917	PSU	1	0
55	2y	37	MIA	1	0
1	2A	2251	OMG	1	0
32	2a	1207	2MG	1	0
1	1A	1915	5MU	1	0
1	1A	1920	OMC	1	0
55	1y	8	4SU	1	0
55	1y	32	PSU	1	0
1	1A	2503	2MA	1	0
55	2y	55	PSU	1	0
43	1l	92	0TD	3	0
54	1w	230	MEQ	1	0
1	1A	2552	OMU	1	0
54	2w	230	MEQ	1	0
55	1y	39	PSU	1	0
55	2x	37	MIA	2	0
32	1a	1402	4OC	3	0
32	2a	1402	4OC	2	0
55	1y	55	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1939	5MU	1	0
55	1x	37	MIA	1	0
1	2A	1915	5MU	1	0
55	1x	8	4SU	1	0
1	1A	1917	PSU	3	0
32	1a	1519	MA6	2	0
32	2a	1518	MA6	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2022 ligands modelled in this entry, 2020 are monoatomic - leaving 2 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	SF4	1d	302	35	0,12,12	-	-	-		
59	SF4	2d	303	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	1d	302	35	-	-	0/6/5/5
59	SF4	2d	303	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1d	302	SF4	3	0
59	2d	303	SF4	2	0

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%)	-0.61	109 (3%)	44	40	10, 27, 82, 98	0
1	2A	2789/2915 (95%)	-0.13	103 (3%)	45	41	25, 49, 84, 97	0
2	1B	120/121 (99%)	-0.39	0	100	100	23, 45, 58, 73	0
2	2B	120/121 (99%)	0.71	4 (3%)	49	45	55, 73, 84, 84	0
3	1D	275/276 (99%)	-0.39	2 (0%)	84	83	12, 27, 44, 70	0
3	2D	275/276 (99%)	0.05	1 (0%)	88	87	21, 43, 56, 67	0
4	1E	204/206 (99%)	-0.41	0	100	100	11, 28, 48, 74	0
4	2E	204/206 (99%)	0.09	1 (0%)	87	86	27, 47, 60, 75	0
5	1F	203/210 (96%)	-0.24	0	100	100	12, 33, 55, 70	0
5	2F	203/210 (96%)	0.37	2 (0%)	79	78	27, 55, 70, 77	0
6	1G	181/182 (99%)	0.42	7 (3%)	43	39	36, 52, 69, 80	0
6	2G	181/182 (99%)	1.23	25 (13%)	6	5	61, 72, 78, 85	0
7	1H	174/180 (96%)	-0.03	1 (0%)	85	85	29, 43, 55, 60	0
7	2H	174/180 (96%)	0.91	13 (7%)	20	17	54, 69, 78, 85	0
8	1I	146/148 (98%)	0.47	3 (2%)	63	61	37, 60, 70, 74	0
8	2I	146/148 (98%)	0.61	4 (2%)	56	53	46, 65, 72, 76	0
9	1N	140/140 (100%)	-0.42	0	100	100	17, 27, 52, 61	0
9	2N	140/140 (100%)	0.27	2 (1%)	73	72	37, 54, 68, 71	0
10	1O	122/122 (100%)	-0.35	0	100	100	18, 30, 49, 55	0
10	2O	122/122 (100%)	-0.16	0	100	100	32, 42, 56, 61	0
11	1P	149/150 (99%)	-0.16	0	100	100	12, 36, 56, 63	0
11	2P	149/150 (99%)	0.51	3 (2%)	65	62	29, 57, 71, 79	0
12	1Q	141/141 (100%)	-0.30	0	100	100	19, 32, 45, 59	0
12	2Q	141/141 (100%)	0.41	3 (2%)	63	61	39, 54, 63, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.45	0 100 100	16, 27, 40, 53	0
13	2R	118/118 (100%)	0.10	0 100 100	31, 46, 55, 64	0
14	1S	110/112 (98%)	-0.02	0 100 100	34, 45, 55, 57	0
14	2S	110/112 (98%)	0.94	10 (9%) 15 12	58, 67, 73, 75	0
15	1T	131/146 (89%)	-0.17	3 (2%) 61 58	24, 36, 62, 75	0
15	2T	131/146 (89%)	0.12	1 (0%) 82 81	34, 48, 65, 74	0
16	1U	116/118 (98%)	-0.49	0 100 100	12, 21, 36, 53	0
16	2U	116/118 (98%)	0.18	0 100 100	35, 50, 61, 67	0
17	1V	101/101 (100%)	-0.50	0 100 100	12, 28, 43, 49	0
17	2V	101/101 (100%)	0.42	1 (0%) 79 78	33, 60, 69, 74	0
18	1W	112/113 (99%)	-0.54	0 100 100	10, 21, 38, 69	0
18	2W	112/113 (99%)	-0.09	0 100 100	32, 42, 61, 82	0
19	1X	95/96 (98%)	-0.26	2 (2%) 63 61	20, 30, 48, 64	0
19	2X	95/96 (98%)	0.55	2 (2%) 63 61	44, 56, 67, 78	0
20	1Y	107/110 (97%)	-0.06	1 (0%) 81 80	26, 39, 59, 70	0
20	2Y	107/110 (97%)	0.75	8 (7%) 20 17	48, 61, 72, 79	0
21	1Z	183/206 (88%)	0.23	1 (0%) 87 86	33, 49, 61, 72	0
21	2Z	186/206 (90%)	0.84	9 (4%) 35 32	54, 67, 74, 80	0
22	10	76/85 (89%)	-0.25	2 (2%) 57 54	20, 30, 49, 61	0
22	20	77/85 (90%)	0.48	3 (3%) 43 39	46, 54, 64, 71	0
23	11	97/98 (98%)	-0.11	1 (1%) 79 78	19, 33, 58, 66	0
23	21	97/98 (98%)	0.30	2 (2%) 63 61	34, 49, 66, 73	0
24	12	70/72 (97%)	0.02	1 (1%) 73 72	27, 39, 51, 68	0
24	22	70/72 (97%)	0.64	4 (5%) 29 26	53, 62, 69, 77	0
25	13	59/60 (98%)	-0.38	0 100 100	17, 26, 48, 60	0
25	23	59/60 (98%)	0.18	0 100 100	41, 53, 64, 68	0
26	14	69/71 (97%)	0.85	9 (13%) 7 6	50, 69, 80, 83	0
26	24	68/71 (95%)	1.48	16 (23%) 2 1	67, 78, 86, 88	0
27	15	59/60 (98%)	-0.58	0 100 100	10, 26, 41, 48	0
27	25	59/60 (98%)	0.04	2 (3%) 48 44	26, 45, 60, 69	0
28	16	53/54 (98%)	-0.26	0 100 100	27, 37, 49, 54	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.33	1 (1%) 66 63	49, 56, 64, 69	0
29	17	48/49 (97%)	-0.23	3 (6%) 26 23	13, 20, 48, 68	0
29	27	48/49 (97%)	0.27	5 (10%) 11 10	26, 36, 60, 66	0
30	18	64/65 (98%)	-0.45	0 100 100	18, 25, 33, 38	0
30	28	64/65 (98%)	0.26	1 (1%) 70 68	35, 46, 52, 63	0
31	19	37/37 (100%)	-0.30	0 100 100	22, 30, 40, 47	0
31	29	37/37 (100%)	0.64	0 100 100	46, 57, 65, 70	0
32	1a	1488/1521 (97%)	0.52	78 (5%) 33 29	23, 64, 86, 97	0
32	2a	1491/1521 (98%)	0.52	67 (4%) 38 34	35, 66, 85, 97	0
33	1b	231/256 (90%)	0.95	15 (6%) 25 22	54, 69, 78, 83	0
33	2b	231/256 (90%)	1.26	38 (16%) 4 4	61, 73, 80, 89	0
34	1c	206/239 (86%)	1.01	19 (9%) 14 12	58, 70, 76, 78	0
34	2c	206/239 (86%)	0.98	18 (8%) 16 13	62, 71, 76, 79	0
35	1d	208/209 (99%)	0.90	18 (8%) 16 13	45, 65, 74, 79	0
35	2d	208/209 (99%)	0.63	7 (3%) 48 44	46, 59, 67, 71	0
36	1e	148/162 (91%)	0.52	2 (1%) 73 72	42, 56, 67, 70	0
36	2e	148/162 (91%)	0.69	4 (2%) 56 53	48, 60, 69, 81	0
37	1f	100/101 (99%)	0.57	4 (4%) 42 38	49, 60, 67, 71	0
37	2f	100/101 (99%)	0.62	2 (2%) 65 62	55, 64, 72, 77	0
38	1g	155/156 (99%)	0.88	11 (7%) 22 19	57, 66, 74, 77	0
38	2g	155/156 (99%)	1.16	23 (14%) 5 4	61, 71, 78, 81	0
39	1h	137/138 (99%)	0.50	1 (0%) 84 83	48, 57, 65, 69	0
39	2h	137/138 (99%)	0.62	7 (5%) 33 29	49, 62, 68, 72	0
40	1i	127/128 (99%)	1.37	26 (20%) 2 2	55, 70, 77, 81	0
40	2i	123/128 (96%)	1.63	39 (31%) 1 1	66, 75, 82, 87	0
41	1j	98/105 (93%)	1.59	27 (27%) 1 1	59, 72, 78, 80	0
41	2j	96/105 (91%)	1.72	30 (31%) 1 1	66, 77, 82, 84	0
42	1k	114/129 (88%)	0.52	1 (0%) 81 80	38, 57, 68, 74	0
42	2k	114/129 (88%)	0.83	5 (4%) 39 35	53, 66, 73, 82	0
43	1l	121/132 (91%)	0.44	4 (3%) 49 45	38, 51, 62, 66	0
43	2l	121/132 (91%)	0.36	4 (3%) 49 45	40, 52, 59, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	118/126 (93%)	1.16	15 (12%) 8 7	55, 68, 76, 78	0
44	2m	115/126 (91%)	1.43	27 (23%) 2 1	63, 73, 79, 82	0
45	1n	60/61 (98%)	1.29	8 (13%) 7 6	58, 68, 75, 78	0
45	2n	60/61 (98%)	1.52	15 (25%) 2 1	63, 72, 77, 78	0
46	1o	88/89 (98%)	0.40	4 (4%) 38 34	39, 56, 67, 72	0
46	2o	88/89 (98%)	0.60	4 (4%) 38 34	50, 61, 71, 75	0
47	1p	82/88 (93%)	1.15	13 (15%) 5 4	53, 64, 72, 76	0
47	2p	82/88 (93%)	0.69	1 (1%) 76 75	47, 57, 65, 73	0
48	1q	99/105 (94%)	0.50	1 (1%) 79 78	44, 56, 66, 72	0
48	2q	99/105 (94%)	0.54	1 (1%) 79 78	48, 58, 65, 76	0
49	1r	68/88 (77%)	0.57	0 100 100	44, 55, 69, 76	0
49	2r	68/88 (77%)	0.83	4 (5%) 28 25	54, 64, 72, 76	0
50	1s	83/93 (89%)	1.48	20 (24%) 2 1	63, 74, 78, 84	0
50	2s	83/93 (89%)	1.46	20 (24%) 2 1	62, 75, 82, 83	0
51	1t	96/106 (90%)	0.76	7 (7%) 21 18	50, 60, 71, 73	0
51	2t	96/106 (90%)	0.80	7 (7%) 21 18	46, 62, 70, 72	0
52	1u	23/27 (85%)	1.54	6 (26%) 1 1	60, 65, 70, 73	0
52	2u	23/27 (85%)	1.69	9 (39%) 1 0	66, 72, 75, 78	0
53	1v	13/24 (54%)	0.32	0 100 100	42, 52, 82, 86	0
53	2v	13/24 (54%)	0.81	0 100 100	56, 65, 85, 88	0
54	1w	248/354 (70%)	0.32	5 (2%) 65 62	25, 58, 72, 80	0
54	2w	252/354 (71%)	0.45	6 (2%) 59 56	40, 64, 76, 82	0
55	1x	68/76 (89%)	-0.10	1 (1%) 72 70	20, 51, 64, 84	0
55	1y	67/76 (88%)	0.96	9 (13%) 7 6	32, 79, 87, 93	0
55	2x	68/76 (89%)	0.20	0 100 100	37, 65, 74, 84	0
55	2y	67/76 (88%)	1.39	14 (20%) 2 2	50, 88, 93, 96	0
56	1z	14/20 (70%)	0.37	0 100 100	25, 35, 61, 67	0
56	2z	14/20 (70%)	0.99	1 (7%) 22 19	43, 58, 70, 73	0
All	All	21290/22342 (95%)	0.24	1019 (4%) 35 32	10, 55, 79, 98	0

The worst 5 of 1019 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1088	A	7.7
32	1a	1026	G	6.5
38	1g	80	VAL	6.5
1	1A	1068	G	6.4
44	1m	2	ALA	6.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	5MU	2y	54	21/22	0.57	0.17	82,91,101,116	0
55	G7M	2y	46	24/25	0.58	0.18	81,91,99,115	0
55	4SU	2y	8	20/21	0.68	0.13	83,87,95,108	0
55	PSU	2y	55	20/21	0.68	0.14	82,90,97,106	0
43	0TD	1l	92	10/11	0.71	0.15	40,51,63,71	0
55	G7M	1y	46	24/25	0.71	0.15	74,84,96,109	0
55	PSU	1y	55	20/21	0.75	0.14	71,81,91,98	0
55	5MU	1y	54	21/22	0.77	0.14	71,81,92,108	0
55	PSU	2y	32	20/21	0.80	0.15	70,80,83,90	0
55	PSU	2y	39	20/21	0.81	0.12	71,80,87,89	0
55	4SU	1y	8	20/21	0.81	0.12	74,80,87,90	0
55	PSU	1y	39	20/21	0.82	0.12	58,75,78,79	0
32	2MG	1a	1207	24/25	0.83	0.14	70,75,81,86	0
55	PSU	1y	32	20/21	0.83	0.11	60,70,75,76	0
32	2MG	2a	1207	24/25	0.83	0.12	60,75,81,87	0
55	MIA	2y	37	29/30	0.84	0.14	68,75,84,94	0
55	G7M	2x	46	24/25	0.85	0.13	62,68,74,93	0
43	0TD	2l	92	10/11	0.86	0.14	53,58,65,74	0
55	MIA	1y	37	29/30	0.87	0.12	58,68,71,82	0
55	PSU	2x	55	20/21	0.87	0.10	55,67,73,78	0
55	PSU	2x	32	20/21	0.87	0.12	61,68,76,77	0
32	M2G	1a	966	25/26	0.88	0.13	42,53,64,65	0
1	5MU	2A	1915	21/22	0.88	0.11	52,57,68,75	0
55	PSU	2x	39	20/21	0.91	0.11	46,64,69,74	0
32	5MC	2a	967	21/22	0.91	0.11	59,63,70,80	0
1	PSU	2A	1911	20/21	0.91	0.09	47,52,58,59	0
55	G7M	1x	46	24/25	0.91	0.09	40,47,62,79	0
32	PSU	2a	516	20/21	0.91	0.11	57,65,72,73	0
32	M2G	2a	966	25/26	0.92	0.11	54,62,72,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	5MU	2x	54	21/22	0.92	0.09	60,65,69,74	0
55	4SU	2x	8	20/21	0.92	0.12	58,65,70,72	0
32	PSU	1a	516	20/21	0.92	0.10	50,58,68,69	0
32	G7M	2a	527	24/25	0.92	0.11	54,62,65,68	0
32	5MC	2a	1400	21/22	0.93	0.10	55,62,66,67	0
32	G7M	1a	527	24/25	0.93	0.10	43,56,63,63	0
55	5MU	1x	54	21/22	0.93	0.11	48,55,60,64	0
1	OMC	2A	1920	21/22	0.93	0.09	44,50,54,55	0
55	PSU	1x	39	20/21	0.93	0.10	35,51,57,59	0
32	MA6	2a	1518	24/25	0.94	0.10	41,51,57,59	0
1	PSU	2A	1917	20/21	0.94	0.07	44,50,57,59	0
32	5MC	1a	967	21/22	0.94	0.10	46,53,63,67	0
32	4OC	2a	1402	22/23	0.94	0.09	46,50,54,59	0
32	5MC	2a	1404	21/22	0.94	0.11	30,44,48,50	0
1	PSU	1A	1911	20/21	0.95	0.10	35,46,53,54	0
54	MEQ	2w	230	10/11	0.95	0.12	42,44,50,51	0
1	5MU	1A	1915	21/22	0.95	0.08	42,48,54,61	0
55	PSU	1x	32	20/21	0.95	0.09	42,51,58,67	0
55	MIA	2x	37	29/30	0.95	0.11	54,62,67,68	0
32	UR3	2a	1498	21/22	0.95	0.10	42,49,55,58	0
55	PSU	1x	55	20/21	0.95	0.09	50,53,60,61	0
32	MA6	2a	1519	24/25	0.95	0.10	41,49,54,57	0
32	5MC	2a	1407	21/22	0.96	0.08	36,42,50,57	0
1	OMC	1A	1920	21/22	0.96	0.09	33,41,45,48	0
55	4SU	1x	8	20/21	0.96	0.07	32,40,47,52	0
1	PSU	1A	1917	20/21	0.96	0.07	34,42,52,54	0
55	MIA	1x	37	29/30	0.96	0.08	37,47,56,58	0
32	5MC	1a	1400	21/22	0.96	0.10	39,47,57,59	0
32	4OC	1a	1402	22/23	0.96	0.09	35,40,44,50	0
32	5MC	1a	1404	21/22	0.96	0.08	30,35,41,48	0
32	MA6	1a	1518	24/25	0.96	0.10	23,35,43,47	0
32	MA6	1a	1519	24/25	0.96	0.09	31,34,38,42	0
54	MEQ	1w	230	10/11	0.97	0.09	20,25,27,29	0
1	5MC	1A	1942	21/22	0.97	0.07	21,28,32,37	0
1	5MC	1A	1962	21/22	0.97	0.07	18,26,29,34	0
1	5MU	2A	1939	21/22	0.97	0.07	28,31,36,36	0
1	5MC	2A	1942	21/22	0.97	0.06	32,38,44,46	0
1	5MC	2A	1962	21/22	0.97	0.08	25,32,36,48	0
1	OMG	2A	2251	24/25	0.97	0.08	25,34,37,45	0
1	2MA	2A	2503	23/24	0.97	0.07	24,29,32,34	0
32	5MC	1a	1407	21/22	0.97	0.07	27,35,39,43	0
1	5MU	1A	1939	21/22	0.98	0.07	13,20,24,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OMG	1A	2251	24/25	0.98	0.06	10,15,18,24	0
1	OMU	2A	2552	21/22	0.98	0.06	22,27,31,35	0
1	PSU	2A	2605	20/21	0.98	0.07	21,28,33,37	0
1	2MA	1A	2503	23/24	0.98	0.06	10,14,17,17	0
1	OMU	1A	2552	21/22	0.98	0.06	12,17,20,23	0
32	UR3	1a	1498	21/22	0.98	0.07	29,34,37,39	0
1	PSU	1A	2605	20/21	0.98	0.07	13,18,22,29	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	3716	1/1	0.43	0.17	42,42,42,42	0
57	MG	1A	3631	1/1	0.44	0.22	65,65,65,65	0
57	MG	2a	1766	1/1	0.46	0.20	64,64,64,64	0
57	MG	2a	1763	1/1	0.51	0.25	82,82,82,82	0
57	MG	1a	1770	1/1	0.60	0.20	73,73,73,73	0
57	MG	2j	202	1/1	0.60	0.24	77,77,77,77	0
57	MG	1a	1738	1/1	0.62	0.28	55,55,55,55	0
57	MG	2A	3024	1/1	0.63	0.21	64,64,64,64	0
57	MG	2A	3585	1/1	0.66	0.17	49,49,49,49	0
57	MG	1A	3751	1/1	0.67	0.24	56,56,56,56	0
57	MG	1A	3549	1/1	0.69	0.16	10,10,10,10	0
57	MG	2A	3046	1/1	0.69	0.20	59,59,59,59	0
57	MG	2a	1749	1/1	0.70	0.29	65,65,65,65	0
57	MG	2A	3625	1/1	0.71	0.15	62,62,62,62	0
57	MG	2A	3634	1/1	0.71	0.14	70,70,70,70	0
57	MG	1a	1751	1/1	0.71	0.22	63,63,63,63	0
57	MG	1A	3352	1/1	0.72	0.17	46,46,46,46	0
57	MG	2A	3068	1/1	0.72	0.22	64,64,64,64	0
57	MG	2a	1666	1/1	0.72	0.41	58,58,58,58	0
57	MG	2A	3446	1/1	0.72	0.13	55,55,55,55	0
57	MG	2a	1759	1/1	0.72	0.31	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1760	1/1	0.72	0.12	52,52,52,52	0
57	MG	2A	3504	1/1	0.72	0.18	60,60,60,60	0
57	MG	14	502	1/1	0.72	0.12	70,70,70,70	0
57	MG	2A	3621	1/1	0.72	0.12	66,66,66,66	0
57	MG	1A	3760	1/1	0.73	0.16	54,54,54,54	0
57	MG	2A	3340	1/1	0.73	0.19	60,60,60,60	0
57	MG	1A	3793	1/1	0.73	0.14	48,48,48,48	0
57	MG	2A	3478	1/1	0.73	0.23	57,57,57,57	0
57	MG	1a	1747	1/1	0.74	0.18	57,57,57,57	0
57	MG	2a	1669	1/1	0.74	0.29	65,65,65,65	0
57	MG	1A	3333	1/1	0.75	0.13	24,24,24,24	0
57	MG	2A	3087	1/1	0.75	0.29	65,65,65,65	0
57	MG	2A	3524	1/1	0.75	0.20	70,70,70,70	0
57	MG	2A	3531	1/1	0.75	0.14	68,68,68,68	0
57	MG	2a	1753	1/1	0.75	0.16	63,63,63,63	0
57	MG	1A	3365	1/1	0.75	0.11	8,8,8,8	0
57	MG	2A	3607	1/1	0.75	0.18	61,61,61,61	0
57	MG	2A	3614	1/1	0.75	0.21	66,66,66,66	0
57	MG	2A	3402	1/1	0.75	0.17	65,65,65,65	0
57	MG	1A	3759	1/1	0.75	0.14	53,53,53,53	0
57	MG	1a	1765	1/1	0.76	0.14	52,52,52,52	0
57	MG	2A	3545	1/1	0.76	0.13	63,63,63,63	0
57	MG	10	103	1/1	0.76	0.18	57,57,57,57	0
57	MG	2D	308	1/1	0.76	0.15	48,48,48,48	0
57	MG	1A	3487	1/1	0.76	0.32	60,60,60,60	0
57	MG	2a	1667	1/1	0.76	0.36	69,69,69,69	0
57	MG	1a	1646	1/1	0.76	0.31	56,56,56,56	0
57	MG	2A	3326	1/1	0.77	0.11	27,27,27,27	0
57	MG	2a	1689	1/1	0.77	0.19	48,48,48,48	0
57	MG	1a	1769	1/1	0.77	0.13	62,62,62,62	0
57	MG	2A	3509	1/1	0.77	0.21	48,48,48,48	0
57	MG	2A	3392	1/1	0.77	0.24	63,63,63,63	0
57	MG	1A	3361	1/1	0.77	0.15	21,21,21,21	0
57	MG	1a	1701	1/1	0.77	0.23	70,70,70,70	0
57	MG	2A	3469	1/1	0.77	0.20	74,74,74,74	0
57	MG	2A	3599	1/1	0.77	0.18	46,46,46,46	0
57	MG	2a	1627	1/1	0.78	0.17	62,62,62,62	0
57	MG	1a	1658	1/1	0.78	0.30	52,52,52,52	0
57	MG	2A	3275	1/1	0.78	0.15	30,30,30,30	0
57	MG	2A	3399	1/1	0.78	0.14	53,53,53,53	0
57	MG	2A	3037	1/1	0.78	0.16	54,54,54,54	0
57	MG	2a	1764	1/1	0.78	0.22	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1725	1/1	0.78	0.14	58,58,58,58	0
57	MG	2a	1736	1/1	0.78	0.35	73,73,73,73	0
57	MG	2k	201	1/1	0.78	0.33	67,67,67,67	0
57	MG	1E	309	1/1	0.79	0.14	30,30,30,30	0
57	MG	1A	3648	1/1	0.79	0.17	46,46,46,46	0
57	MG	1A	3607	1/1	0.79	0.10	38,38,38,38	0
57	MG	2A	3140	1/1	0.79	0.21	62,62,62,62	0
57	MG	1a	1605	1/1	0.79	0.16	61,61,61,61	0
57	MG	1A	3368	1/1	0.79	0.14	46,46,46,46	0
57	MG	2x	108	1/1	0.79	0.29	65,65,65,65	0
57	MG	2A	3393	1/1	0.80	0.16	67,67,67,67	0
57	MG	1a	1601	1/1	0.80	0.23	62,62,62,62	0
57	MG	1a	1732	1/1	0.80	0.19	58,58,58,58	0
57	MG	2a	1756	1/1	0.80	0.24	63,63,63,63	0
57	MG	2N	201	1/1	0.80	0.07	61,61,61,61	0
57	MG	2A	3578	1/1	0.80	0.19	59,59,59,59	0
57	MG	1A	3485	1/1	0.80	0.21	52,52,52,52	0
57	MG	1a	1632	1/1	0.80	0.26	52,52,52,52	0
57	MG	1A	3764	1/1	0.80	0.13	31,31,31,31	0
57	MG	2a	1670	1/1	0.80	0.22	72,72,72,72	0
57	MG	2A	3360	1/1	0.80	0.19	68,68,68,68	0
57	MG	1A	3730	1/1	0.80	0.22	65,65,65,65	0
57	MG	1a	1784	1/1	0.81	0.15	62,62,62,62	0
57	MG	1a	1618	1/1	0.81	0.22	56,56,56,56	0
57	MG	2a	1673	1/1	0.81	0.26	61,61,61,61	0
57	MG	2A	3026	1/1	0.81	0.51	49,49,49,49	0
57	MG	2a	1697	1/1	0.81	0.15	60,60,60,60	0
57	MG	1A	3683	1/1	0.81	0.20	60,60,60,60	0
57	MG	1A	3474	1/1	0.81	0.14	30,30,30,30	0
57	MG	1a	1761	1/1	0.81	0.17	42,42,42,42	0
57	MG	1A	3724	1/1	0.81	0.46	48,48,48,48	0
57	MG	2A	3414	1/1	0.81	0.19	33,33,33,33	0
57	MG	1A	3626	1/1	0.81	0.13	36,36,36,36	0
57	MG	2A	3452	1/1	0.81	0.19	55,55,55,55	0
57	MG	2A	3145	1/1	0.81	0.20	56,56,56,56	0
57	MG	2A	3167	1/1	0.81	0.33	50,50,50,50	0
57	MG	2X	103	1/1	0.81	0.14	71,71,71,71	0
57	MG	2A	3272	1/1	0.81	0.13	49,49,49,49	0
57	MG	1A	3741	1/1	0.81	0.12	36,36,36,36	0
57	MG	2A	3277	1/1	0.81	0.18	67,67,67,67	0
57	MG	2A	3415	1/1	0.82	0.17	55,55,55,55	0
57	MG	2A	3436	1/1	0.82	0.14	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	1A	3707	1/1	0.82	0.12	47,47,47,47	0
57	MG	2A	3162	1/1	0.82	0.17	48,48,48,48	0
57	MG	1A	3562	1/1	0.82	0.10	26,26,26,26	0
57	MG	1A	3723	1/1	0.82	0.24	25,25,25,25	0
57	MG	1a	1787	1/1	0.82	0.25	49,49,49,49	0
57	MG	1a	1704	1/1	0.82	0.13	64,64,64,64	0
57	MG	2A	3293	1/1	0.82	0.15	56,56,56,56	0
57	MG	2A	3296	1/1	0.82	0.12	36,36,36,36	0
57	MG	2a	1698	1/1	0.82	0.16	68,68,68,68	0
57	MG	2A	3543	1/1	0.82	0.19	51,51,51,51	0
57	MG	2a	1729	1/1	0.82	0.16	68,68,68,68	0
57	MG	2a	1734	1/1	0.82	0.28	65,65,65,65	0
57	MG	1A	3374	1/1	0.82	0.11	26,26,26,26	0
57	MG	2A	3562	1/1	0.82	0.14	61,61,61,61	0
57	MG	1A	3331	1/1	0.82	0.12	24,24,24,24	0
57	MG	2A	3358	1/1	0.82	0.21	62,62,62,62	0
57	MG	2A	3596	1/1	0.82	0.17	58,58,58,58	0
57	MG	1A	3018	1/1	0.82	0.20	37,37,37,37	0
57	MG	2A	3051	1/1	0.82	0.13	50,50,50,50	0
57	MG	1A	3638	1/1	0.82	0.09	26,26,26,26	0
57	MG	2A	3398	1/1	0.82	0.13	47,47,47,47	0
57	MG	1A	3019	1/1	0.82	0.15	47,47,47,47	0
57	MG	2A	3117	1/1	0.82	0.21	65,65,65,65	0
57	MG	1A	3372	1/1	0.82	0.13	32,32,32,32	0
57	MG	2A	3239	1/1	0.83	0.13	30,30,30,30	0
57	MG	2a	1711	1/1	0.83	0.20	57,57,57,57	0
57	MG	2A	3480	1/1	0.83	0.17	65,65,65,65	0
57	MG	2A	3252	1/1	0.83	0.13	53,53,53,53	0
57	MG	1x	108	1/1	0.83	0.10	42,42,42,42	0
57	MG	2a	1735	1/1	0.83	0.15	62,62,62,62	0
57	MG	1A	3398	1/1	0.83	0.15	48,48,48,48	0
57	MG	1A	3664	1/1	0.83	0.12	39,39,39,39	0
57	MG	2A	3290	1/1	0.83	0.21	44,44,44,44	0
57	MG	2a	1755	1/1	0.83	0.13	64,64,64,64	0
57	MG	1A	3127	1/1	0.83	0.24	71,71,71,71	0
57	MG	1A	3385	1/1	0.83	0.14	39,39,39,39	0
57	MG	2A	3574	1/1	0.83	0.15	68,68,68,68	0
57	MG	1A	3588	1/1	0.83	0.16	14,14,14,14	0
57	MG	2A	3054	1/1	0.83	0.25	53,53,53,53	0
57	MG	2A	3346	1/1	0.83	0.10	50,50,50,50	0
57	MG	2a	1680	1/1	0.83	0.25	59,59,59,59	0
57	MG	2A	3461	1/1	0.83	0.16	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2x	106	1/1	0.83	0.26	72,72,72,72	0
57	MG	2A	3183	1/1	0.83	0.35	56,56,56,56	0
57	MG	2A	3077	1/1	0.84	0.18	56,56,56,56	0
57	MG	2A	3520	1/1	0.84	0.17	63,63,63,63	0
57	MG	1a	1640	1/1	0.84	0.21	69,69,69,69	0
57	MG	1E	305	1/1	0.84	0.24	57,57,57,57	0
57	MG	1a	1781	1/1	0.84	0.14	53,53,53,53	0
57	MG	1a	1647	1/1	0.84	0.24	47,47,47,47	0
57	MG	2A	3546	1/1	0.84	0.24	60,60,60,60	0
57	MG	2A	3556	1/1	0.84	0.12	45,45,45,45	0
57	MG	1A	3027	1/1	0.84	0.12	44,44,44,44	0
57	MG	2a	1713	1/1	0.84	0.22	60,60,60,60	0
57	MG	1v	101	1/1	0.84	0.13	65,65,65,65	0
57	MG	2a	1726	1/1	0.84	0.21	69,69,69,69	0
57	MG	1w	403	1/1	0.84	0.17	54,54,54,54	0
57	MG	2A	3209	1/1	0.84	0.23	47,47,47,47	0
57	MG	1A	3591	1/1	0.84	0.09	29,29,29,29	0
57	MG	2A	3597	1/1	0.84	0.10	56,56,56,56	0
57	MG	1A	3519	1/1	0.84	0.11	39,39,39,39	0
57	MG	2A	3258	1/1	0.84	0.16	42,42,42,42	0
57	MG	2A	3444	1/1	0.84	0.24	59,59,59,59	0
57	MG	1A	3109	1/1	0.84	0.19	50,50,50,50	0
57	MG	1A	3768	1/1	0.84	0.13	33,33,33,33	0
57	MG	1a	1614	1/1	0.84	0.20	71,71,71,71	0
57	MG	1a	1616	1/1	0.84	0.29	58,58,58,58	0
57	MG	2A	3472	1/1	0.84	0.10	39,39,39,39	0
57	MG	1A	3390	1/1	0.84	0.17	50,50,50,50	0
57	MG	2a	1618	1/1	0.84	0.20	61,61,61,61	0
57	MG	2a	1626	1/1	0.84	0.26	48,48,48,48	0
57	MG	2A	3057	1/1	0.84	0.24	58,58,58,58	0
57	MG	1B	202	1/1	0.84	0.20	43,43,43,43	0
57	MG	2A	3537	1/1	0.85	0.18	53,53,53,53	0
57	MG	1a	1721	1/1	0.85	0.18	63,63,63,63	0
57	MG	2A	3193	1/1	0.85	0.20	57,57,57,57	0
57	MG	2A	3002	1/1	0.85	0.12	52,52,52,52	0
57	MG	2A	3550	1/1	0.85	0.18	55,55,55,55	0
57	MG	1B	209	1/1	0.85	0.22	51,51,51,51	0
57	MG	1A	3601	1/1	0.85	0.09	18,18,18,18	0
57	MG	1a	1625	1/1	0.85	0.14	56,56,56,56	0
57	MG	2A	3432	1/1	0.85	0.18	60,60,60,60	0
57	MG	2A	3581	1/1	0.85	0.08	69,69,69,69	0
57	MG	2A	3264	1/1	0.85	0.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3577	1/1	0.85	0.09	30,30,30,30	0
57	MG	1a	1638	1/1	0.85	0.21	54,54,54,54	0
57	MG	1U	204	1/1	0.85	0.17	37,37,37,37	0
57	MG	1a	1768	1/1	0.85	0.33	71,71,71,71	0
57	MG	2A	3466	1/1	0.85	0.22	58,58,58,58	0
57	MG	1A	3262	1/1	0.85	0.17	40,40,40,40	0
57	MG	1A	3735	1/1	0.85	0.10	12,12,12,12	0
57	MG	1a	1648	1/1	0.85	0.27	60,60,60,60	0
57	MG	2D	306	1/1	0.85	0.10	55,55,55,55	0
57	MG	1a	1782	1/1	0.85	0.15	74,74,74,74	0
57	MG	2A	3499	1/1	0.85	0.15	56,56,56,56	0
57	MG	1A	3785	1/1	0.85	0.30	58,58,58,58	0
57	MG	2A	3507	1/1	0.85	0.17	37,37,37,37	0
57	MG	2f	201	1/1	0.85	0.14	64,64,64,64	0
57	MG	1a	1688	1/1	0.85	0.25	55,55,55,55	0
57	MG	1A	3358	1/1	0.85	0.12	38,38,38,38	0
57	MG	2A	3383	1/1	0.85	0.28	54,54,54,54	0
57	MG	1A	3600	1/1	0.85	0.12	29,29,29,29	0
57	MG	2A	3113	1/1	0.86	0.22	64,64,64,64	0
57	MG	1A	3595	1/1	0.86	0.10	38,38,38,38	0
57	MG	1A	3111	1/1	0.86	0.17	54,54,54,54	0
57	MG	2A	3390	1/1	0.86	0.15	43,43,43,43	0
57	MG	1A	3276	1/1	0.86	0.09	52,52,52,52	0
57	MG	1A	3336	1/1	0.86	0.10	32,32,32,32	0
57	MG	2A	3395	1/1	0.86	0.14	48,48,48,48	0
57	MG	1A	3448	1/1	0.86	0.13	54,54,54,54	0
57	MG	1a	1706	1/1	0.86	0.14	45,45,45,45	0
57	MG	1a	1717	1/1	0.86	0.08	69,69,69,69	0
57	MG	1A	3729	1/1	0.86	0.13	22,22,22,22	0
57	MG	2A	3230	1/1	0.86	0.15	48,48,48,48	0
57	MG	1A	3281	1/1	0.86	0.18	49,49,49,49	0
57	MG	1a	1735	1/1	0.86	0.16	54,54,54,54	0
57	MG	2A	3590	1/1	0.86	0.09	48,48,48,48	0
57	MG	1B	206	1/1	0.86	0.15	34,34,34,34	0
57	MG	1a	1627	1/1	0.86	0.17	67,67,67,67	0
57	MG	2A	3270	1/1	0.86	0.14	52,52,52,52	0
57	MG	2A	3050	1/1	0.86	0.24	60,60,60,60	0
57	MG	1A	3475	1/1	0.86	0.14	39,39,39,39	0
57	MG	1a	1634	1/1	0.86	0.33	60,60,60,60	0
57	MG	1A	3737	1/1	0.86	0.14	32,32,32,32	0
57	MG	2A	3633	1/1	0.86	0.14	73,73,73,73	0
57	MG	2A	3477	1/1	0.86	0.19	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	2A	3640	1/1	0.86	0.12	49,49,49,49	0
57	MG	1A	3589	1/1	0.86	0.11	16,16,16,16	0
57	MG	2A	3073	1/1	0.86	0.25	61,61,61,61	0
57	MG	2A	3319	1/1	0.86	0.10	49,49,49,49	0
57	MG	2P	202	1/1	0.86	0.19	72,72,72,72	0
57	MG	1Q	205	1/1	0.86	0.12	48,48,48,48	0
57	MG	1A	3311	1/1	0.86	0.11	24,24,24,24	0
57	MG	2A	3112	1/1	0.86	0.20	55,55,55,55	0
57	MG	2x	109	1/1	0.86	0.17	51,51,51,51	0
57	MG	2A	3426	1/1	0.87	0.11	58,58,58,58	0
57	MG	2A	3228	1/1	0.87	0.16	51,51,51,51	0
57	MG	1B	203	1/1	0.87	0.13	54,54,54,54	0
57	MG	2A	3638	1/1	0.87	0.15	45,45,45,45	0
57	MG	2A	3236	1/1	0.87	0.15	68,68,68,68	0
57	MG	2B	208	1/1	0.87	0.19	54,54,54,54	0
57	MG	1A	3415	1/1	0.87	0.08	26,26,26,26	0
57	MG	1a	1719	1/1	0.87	0.13	54,54,54,54	0
57	MG	1A	3320	1/1	0.87	0.08	41,41,41,41	0
57	MG	1A	3377	1/1	0.87	0.12	40,40,40,40	0
57	MG	2A	3043	1/1	0.87	0.15	50,50,50,50	0
57	MG	2a	1602	1/1	0.87	0.14	64,64,64,64	0
57	MG	2a	1603	1/1	0.87	0.18	62,62,62,62	0
57	MG	1A	3568	1/1	0.87	0.09	30,30,30,30	0
57	MG	2a	1625	1/1	0.87	0.19	49,49,49,49	0
57	MG	1F	309	1/1	0.87	0.32	38,38,38,38	0
57	MG	1N	204	1/1	0.87	0.12	33,33,33,33	0
57	MG	2a	1630	1/1	0.87	0.09	56,56,56,56	0
57	MG	2a	1644	1/1	0.87	0.23	66,66,66,66	0
57	MG	2a	1655	1/1	0.87	0.17	68,68,68,68	0
57	MG	2a	1664	1/1	0.87	0.26	50,50,50,50	0
57	MG	2A	3278	1/1	0.87	0.08	49,49,49,49	0
57	MG	2A	3487	1/1	0.87	0.12	66,66,66,66	0
57	MG	2A	3490	1/1	0.87	0.13	44,44,44,44	0
57	MG	2A	3493	1/1	0.87	0.18	69,69,69,69	0
57	MG	1a	1749	1/1	0.87	0.09	51,51,51,51	0
57	MG	1A	3720	1/1	0.87	0.17	21,21,21,21	0
57	MG	1a	1752	1/1	0.87	0.18	60,60,60,60	0
57	MG	2A	3307	1/1	0.87	0.12	47,47,47,47	0
57	MG	2A	3515	1/1	0.87	0.16	52,52,52,52	0
57	MG	2A	3313	1/1	0.87	0.19	41,41,41,41	0
57	MG	1A	3263	1/1	0.87	0.09	48,48,48,48	0
57	MG	2a	1716	1/1	0.87	0.16	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	1719	1/1	0.87	0.21	53,53,53,53	0
57	MG	1A	3477	1/1	0.87	0.12	44,44,44,44	0
57	MG	1A	3784	1/1	0.87	0.21	50,50,50,50	0
57	MG	1a	1651	1/1	0.87	0.09	66,66,66,66	0
57	MG	2a	1730	1/1	0.87	0.09	54,54,54,54	0
57	MG	18	101	1/1	0.87	0.18	38,38,38,38	0
57	MG	1a	1771	1/1	0.87	0.13	67,67,67,67	0
57	MG	2A	3547	1/1	0.87	0.10	41,41,41,41	0
57	MG	2a	1739	1/1	0.87	0.26	61,61,61,61	0
57	MG	2A	3368	1/1	0.87	0.15	57,57,57,57	0
57	MG	2A	3132	1/1	0.87	0.10	45,45,45,45	0
57	MG	1a	1660	1/1	0.87	0.25	64,64,64,64	0
57	MG	1a	1679	1/1	0.87	0.33	67,67,67,67	0
57	MG	1a	1686	1/1	0.87	0.18	48,48,48,48	0
57	MG	1A	3354	1/1	0.87	0.12	22,22,22,22	0
57	MG	2A	3583	1/1	0.87	0.11	40,40,40,40	0
57	MG	2A	3169	1/1	0.87	0.24	47,47,47,47	0
57	MG	1A	3235	1/1	0.87	0.23	49,49,49,49	0
57	MG	1A	3659	1/1	0.87	0.15	39,39,39,39	0
57	MG	2A	3405	1/1	0.87	0.16	42,42,42,42	0
57	MG	2A	3408	1/1	0.87	0.12	27,27,27,27	0
57	MG	2A	3206	1/1	0.87	0.07	61,61,61,61	0
57	MG	1x	106	1/1	0.87	0.12	52,52,52,52	0
57	MG	2A	3416	1/1	0.87	0.11	33,33,33,33	0
57	MG	1A	3620	1/1	0.88	0.14	51,51,51,51	0
57	MG	1a	1693	1/1	0.88	0.20	60,60,60,60	0
57	MG	2A	3418	1/1	0.88	0.20	61,61,61,61	0
57	MG	1a	1698	1/1	0.88	0.21	53,53,53,53	0
57	MG	2B	204	1/1	0.88	0.26	51,51,51,51	0
57	MG	1A	3408	1/1	0.88	0.09	29,29,29,29	0
57	MG	2B	209	1/1	0.88	0.21	45,45,45,45	0
57	MG	2A	3012	1/1	0.88	0.09	52,52,52,52	0
57	MG	1A	3515	1/1	0.88	0.13	31,31,31,31	0
57	MG	2F	305	1/1	0.88	0.25	45,45,45,45	0
57	MG	2A	3253	1/1	0.88	0.15	58,58,58,58	0
57	MG	1A	3286	1/1	0.88	0.15	44,44,44,44	0
57	MG	2A	3454	1/1	0.88	0.34	43,43,43,43	0
57	MG	26	101	1/1	0.88	0.10	62,62,62,62	0
57	MG	1a	1712	1/1	0.88	0.16	65,65,65,65	0
57	MG	2A	3465	1/1	0.88	0.17	49,49,49,49	0
57	MG	2a	1617	1/1	0.88	0.27	56,56,56,56	0
57	MG	2A	3269	1/1	0.88	0.11	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	1A	3426	1/1	0.88	0.09	21,21,21,21	0
57	MG	1A	3432	1/1	0.88	0.14	54,54,54,54	0
57	MG	1A	3446	1/1	0.88	0.10	52,52,52,52	0
57	MG	1A	3680	1/1	0.88	0.09	41,41,41,41	0
57	MG	2a	1635	1/1	0.88	0.15	58,58,58,58	0
57	MG	1A	3795	1/1	0.88	0.11	47,47,47,47	0
57	MG	2a	1646	1/1	0.88	0.29	59,59,59,59	0
57	MG	2A	3286	1/1	0.88	0.12	61,61,61,61	0
57	MG	2a	1661	1/1	0.88	0.17	39,39,39,39	0
57	MG	1A	3359	1/1	0.88	0.09	34,34,34,34	0
57	MG	2A	3064	1/1	0.88	0.25	50,50,50,50	0
57	MG	1a	1744	1/1	0.88	0.12	55,55,55,55	0
57	MG	2A	3297	1/1	0.88	0.11	47,47,47,47	0
57	MG	2A	3300	1/1	0.88	0.07	34,34,34,34	0
57	MG	1A	3582	1/1	0.88	0.10	33,33,33,33	0
57	MG	2A	3513	1/1	0.88	0.07	36,36,36,36	0
57	MG	2A	3074	1/1	0.88	0.08	54,54,54,54	0
57	MG	2a	1692	1/1	0.88	0.13	27,27,27,27	0
57	MG	1A	3586	1/1	0.88	0.08	16,16,16,16	0
57	MG	1A	3587	1/1	0.88	0.10	27,27,27,27	0
57	MG	2a	1702	1/1	0.88	0.15	61,61,61,61	0
57	MG	1a	1641	1/1	0.88	0.26	63,63,63,63	0
57	MG	2A	3344	1/1	0.88	0.13	37,37,37,37	0
57	MG	2A	3345	1/1	0.88	0.07	67,67,67,67	0
57	MG	2a	1717	1/1	0.88	0.11	40,40,40,40	0
57	MG	1A	3452	1/1	0.88	0.13	19,19,19,19	0
57	MG	1A	3460	1/1	0.88	0.12	29,29,29,29	0
57	MG	2A	3127	1/1	0.88	0.14	45,45,45,45	0
57	MG	2a	1728	1/1	0.88	0.18	64,64,64,64	0
57	MG	2A	3361	1/1	0.88	0.08	52,52,52,52	0
57	MG	2A	3551	1/1	0.88	0.13	25,25,25,25	0
57	MG	1A	3471	1/1	0.88	0.10	57,57,57,57	0
57	MG	2A	3558	1/1	0.88	0.18	60,60,60,60	0
57	MG	1A	3224	1/1	0.88	0.11	59,59,59,59	0
57	MG	2A	3568	1/1	0.88	0.09	66,66,66,66	0
57	MG	2A	3386	1/1	0.88	0.10	60,60,60,60	0
57	MG	2A	3387	1/1	0.88	0.14	54,54,54,54	0
57	MG	2a	1754	1/1	0.88	0.18	58,58,58,58	0
57	MG	1a	1653	1/1	0.88	0.14	63,63,63,63	0
57	MG	2A	3391	1/1	0.88	0.10	22,22,22,22	0
57	MG	2A	3158	1/1	0.88	0.18	60,60,60,60	0
57	MG	1A	3124	1/1	0.88	0.18	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	3592	1/1	0.88	0.16	51,51,51,51	0
57	MG	1R	203	1/1	0.88	0.17	42,42,42,42	0
57	MG	1a	1678	1/1	0.88	0.34	56,56,56,56	0
57	MG	2A	3171	1/1	0.88	0.32	59,59,59,59	0
57	MG	2A	3178	1/1	0.88	0.16	52,52,52,52	0
57	MG	2A	3610	1/1	0.88	0.13	51,51,51,51	0
57	MG	1A	3367	1/1	0.88	0.17	54,54,54,54	0
57	MG	1a	1680	1/1	0.88	0.22	61,61,61,61	0
57	MG	1A	3050	1/1	0.88	0.12	40,40,40,40	0
58	ZN	14	501	1/1	0.88	0.17	124,124,124,124	0
57	MG	1a	1731	1/1	0.89	0.10	39,39,39,39	0
57	MG	1A	3583	1/1	0.89	0.10	55,55,55,55	0
57	MG	1A	3643	1/1	0.89	0.07	22,22,22,22	0
57	MG	2a	1632	1/1	0.89	0.25	56,56,56,56	0
57	MG	1A	3247	1/1	0.89	0.08	40,40,40,40	0
57	MG	1a	1742	1/1	0.89	0.16	48,48,48,48	0
57	MG	1A	3191	1/1	0.89	0.06	48,48,48,48	0
57	MG	1a	1746	1/1	0.89	0.10	49,49,49,49	0
57	MG	2a	1659	1/1	0.89	0.28	53,53,53,53	0
57	MG	2a	1660	1/1	0.89	0.17	45,45,45,45	0
57	MG	1A	3755	1/1	0.89	0.17	25,25,25,25	0
57	MG	2a	1662	1/1	0.89	0.12	50,50,50,50	0
57	MG	2A	3053	1/1	0.89	0.20	58,58,58,58	0
57	MG	1A	3429	1/1	0.89	0.15	54,54,54,54	0
57	MG	1A	3674	1/1	0.89	0.12	41,41,41,41	0
57	MG	2a	1668	1/1	0.89	0.12	52,52,52,52	0
57	MG	2A	3265	1/1	0.89	0.07	25,25,25,25	0
57	MG	2A	3410	1/1	0.89	0.18	53,53,53,53	0
57	MG	1A	3323	1/1	0.89	0.16	39,39,39,39	0
57	MG	2a	1677	1/1	0.89	0.18	50,50,50,50	0
57	MG	2A	3066	1/1	0.89	0.10	46,46,46,46	0
57	MG	2A	3067	1/1	0.89	0.27	58,58,58,58	0
57	MG	1A	3765	1/1	0.89	0.25	50,50,50,50	0
57	MG	2A	3423	1/1	0.89	0.09	43,43,43,43	0
57	MG	1A	3509	1/1	0.89	0.08	14,14,14,14	0
57	MG	1a	1603	1/1	0.89	0.18	46,46,46,46	0
57	MG	2a	1708	1/1	0.89	0.17	57,57,57,57	0
57	MG	2A	3593	1/1	0.89	0.11	54,54,54,54	0
57	MG	2A	3284	1/1	0.89	0.14	66,66,66,66	0
57	MG	2A	3437	1/1	0.89	0.09	36,36,36,36	0
57	MG	1A	3782	1/1	0.89	0.10	39,39,39,39	0
57	MG	1A	3688	1/1	0.89	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3201	1/1	0.89	0.33	33,33,33,33	0
57	MG	2A	3612	1/1	0.89	0.16	49,49,49,49	0
57	MG	1a	1773	1/1	0.89	0.30	62,62,62,62	0
57	MG	1a	1774	1/1	0.89	0.20	82,82,82,82	0
57	MG	2A	3464	1/1	0.89	0.12	58,58,58,58	0
57	MG	2A	3122	1/1	0.89	0.33	59,59,59,59	0
57	MG	1A	3715	1/1	0.89	0.15	35,35,35,35	0
57	MG	2A	3312	1/1	0.89	0.12	30,30,30,30	0
57	MG	2a	1738	1/1	0.89	0.15	59,59,59,59	0
57	MG	1a	1621	1/1	0.89	0.20	57,57,57,57	0
57	MG	2A	3137	1/1	0.89	0.14	61,61,61,61	0
57	MG	1A	3219	1/1	0.89	0.18	50,50,50,50	0
57	MG	1A	3392	1/1	0.89	0.12	24,24,24,24	0
57	MG	2A	3155	1/1	0.89	0.63	44,44,44,44	0
57	MG	1n	101	1/1	0.89	0.11	63,63,63,63	0
57	MG	1A	3454	1/1	0.89	0.12	36,36,36,36	0
57	MG	1w	401	1/1	0.89	0.22	51,51,51,51	0
57	MG	2A	3503	1/1	0.89	0.16	61,61,61,61	0
57	MG	1A	3396	1/1	0.89	0.11	35,35,35,35	0
57	MG	2a	1765	1/1	0.89	0.17	53,53,53,53	0
57	MG	20	101	1/1	0.89	0.10	49,49,49,49	0
57	MG	1A	3114	1/1	0.89	0.17	42,42,42,42	0
57	MG	2A	3508	1/1	0.89	0.11	49,49,49,49	0
57	MG	1A	3161	1/1	0.89	0.11	24,24,24,24	0
57	MG	2a	1612	1/1	0.89	0.18	58,58,58,58	0
57	MG	2A	3382	1/1	0.89	0.11	65,65,65,65	0
57	MG	1a	1727	1/1	0.89	0.11	58,58,58,58	0
57	MG	2A	3384	1/1	0.89	0.12	49,49,49,49	0
57	MG	1A	3315	1/1	0.90	0.11	17,17,17,17	0
57	MG	2R	203	1/1	0.90	0.09	45,45,45,45	0
57	MG	1A	3316	1/1	0.90	0.11	40,40,40,40	0
57	MG	1A	3205	1/1	0.90	0.24	39,39,39,39	0
57	MG	2A	3279	1/1	0.90	0.15	51,51,51,51	0
57	MG	1P	204	1/1	0.90	0.09	32,32,32,32	0
57	MG	1A	3404	1/1	0.90	0.08	17,17,17,17	0
57	MG	1a	1755	1/1	0.90	0.20	47,47,47,47	0
57	MG	2a	1615	1/1	0.90	0.18	52,52,52,52	0
57	MG	2A	3083	1/1	0.90	0.27	48,48,48,48	0
57	MG	2A	3483	1/1	0.90	0.22	46,46,46,46	0
57	MG	1a	1656	1/1	0.90	0.13	55,55,55,55	0
57	MG	2A	3095	1/1	0.90	0.36	61,61,61,61	0
57	MG	2A	3492	1/1	0.90	0.17	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	3102	1/1	0.90	0.11	50,50,50,50	0
57	MG	2A	3496	1/1	0.90	0.12	47,47,47,47	0
57	MG	2A	3497	1/1	0.90	0.14	50,50,50,50	0
57	MG	2a	1637	1/1	0.90	0.16	43,43,43,43	0
57	MG	2A	3103	1/1	0.90	0.20	59,59,59,59	0
57	MG	1A	3322	1/1	0.90	0.18	48,48,48,48	0
57	MG	2a	1648	1/1	0.90	0.19	49,49,49,49	0
57	MG	2a	1651	1/1	0.90	0.10	46,46,46,46	0
57	MG	2a	1654	1/1	0.90	0.28	63,63,63,63	0
57	MG	1A	3758	1/1	0.90	0.20	28,28,28,28	0
57	MG	2A	3114	1/1	0.90	0.14	42,42,42,42	0
57	MG	1a	1668	1/1	0.90	0.13	55,55,55,55	0
57	MG	2A	3327	1/1	0.90	0.14	53,53,53,53	0
57	MG	1a	1671	1/1	0.90	0.19	50,50,50,50	0
57	MG	1A	3149	1/1	0.90	0.11	29,29,29,29	0
57	MG	11	103	1/1	0.90	0.27	48,48,48,48	0
57	MG	12	101	1/1	0.90	0.10	32,32,32,32	0
57	MG	2A	3525	1/1	0.90	0.14	65,65,65,65	0
57	MG	1A	3326	1/1	0.90	0.12	16,16,16,16	0
57	MG	2A	3533	1/1	0.90	0.12	63,63,63,63	0
57	MG	1a	1687	1/1	0.90	0.37	64,64,64,64	0
57	MG	2a	1674	1/1	0.90	0.32	63,63,63,63	0
57	MG	2a	1676	1/1	0.90	0.22	61,61,61,61	0
57	MG	2A	3539	1/1	0.90	0.20	56,56,56,56	0
57	MG	15	104	1/1	0.90	0.28	35,35,35,35	0
57	MG	2a	1685	1/1	0.90	0.22	52,52,52,52	0
57	MG	2a	1686	1/1	0.90	0.23	49,49,49,49	0
57	MG	2A	3366	1/1	0.90	0.15	51,51,51,51	0
57	MG	1A	3020	1/1	0.90	0.19	56,56,56,56	0
57	MG	2A	3373	1/1	0.90	0.13	56,56,56,56	0
57	MG	2A	3159	1/1	0.90	0.31	58,58,58,58	0
57	MG	1a	1789	1/1	0.90	0.15	58,58,58,58	0
57	MG	1a	1694	1/1	0.90	0.16	61,61,61,61	0
57	MG	1A	3513	1/1	0.90	0.20	48,48,48,48	0
57	MG	1A	3599	1/1	0.90	0.10	52,52,52,52	0
57	MG	2A	3172	1/1	0.90	0.09	38,38,38,38	0
57	MG	2A	3174	1/1	0.90	0.22	63,63,63,63	0
57	MG	1a	1703	1/1	0.90	0.18	55,55,55,55	0
57	MG	1x	103	1/1	0.90	0.18	60,60,60,60	0
57	MG	2A	3394	1/1	0.90	0.13	22,22,22,22	0
57	MG	1A	3776	1/1	0.90	0.06	7,7,7,7	0
57	MG	2A	3199	1/1	0.90	0.31	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	3200	1/1	0.90	0.28	62,62,62,62	0
57	MG	2a	1733	1/1	0.90	0.22	46,46,46,46	0
57	MG	1A	3699	1/1	0.90	0.07	42,42,42,42	0
57	MG	1A	3029	1/1	0.90	0.10	56,56,56,56	0
57	MG	2A	3212	1/1	0.90	0.21	45,45,45,45	0
57	MG	2A	3216	1/1	0.90	0.25	57,57,57,57	0
57	MG	2A	3413	1/1	0.90	0.13	58,58,58,58	0
57	MG	1A	3711	1/1	0.90	0.08	33,33,33,33	0
57	MG	1A	3786	1/1	0.90	0.08	49,49,49,49	0
57	MG	2A	3613	1/1	0.90	0.15	41,41,41,41	0
57	MG	2A	3235	1/1	0.90	0.12	51,51,51,51	0
57	MG	1A	3246	1/1	0.90	0.06	28,28,28,28	0
57	MG	1A	3383	1/1	0.90	0.10	23,23,23,23	0
57	MG	2A	3247	1/1	0.90	0.17	40,40,40,40	0
57	MG	1a	1728	1/1	0.90	0.14	46,46,46,46	0
57	MG	2A	3636	1/1	0.90	0.12	46,46,46,46	0
57	MG	2A	3434	1/1	0.90	0.08	31,31,31,31	0
57	MG	1A	3618	1/1	0.90	0.11	38,38,38,38	0
57	MG	1A	3292	1/1	0.90	0.09	37,37,37,37	0
57	MG	1a	1635	1/1	0.90	0.32	56,56,56,56	0
57	MG	1A	3045	1/1	0.90	0.09	47,47,47,47	0
57	MG	2x	102	1/1	0.90	0.22	55,55,55,55	0
57	MG	2A	3451	1/1	0.90	0.21	47,47,47,47	0
57	MG	1A	3628	1/1	0.90	0.12	38,38,38,38	0
57	MG	1A	3630	1/1	0.90	0.11	54,54,54,54	0
57	MG	1a	1745	1/1	0.90	0.25	59,59,59,59	0
57	MG	1A	3511	1/1	0.91	0.10	30,30,30,30	0
57	MG	1E	304	1/1	0.91	0.13	44,44,44,44	0
57	MG	2A	3329	1/1	0.91	0.08	29,29,29,29	0
57	MG	1A	3220	1/1	0.91	0.20	37,37,37,37	0
57	MG	1A	3661	1/1	0.91	0.06	34,34,34,34	0
57	MG	1A	3121	1/1	0.91	0.07	15,15,15,15	0
57	MG	1N	203	1/1	0.91	0.10	26,26,26,26	0
57	MG	2A	3079	1/1	0.91	0.11	50,50,50,50	0
57	MG	2A	3600	1/1	0.91	0.14	56,56,56,56	0
57	MG	2A	3601	1/1	0.91	0.12	53,53,53,53	0
57	MG	2A	3606	1/1	0.91	0.12	50,50,50,50	0
57	MG	1A	3665	1/1	0.91	0.06	31,31,31,31	0
57	MG	2A	3609	1/1	0.91	0.09	31,31,31,31	0
57	MG	2A	3086	1/1	0.91	0.11	47,47,47,47	0
57	MG	1A	3666	1/1	0.91	0.24	38,38,38,38	0
57	MG	2A	3094	1/1	0.91	0.07	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	1a	1720	1/1	0.91	0.13	59,59,59,59	0
57	MG	2A	3619	1/1	0.91	0.08	45,45,45,45	0
57	MG	2A	3101	1/1	0.91	0.40	45,45,45,45	0
57	MG	2A	3623	1/1	0.91	0.10	46,46,46,46	0
57	MG	1A	3410	1/1	0.91	0.10	14,14,14,14	0
57	MG	2A	3631	1/1	0.91	0.29	58,58,58,58	0
57	MG	1A	3520	1/1	0.91	0.18	48,48,48,48	0
57	MG	2A	3104	1/1	0.91	0.23	49,49,49,49	0
57	MG	1A	3534	1/1	0.91	0.12	10,10,10,10	0
57	MG	1a	1730	1/1	0.91	0.17	59,59,59,59	0
57	MG	1W	201	1/1	0.91	0.22	47,47,47,47	0
57	MG	2B	202	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3539	1/1	0.91	0.09	16,16,16,16	0
57	MG	2B	206	1/1	0.91	0.23	55,55,55,55	0
57	MG	2B	207	1/1	0.91	0.37	57,57,57,57	0
57	MG	2A	3121	1/1	0.91	0.16	39,39,39,39	0
57	MG	1A	3693	1/1	0.91	0.15	47,47,47,47	0
57	MG	1a	1737	1/1	0.91	0.13	44,44,44,44	0
57	MG	2A	3130	1/1	0.91	0.18	54,54,54,54	0
57	MG	2E	304	1/1	0.91	0.12	24,24,24,24	0
57	MG	1A	3540	1/1	0.91	0.07	12,12,12,12	0
57	MG	1a	1740	1/1	0.91	0.13	43,43,43,43	0
57	MG	2A	3403	1/1	0.91	0.12	61,61,61,61	0
57	MG	2R	202	1/1	0.91	0.33	44,44,44,44	0
57	MG	2A	3404	1/1	0.91	0.17	34,34,34,34	0
57	MG	2A	3138	1/1	0.91	0.06	50,50,50,50	0
57	MG	2A	3407	1/1	0.91	0.12	38,38,38,38	0
57	MG	13	102	1/1	0.91	0.07	13,13,13,13	0
57	MG	2A	3409	1/1	0.91	0.07	34,34,34,34	0
57	MG	2A	3143	1/1	0.91	0.29	54,54,54,54	0
57	MG	2A	3412	1/1	0.91	0.21	35,35,35,35	0
57	MG	2a	1614	1/1	0.91	0.13	53,53,53,53	0
57	MG	1A	3703	1/1	0.91	0.10	22,22,22,22	0
57	MG	2A	3151	1/1	0.91	0.06	45,45,45,45	0
57	MG	1A	3543	1/1	0.91	0.10	36,36,36,36	0
57	MG	1A	3546	1/1	0.91	0.09	23,23,23,23	0
57	MG	1A	3225	1/1	0.91	0.26	47,47,47,47	0
57	MG	1A	3561	1/1	0.91	0.07	12,12,12,12	0
57	MG	2A	3163	1/1	0.91	0.14	36,36,36,36	0
57	MG	2A	3429	1/1	0.91	0.19	45,45,45,45	0
57	MG	2A	3430	1/1	0.91	0.10	25,25,25,25	0
57	MG	1A	3420	1/1	0.91	0.06	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1642	1/1	0.91	0.10	37,37,37,37	0
57	MG	1a	1612	1/1	0.91	0.16	50,50,50,50	0
57	MG	1A	3234	1/1	0.91	0.11	40,40,40,40	0
57	MG	1A	3428	1/1	0.91	0.09	15,15,15,15	0
57	MG	2a	1649	1/1	0.91	0.20	60,60,60,60	0
57	MG	2A	3443	1/1	0.91	0.09	37,37,37,37	0
57	MG	1a	1763	1/1	0.91	0.12	67,67,67,67	0
57	MG	1A	3168	1/1	0.91	0.09	19,19,19,19	0
57	MG	2A	3182	1/1	0.91	0.09	48,48,48,48	0
57	MG	1A	3431	1/1	0.91	0.12	17,17,17,17	0
57	MG	2A	3186	1/1	0.91	0.08	57,57,57,57	0
57	MG	2A	3455	1/1	0.91	0.24	55,55,55,55	0
57	MG	1A	3186	1/1	0.91	0.11	33,33,33,33	0
57	MG	2A	3463	1/1	0.91	0.15	37,37,37,37	0
57	MG	1A	3190	1/1	0.91	0.20	22,22,22,22	0
57	MG	1A	3091	1/1	0.91	0.09	42,42,42,42	0
57	MG	2A	3203	1/1	0.91	0.14	48,48,48,48	0
57	MG	1A	3742	1/1	0.91	0.07	43,43,43,43	0
57	MG	2A	3207	1/1	0.91	0.19	66,66,66,66	0
57	MG	2A	3475	1/1	0.91	0.14	46,46,46,46	0
57	MG	1A	3329	1/1	0.91	0.14	6,6,6,6	0
57	MG	1A	3752	1/1	0.91	0.08	33,33,33,33	0
57	MG	1A	3590	1/1	0.91	0.14	34,34,34,34	0
57	MG	2a	1684	1/1	0.91	0.09	55,55,55,55	0
57	MG	1A	3198	1/1	0.91	0.13	39,39,39,39	0
57	MG	1A	3456	1/1	0.91	0.11	40,40,40,40	0
57	MG	1a	1788	1/1	0.91	0.11	66,66,66,66	0
57	MG	1A	3384	1/1	0.91	0.08	53,53,53,53	0
57	MG	1d	301	1/1	0.91	0.20	34,34,34,34	0
57	MG	1A	3462	1/1	0.91	0.12	44,44,44,44	0
57	MG	2a	1701	1/1	0.91	0.14	65,65,65,65	0
57	MG	2A	3251	1/1	0.91	0.13	58,58,58,58	0
57	MG	2a	1703	1/1	0.91	0.19	39,39,39,39	0
57	MG	1A	3464	1/1	0.91	0.10	16,16,16,16	0
57	MG	1A	3767	1/1	0.91	0.12	35,35,35,35	0
57	MG	1A	3469	1/1	0.91	0.08	35,35,35,35	0
57	MG	2a	1714	1/1	0.91	0.14	34,34,34,34	0
57	MG	1x	102	1/1	0.91	0.11	33,33,33,33	0
57	MG	1A	3613	1/1	0.91	0.11	45,45,45,45	0
57	MG	2A	3268	1/1	0.91	0.12	67,67,67,67	0
57	MG	2a	1723	1/1	0.91	0.24	62,62,62,62	0
57	MG	1a	1659	1/1	0.91	0.25	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3514	1/1	0.91	0.08	57,57,57,57	0
57	MG	1A	3067	1/1	0.91	0.15	30,30,30,30	0
57	MG	1A	3783	1/1	0.91	0.09	27,27,27,27	0
57	MG	2A	3008	1/1	0.91	0.15	46,46,46,46	0
57	MG	1A	3130	1/1	0.91	0.05	15,15,15,15	0
57	MG	2A	3527	1/1	0.91	0.15	39,39,39,39	0
57	MG	2A	3528	1/1	0.91	0.10	42,42,42,42	0
57	MG	2A	3529	1/1	0.91	0.12	52,52,52,52	0
57	MG	1a	1676	1/1	0.91	0.35	54,54,54,54	0
57	MG	1A	3338	1/1	0.91	0.09	33,33,33,33	0
57	MG	2A	3534	1/1	0.91	0.12	71,71,71,71	0
57	MG	2a	1752	1/1	0.91	0.21	48,48,48,48	0
57	MG	2A	3535	1/1	0.91	0.10	47,47,47,47	0
57	MG	2A	3281	1/1	0.91	0.13	36,36,36,36	0
57	MG	1A	3117	1/1	0.91	0.07	24,24,24,24	0
57	MG	1A	3288	1/1	0.91	0.23	30,30,30,30	0
57	MG	1a	1682	1/1	0.91	0.14	44,44,44,44	0
57	MG	1a	1685	1/1	0.91	0.11	35,35,35,35	0
57	MG	1A	3399	1/1	0.91	0.09	14,14,14,14	0
57	MG	2A	3052	1/1	0.91	0.27	65,65,65,65	0
57	MG	1B	201	1/1	0.91	0.09	43,43,43,43	0
57	MG	1A	3635	1/1	0.91	0.43	19,19,19,19	0
57	MG	2e	201	1/1	0.91	0.12	56,56,56,56	0
57	MG	1A	3499	1/1	0.91	0.10	52,52,52,52	0
57	MG	2A	3559	1/1	0.91	0.11	57,57,57,57	0
57	MG	2A	3058	1/1	0.91	0.15	50,50,50,50	0
57	MG	2x	101	1/1	0.91	0.15	54,54,54,54	0
57	MG	2A	3314	1/1	0.91	0.08	28,28,28,28	0
57	MG	2x	105	1/1	0.91	0.14	36,36,36,36	0
57	MG	1A	3403	1/1	0.91	0.06	15,15,15,15	0
57	MG	2A	3577	1/1	0.91	0.08	61,61,61,61	0
57	MG	2A	3320	1/1	0.91	0.09	29,29,29,29	0
57	MG	2A	3325	1/1	0.91	0.09	39,39,39,39	0
57	MG	1a	1626	1/1	0.92	0.07	45,45,45,45	0
57	MG	2A	3238	1/1	0.92	0.11	56,56,56,56	0
57	MG	2B	205	1/1	0.92	0.11	56,56,56,56	0
57	MG	1A	3378	1/1	0.92	0.06	38,38,38,38	0
57	MG	1A	3177	1/1	0.92	0.17	35,35,35,35	0
57	MG	2A	3442	1/1	0.92	0.13	41,41,41,41	0
57	MG	1a	1633	1/1	0.92	0.15	50,50,50,50	0
57	MG	2B	211	1/1	0.92	0.08	56,56,56,56	0
57	MG	2D	304	1/1	0.92	0.69	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1734	1/1	0.92	0.18	65,65,65,65	0
57	MG	1A	3439	1/1	0.92	0.07	39,39,39,39	0
57	MG	2A	3254	1/1	0.92	0.10	52,52,52,52	0
57	MG	1a	1736	1/1	0.92	0.10	61,61,61,61	0
57	MG	1A	3710	1/1	0.92	0.08	17,17,17,17	0
57	MG	1A	3603	1/1	0.92	0.07	36,36,36,36	0
57	MG	2Q	201	1/1	0.92	0.08	45,45,45,45	0
57	MG	1a	1739	1/1	0.92	0.19	45,45,45,45	0
57	MG	1A	3714	1/1	0.92	0.14	13,13,13,13	0
57	MG	1A	3223	1/1	0.92	0.24	44,44,44,44	0
57	MG	1A	3059	1/1	0.92	0.11	30,30,30,30	0
57	MG	1B	210	1/1	0.92	0.15	48,48,48,48	0
57	MG	1A	3387	1/1	0.92	0.12	36,36,36,36	0
57	MG	2A	3470	1/1	0.92	0.10	59,59,59,59	0
57	MG	2A	3471	1/1	0.92	0.16	43,43,43,43	0
57	MG	1a	1650	1/1	0.92	0.16	32,32,32,32	0
57	MG	2A	3473	1/1	0.92	0.08	31,31,31,31	0
57	MG	1A	3721	1/1	0.92	0.14	24,24,24,24	0
57	MG	1A	3343	1/1	0.92	0.09	30,30,30,30	0
57	MG	2a	1624	1/1	0.92	0.10	41,41,41,41	0
57	MG	1a	1655	1/1	0.92	0.18	40,40,40,40	0
57	MG	2A	3285	1/1	0.92	0.16	38,38,38,38	0
57	MG	1A	3350	1/1	0.92	0.07	25,25,25,25	0
57	MG	1a	1758	1/1	0.92	0.22	49,49,49,49	0
57	MG	1A	3728	1/1	0.92	0.09	27,27,27,27	0
57	MG	2a	1634	1/1	0.92	0.15	50,50,50,50	0
57	MG	2A	3491	1/1	0.92	0.15	55,55,55,55	0
57	MG	2a	1636	1/1	0.92	0.23	48,48,48,48	0
57	MG	2A	3295	1/1	0.92	0.09	37,37,37,37	0
57	MG	1A	3627	1/1	0.92	0.09	39,39,39,39	0
57	MG	1a	1764	1/1	0.92	0.12	53,53,53,53	0
57	MG	1A	3542	1/1	0.92	0.08	21,21,21,21	0
57	MG	2A	3305	1/1	0.92	0.10	44,44,44,44	0
57	MG	1a	1767	1/1	0.92	0.07	71,71,71,71	0
57	MG	2A	3310	1/1	0.92	0.10	39,39,39,39	0
57	MG	2A	3116	1/1	0.92	0.17	51,51,51,51	0
57	MG	1a	1661	1/1	0.92	0.15	43,43,43,43	0
57	MG	1a	1662	1/1	0.92	0.22	34,34,34,34	0
57	MG	2A	3510	1/1	0.92	0.10	41,41,41,41	0
57	MG	1A	3030	1/1	0.92	0.24	49,49,49,49	0
57	MG	1Q	206	1/1	0.92	0.12	32,32,32,32	0
57	MG	1a	1674	1/1	0.92	0.15	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	3300	1/1	0.92	0.21	31,31,31,31	0
57	MG	1a	1775	1/1	0.92	0.20	58,58,58,58	0
57	MG	1a	1776	1/1	0.92	0.20	49,49,49,49	0
57	MG	2A	3330	1/1	0.92	0.12	51,51,51,51	0
57	MG	2A	3333	1/1	0.92	0.16	55,55,55,55	0
57	MG	1A	3632	1/1	0.92	0.14	49,49,49,49	0
57	MG	1A	3357	1/1	0.92	0.10	43,43,43,43	0
57	MG	2A	3532	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3113	1/1	0.92	0.27	57,57,57,57	0
57	MG	2A	3147	1/1	0.92	0.12	46,46,46,46	0
57	MG	2a	1682	1/1	0.92	0.13	52,52,52,52	0
57	MG	2A	3348	1/1	0.92	0.09	60,60,60,60	0
57	MG	2A	3353	1/1	0.92	0.12	38,38,38,38	0
57	MG	2A	3538	1/1	0.92	0.12	28,28,28,28	0
57	MG	2A	3356	1/1	0.92	0.13	45,45,45,45	0
57	MG	2a	1691	1/1	0.92	0.17	44,44,44,44	0
57	MG	1a	1681	1/1	0.92	0.08	44,44,44,44	0
57	MG	1A	3196	1/1	0.92	0.12	29,29,29,29	0
57	MG	1A	3086	1/1	0.92	0.08	23,23,23,23	0
57	MG	1A	3756	1/1	0.92	0.09	14,14,14,14	0
57	MG	1k	201	1/1	0.92	0.12	52,52,52,52	0
57	MG	1A	3156	1/1	0.92	0.18	50,50,50,50	0
57	MG	2A	3374	1/1	0.92	0.07	26,26,26,26	0
57	MG	2A	3381	1/1	0.92	0.07	55,55,55,55	0
57	MG	1A	3250	1/1	0.92	0.15	49,49,49,49	0
57	MG	1v	102	1/1	0.92	0.13	44,44,44,44	0
57	MG	2A	3563	1/1	0.92	0.17	54,54,54,54	0
57	MG	17	106	1/1	0.92	0.15	38,38,38,38	0
57	MG	2A	3570	1/1	0.92	0.10	62,62,62,62	0
57	MG	1A	3482	1/1	0.92	0.14	37,37,37,37	0
57	MG	2A	3173	1/1	0.92	0.23	49,49,49,49	0
57	MG	1A	3051	1/1	0.92	0.09	29,29,29,29	0
57	MG	1A	3212	1/1	0.92	0.23	28,28,28,28	0
57	MG	2A	3180	1/1	0.92	0.26	51,51,51,51	0
57	MG	1A	3673	1/1	0.92	0.08	46,46,46,46	0
57	MG	2a	1732	1/1	0.92	0.12	48,48,48,48	0
57	MG	2A	3589	1/1	0.92	0.16	46,46,46,46	0
57	MG	1a	1611	1/1	0.92	0.14	46,46,46,46	0
57	MG	1y	101	1/1	0.92	0.15	55,55,55,55	0
57	MG	2A	3187	1/1	0.92	0.10	44,44,44,44	0
57	MG	1A	3493	1/1	0.92	0.14	31,31,31,31	0
57	MG	2A	3401	1/1	0.92	0.08	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1743	1/1	0.92	0.15	64,64,64,64	0
57	MG	2a	1745	1/1	0.92	0.14	47,47,47,47	0
57	MG	2a	1747	1/1	0.92	0.17	62,62,62,62	0
57	MG	2A	3194	1/1	0.92	0.12	29,29,29,29	0
57	MG	2A	3197	1/1	0.92	0.10	52,52,52,52	0
57	MG	1A	3678	1/1	0.92	0.14	50,50,50,50	0
57	MG	1a	1716	1/1	0.92	0.19	48,48,48,48	0
57	MG	1A	3270	1/1	0.92	0.15	26,26,26,26	0
57	MG	2A	3204	1/1	0.92	0.09	46,46,46,46	0
57	MG	1a	1718	1/1	0.92	0.09	59,59,59,59	0
57	MG	2A	3611	1/1	0.92	0.10	46,46,46,46	0
57	MG	2a	1761	1/1	0.92	0.18	57,57,57,57	0
57	MG	2A	3032	1/1	0.92	0.17	47,47,47,47	0
57	MG	2A	3411	1/1	0.92	0.11	40,40,40,40	0
57	MG	2A	3034	1/1	0.92	0.11	55,55,55,55	0
57	MG	1A	3500	1/1	0.92	0.08	44,44,44,44	0
57	MG	2a	1767	1/1	0.92	0.12	62,62,62,62	0
57	MG	2d	301	1/1	0.92	0.33	56,56,56,56	0
57	MG	1a	1620	1/1	0.92	0.06	55,55,55,55	0
57	MG	2A	3221	1/1	0.92	0.18	34,34,34,34	0
57	MG	2A	3624	1/1	0.92	0.21	37,37,37,37	0
57	MG	2A	3222	1/1	0.92	0.38	50,50,50,50	0
57	MG	2v	101	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3626	1/1	0.92	0.12	67,67,67,67	0
57	MG	2A	3417	1/1	0.92	0.09	40,40,40,40	0
57	MG	2x	103	1/1	0.92	0.16	46,46,46,46	0
57	MG	2x	104	1/1	0.92	0.18	48,48,48,48	0
57	MG	2A	3227	1/1	0.92	0.26	45,45,45,45	0
57	MG	1A	3506	1/1	0.92	0.11	57,57,57,57	0
57	MG	2A	3049	1/1	0.92	0.18	58,58,58,58	0
57	MG	2A	3231	1/1	0.92	0.11	47,47,47,47	0
57	MG	1A	3101	1/1	0.92	0.17	28,28,28,28	0
57	MG	1A	3445	1/1	0.93	0.08	13,13,13,13	0
57	MG	2A	3195	1/1	0.93	0.20	47,47,47,47	0
57	MG	1A	3169	1/1	0.93	0.15	33,33,33,33	0
57	MG	2A	3630	1/1	0.93	0.07	57,57,57,57	0
57	MG	2A	3198	1/1	0.93	0.34	53,53,53,53	0
57	MG	1A	3173	1/1	0.93	0.10	29,29,29,29	0
57	MG	1F	310	1/1	0.93	0.07	39,39,39,39	0
57	MG	1a	1684	1/1	0.93	0.20	59,59,59,59	0
57	MG	1x	104	1/1	0.93	0.12	34,34,34,34	0
57	MG	2A	3639	1/1	0.93	0.10	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3205	1/1	0.93	0.17	51,51,51,51	0
57	MG	2B	201	1/1	0.93	0.14	59,59,59,59	0
57	MG	1G	201	1/1	0.93	0.10	55,55,55,55	0
57	MG	1N	202	1/1	0.93	0.05	31,31,31,31	0
57	MG	2A	3208	1/1	0.93	0.24	48,48,48,48	0
57	MG	1A	3449	1/1	0.93	0.11	24,24,24,24	0
57	MG	1A	3559	1/1	0.93	0.08	25,25,25,25	0
57	MG	1a	1690	1/1	0.93	0.17	45,45,45,45	0
57	MG	2A	3419	1/1	0.93	0.07	44,44,44,44	0
57	MG	2A	3420	1/1	0.93	0.06	35,35,35,35	0
57	MG	2A	3219	1/1	0.93	0.21	48,48,48,48	0
57	MG	1A	3230	1/1	0.93	0.10	35,35,35,35	0
57	MG	2A	3018	1/1	0.93	0.15	43,43,43,43	0
57	MG	2A	3020	1/1	0.93	0.11	49,49,49,49	0
57	MG	1Q	201	1/1	0.93	0.31	38,38,38,38	0
57	MG	1a	1696	1/1	0.93	0.22	41,41,41,41	0
57	MG	1A	3453	1/1	0.93	0.07	21,21,21,21	0
57	MG	2A	3232	1/1	0.93	0.10	44,44,44,44	0
57	MG	2A	3438	1/1	0.93	0.09	48,48,48,48	0
57	MG	2A	3440	1/1	0.93	0.13	53,53,53,53	0
57	MG	1a	1699	1/1	0.93	0.25	70,70,70,70	0
57	MG	1A	3706	1/1	0.93	0.08	25,25,25,25	0
57	MG	20	102	1/1	0.93	0.11	57,57,57,57	0
57	MG	1a	1702	1/1	0.93	0.17	49,49,49,49	0
57	MG	1A	3032	1/1	0.93	0.06	23,23,23,23	0
57	MG	2A	3244	1/1	0.93	0.10	36,36,36,36	0
57	MG	2a	1608	1/1	0.93	0.17	55,55,55,55	0
57	MG	1A	3007	1/1	0.93	0.08	31,31,31,31	0
57	MG	2A	3249	1/1	0.93	0.21	52,52,52,52	0
57	MG	2A	3250	1/1	0.93	0.08	38,38,38,38	0
57	MG	2a	1616	1/1	0.93	0.18	41,41,41,41	0
57	MG	1A	3579	1/1	0.93	0.14	43,43,43,43	0
57	MG	1a	1707	1/1	0.93	0.13	36,36,36,36	0
57	MG	1W	202	1/1	0.93	0.07	22,22,22,22	0
57	MG	1A	3580	1/1	0.93	0.10	18,18,18,18	0
57	MG	1A	3240	1/1	0.93	0.07	31,31,31,31	0
57	MG	1A	3093	1/1	0.93	0.12	34,34,34,34	0
57	MG	1A	3327	1/1	0.93	0.12	41,41,41,41	0
57	MG	2A	3059	1/1	0.93	0.16	56,56,56,56	0
57	MG	2a	1633	1/1	0.93	0.16	51,51,51,51	0
57	MG	1A	3466	1/1	0.93	0.11	25,25,25,25	0
57	MG	15	101	1/1	0.93	0.27	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3271	1/1	0.93	0.11	52,52,52,52	0
57	MG	2A	3476	1/1	0.93	0.18	55,55,55,55	0
57	MG	1A	3126	1/1	0.93	0.09	30,30,30,30	0
57	MG	2A	3273	1/1	0.93	0.12	43,43,43,43	0
57	MG	2a	1645	1/1	0.93	0.11	45,45,45,45	0
57	MG	1A	3015	1/1	0.93	0.24	36,36,36,36	0
57	MG	2A	3070	1/1	0.93	0.11	34,34,34,34	0
57	MG	17	107	1/1	0.93	0.13	58,58,58,58	0
57	MG	2A	3489	1/1	0.93	0.10	45,45,45,45	0
57	MG	2a	1653	1/1	0.93	0.33	47,47,47,47	0
57	MG	1A	3391	1/1	0.93	0.11	38,38,38,38	0
57	MG	1A	3255	1/1	0.93	0.09	67,67,67,67	0
57	MG	2a	1656	1/1	0.93	0.19	55,55,55,55	0
57	MG	1A	3593	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3197	1/1	0.93	0.23	41,41,41,41	0
57	MG	2A	3494	1/1	0.93	0.10	47,47,47,47	0
57	MG	2A	3495	1/1	0.93	0.07	35,35,35,35	0
57	MG	2a	1663	1/1	0.93	0.11	52,52,52,52	0
57	MG	2A	3084	1/1	0.93	0.17	45,45,45,45	0
57	MG	1A	3480	1/1	0.93	0.10	37,37,37,37	0
57	MG	2A	3292	1/1	0.93	0.10	19,19,19,19	0
57	MG	1A	3738	1/1	0.93	0.25	27,27,27,27	0
57	MG	1A	3001	1/1	0.93	0.10	20,20,20,20	0
57	MG	1A	3269	1/1	0.93	0.31	50,50,50,50	0
57	MG	1A	3486	1/1	0.93	0.08	26,26,26,26	0
57	MG	2A	3299	1/1	0.93	0.12	39,39,39,39	0
57	MG	1A	3133	1/1	0.93	0.07	42,42,42,42	0
57	MG	2A	3301	1/1	0.93	0.11	25,25,25,25	0
57	MG	1A	3491	1/1	0.93	0.09	45,45,45,45	0
57	MG	1A	3006	1/1	0.93	0.08	41,41,41,41	0
57	MG	2A	3517	1/1	0.93	0.07	35,35,35,35	0
57	MG	2A	3308	1/1	0.93	0.13	22,22,22,22	0
57	MG	2A	3521	1/1	0.93	0.22	62,62,62,62	0
57	MG	1A	3206	1/1	0.93	0.18	44,44,44,44	0
57	MG	2A	3311	1/1	0.93	0.07	26,26,26,26	0
57	MG	1A	3355	1/1	0.93	0.13	33,33,33,33	0
57	MG	2a	1695	1/1	0.93	0.15	41,41,41,41	0
57	MG	1a	1629	1/1	0.93	0.11	51,51,51,51	0
57	MG	1A	3031	1/1	0.93	0.09	20,20,20,20	0
57	MG	2A	3315	1/1	0.93	0.10	27,27,27,27	0
57	MG	1A	3761	1/1	0.93	0.07	49,49,49,49	0
57	MG	2A	3118	1/1	0.93	0.16	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	1705	1/1	0.93	0.12	54,54,54,54	0
57	MG	1A	3763	1/1	0.93	0.07	35,35,35,35	0
57	MG	2a	1710	1/1	0.93	0.10	47,47,47,47	0
57	MG	1a	1756	1/1	0.93	0.19	65,65,65,65	0
57	MG	2A	3123	1/1	0.93	0.23	44,44,44,44	0
57	MG	2A	3126	1/1	0.93	0.18	45,45,45,45	0
57	MG	2a	1715	1/1	0.93	0.10	63,63,63,63	0
57	MG	1A	3287	1/1	0.93	0.09	31,31,31,31	0
57	MG	2A	3540	1/1	0.93	0.16	75,75,75,75	0
57	MG	1A	3421	1/1	0.93	0.10	16,16,16,16	0
57	MG	2A	3334	1/1	0.93	0.08	24,24,24,24	0
57	MG	2A	3339	1/1	0.93	0.09	26,26,26,26	0
57	MG	1a	1762	1/1	0.93	0.17	62,62,62,62	0
57	MG	2a	1727	1/1	0.93	0.25	40,40,40,40	0
57	MG	1A	3159	1/1	0.93	0.09	55,55,55,55	0
57	MG	1A	3073	1/1	0.93	0.27	53,53,53,53	0
57	MG	2A	3555	1/1	0.93	0.15	54,54,54,54	0
57	MG	1A	3769	1/1	0.93	0.09	49,49,49,49	0
57	MG	1A	3364	1/1	0.93	0.07	33,33,33,33	0
57	MG	1A	3115	1/1	0.93	0.09	28,28,28,28	0
57	MG	2A	3146	1/1	0.93	0.15	40,40,40,40	0
57	MG	2A	3357	1/1	0.93	0.15	60,60,60,60	0
57	MG	2a	1737	1/1	0.93	0.16	43,43,43,43	0
57	MG	2A	3566	1/1	0.93	0.10	60,60,60,60	0
57	MG	1A	3639	1/1	0.93	0.08	10,10,10,10	0
57	MG	2a	1741	1/1	0.93	0.20	58,58,58,58	0
57	MG	2A	3150	1/1	0.93	0.26	51,51,51,51	0
57	MG	2A	3572	1/1	0.93	0.10	42,42,42,42	0
57	MG	2a	1746	1/1	0.93	0.12	56,56,56,56	0
57	MG	2A	3573	1/1	0.93	0.15	61,61,61,61	0
57	MG	1A	3521	1/1	0.93	0.06	34,34,34,34	0
57	MG	2a	1750	1/1	0.93	0.17	57,57,57,57	0
57	MG	2a	1751	1/1	0.93	0.15	43,43,43,43	0
57	MG	2A	3575	1/1	0.93	0.12	47,47,47,47	0
57	MG	1A	3646	1/1	0.93	0.27	42,42,42,42	0
57	MG	2A	3156	1/1	0.93	0.19	61,61,61,61	0
57	MG	2A	3370	1/1	0.93	0.09	47,47,47,47	0
57	MG	2A	3372	1/1	0.93	0.10	53,53,53,53	0
57	MG	2a	1758	1/1	0.93	0.15	62,62,62,62	0
57	MG	1a	1772	1/1	0.93	0.12	62,62,62,62	0
57	MG	1A	3522	1/1	0.93	0.06	29,29,29,29	0
57	MG	1A	3526	1/1	0.93	0.10	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3591	1/1	0.93	0.13	46,46,46,46	0
57	MG	1A	3528	1/1	0.93	0.12	33,33,33,33	0
57	MG	1A	3366	1/1	0.93	0.12	7,7,7,7	0
57	MG	1A	3538	1/1	0.93	0.09	25,25,25,25	0
57	MG	1A	3438	1/1	0.93	0.10	20,20,20,20	0
57	MG	1A	3670	1/1	0.93	0.06	67,67,67,67	0
57	MG	2A	3388	1/1	0.93	0.18	59,59,59,59	0
57	MG	1a	1786	1/1	0.93	0.08	47,47,47,47	0
57	MG	1a	1664	1/1	0.93	0.24	46,46,46,46	0
57	MG	1A	3672	1/1	0.93	0.08	39,39,39,39	0
57	MG	2k	202	1/1	0.93	0.07	60,60,60,60	0
57	MG	1A	3309	1/1	0.93	0.10	30,30,30,30	0
57	MG	1B	213	1/1	0.93	0.11	47,47,47,47	0
57	MG	1E	303	1/1	0.93	0.08	9,9,9,9	0
57	MG	2A	3396	1/1	0.93	0.14	29,29,29,29	0
57	MG	1m	3001	1/1	0.93	0.10	58,58,58,58	0
57	MG	1a	1677	1/1	0.93	0.19	41,41,41,41	0
57	MG	2A	3618	1/1	0.93	0.05	45,45,45,45	0
57	MG	2A	3400	1/1	0.93	0.15	28,28,28,28	0
57	MG	2A	3191	1/1	0.93	0.23	54,54,54,54	0
57	MG	1A	3541	1/1	0.93	0.09	29,29,29,29	0
57	MG	1A	3268	1/1	0.94	0.13	29,29,29,29	0
57	MG	1A	3679	1/1	0.94	0.09	8,8,8,8	0
57	MG	2A	3129	1/1	0.94	0.39	53,53,53,53	0
57	MG	1A	3096	1/1	0.94	0.33	29,29,29,29	0
57	MG	1A	3682	1/1	0.94	0.10	38,38,38,38	0
57	MG	2A	3376	1/1	0.94	0.17	45,45,45,45	0
57	MG	2A	3134	1/1	0.94	0.06	45,45,45,45	0
57	MG	1A	3192	1/1	0.94	0.09	20,20,20,20	0
57	MG	1A	3684	1/1	0.94	0.09	37,37,37,37	0
57	MG	1W	205	1/1	0.94	0.07	26,26,26,26	0
57	MG	1X	101	1/1	0.94	0.07	39,39,39,39	0
57	MG	2A	3144	1/1	0.94	0.06	67,67,67,67	0
57	MG	10	102	1/1	0.94	0.11	38,38,38,38	0
57	MG	1A	3062	1/1	0.94	0.09	36,36,36,36	0
57	MG	11	102	1/1	0.94	0.17	32,32,32,32	0
57	MG	1A	3104	1/1	0.94	0.08	32,32,32,32	0
57	MG	1A	3129	1/1	0.94	0.14	28,28,28,28	0
57	MG	1A	3550	1/1	0.94	0.09	18,18,18,18	0
57	MG	1A	3704	1/1	0.94	0.07	37,37,37,37	0
57	MG	1A	3558	1/1	0.94	0.08	51,51,51,51	0
57	MG	1A	3450	1/1	0.94	0.07	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	3161	1/1	0.94	0.18	58,58,58,58	0
57	MG	1A	3708	1/1	0.94	0.26	52,52,52,52	0
57	MG	1A	3107	1/1	0.94	0.21	51,51,51,51	0
57	MG	2A	3164	1/1	0.94	0.16	29,29,29,29	0
57	MG	1A	3204	1/1	0.94	0.17	43,43,43,43	0
57	MG	1A	3563	1/1	0.94	0.08	42,42,42,42	0
57	MG	1a	1759	1/1	0.94	0.22	40,40,40,40	0
57	MG	2A	3406	1/1	0.94	0.11	51,51,51,51	0
57	MG	1a	1602	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3290	1/1	0.94	0.07	11,11,11,11	0
57	MG	1a	1604	1/1	0.94	0.16	43,43,43,43	0
57	MG	2A	3175	1/1	0.94	0.14	29,29,29,29	0
57	MG	2E	301	1/1	0.94	0.18	35,35,35,35	0
57	MG	2E	303	1/1	0.94	0.08	51,51,51,51	0
57	MG	1A	3576	1/1	0.94	0.09	39,39,39,39	0
57	MG	2F	303	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3455	1/1	0.94	0.06	16,16,16,16	0
57	MG	2F	307	1/1	0.94	0.06	31,31,31,31	0
57	MG	1A	3132	1/1	0.94	0.09	15,15,15,15	0
57	MG	1A	3457	1/1	0.94	0.07	16,16,16,16	0
57	MG	1A	3298	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3064	1/1	0.94	0.06	19,19,19,19	0
57	MG	1A	3584	1/1	0.94	0.06	10,10,10,10	0
57	MG	1A	3463	1/1	0.94	0.07	13,13,13,13	0
57	MG	1A	3308	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3134	1/1	0.94	0.31	28,28,28,28	0
57	MG	1A	3467	1/1	0.94	0.08	42,42,42,42	0
57	MG	1A	3739	1/1	0.94	0.07	31,31,31,31	0
57	MG	1a	1630	1/1	0.94	0.13	38,38,38,38	0
57	MG	2a	1605	1/1	0.94	0.10	52,52,52,52	0
57	MG	2a	1607	1/1	0.94	0.27	42,42,42,42	0
57	MG	1A	3382	1/1	0.94	0.10	35,35,35,35	0
57	MG	2a	1609	1/1	0.94	0.13	54,54,54,54	0
57	MG	2a	1610	1/1	0.94	0.24	53,53,53,53	0
57	MG	2A	3202	1/1	0.94	0.16	45,45,45,45	0
57	MG	2a	1613	1/1	0.94	0.20	51,51,51,51	0
57	MG	1A	3310	1/1	0.94	0.08	13,13,13,13	0
57	MG	1A	3744	1/1	0.94	0.11	26,26,26,26	0
57	MG	1A	3745	1/1	0.94	0.10	38,38,38,38	0
57	MG	1A	3748	1/1	0.94	0.06	12,12,12,12	0
57	MG	1A	3750	1/1	0.94	0.08	15,15,15,15	0
57	MG	2a	1620	1/1	0.94	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1621	1/1	0.94	0.07	43,43,43,43	0
57	MG	2a	1622	1/1	0.94	0.09	46,46,46,46	0
57	MG	2a	1623	1/1	0.94	0.33	54,54,54,54	0
57	MG	1A	3472	1/1	0.94	0.16	43,43,43,43	0
57	MG	1f	201	1/1	0.94	0.06	34,34,34,34	0
57	MG	1A	3218	1/1	0.94	0.12	26,26,26,26	0
57	MG	2A	3445	1/1	0.94	0.13	35,35,35,35	0
57	MG	2a	1629	1/1	0.94	0.19	54,54,54,54	0
57	MG	1A	3597	1/1	0.94	0.10	22,22,22,22	0
57	MG	2A	3448	1/1	0.94	0.13	46,46,46,46	0
57	MG	2A	3218	1/1	0.94	0.06	27,27,27,27	0
57	MG	1A	3598	1/1	0.94	0.05	40,40,40,40	0
57	MG	1A	3312	1/1	0.94	0.12	32,32,32,32	0
57	MG	1A	3476	1/1	0.94	0.10	19,19,19,19	0
57	MG	2A	3458	1/1	0.94	0.13	52,52,52,52	0
57	MG	2A	3223	1/1	0.94	0.18	35,35,35,35	0
57	MG	2a	1643	1/1	0.94	0.20	40,40,40,40	0
57	MG	2A	3225	1/1	0.94	0.16	42,42,42,42	0
57	MG	1a	1652	1/1	0.94	0.23	51,51,51,51	0
57	MG	1A	3314	1/1	0.94	0.15	42,42,42,42	0
57	MG	1a	1654	1/1	0.94	0.13	45,45,45,45	0
57	MG	2A	3468	1/1	0.94	0.07	51,51,51,51	0
57	MG	2a	1650	1/1	0.94	0.13	53,53,53,53	0
57	MG	1A	3046	1/1	0.94	0.07	18,18,18,18	0
57	MG	1A	3150	1/1	0.94	0.06	31,31,31,31	0
57	MG	1a	1657	1/1	0.94	0.10	48,48,48,48	0
57	MG	1A	3112	1/1	0.94	0.08	28,28,28,28	0
57	MG	2A	3237	1/1	0.94	0.11	29,29,29,29	0
57	MG	1A	3614	1/1	0.94	0.09	21,21,21,21	0
57	MG	1A	3615	1/1	0.94	0.17	50,50,50,50	0
57	MG	2A	3241	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3004	1/1	0.94	0.22	58,58,58,58	0
57	MG	2A	3479	1/1	0.94	0.11	35,35,35,35	0
57	MG	2A	3246	1/1	0.94	0.17	50,50,50,50	0
57	MG	2A	3482	1/1	0.94	0.09	35,35,35,35	0
57	MG	1A	3394	1/1	0.94	0.11	29,29,29,29	0
57	MG	2A	3486	1/1	0.94	0.29	34,34,34,34	0
57	MG	1A	3071	1/1	0.94	0.06	39,39,39,39	0
57	MG	2A	3014	1/1	0.94	0.14	33,33,33,33	0
57	MG	1a	1663	1/1	0.94	0.31	47,47,47,47	0
57	MG	1A	3489	1/1	0.94	0.15	57,57,57,57	0
57	MG	2A	3021	1/1	0.94	0.07	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3023	1/1	0.94	0.26	47,47,47,47	0
57	MG	2a	1679	1/1	0.94	0.34	52,52,52,52	0
57	MG	2A	3256	1/1	0.94	0.13	54,54,54,54	0
57	MG	1A	3777	1/1	0.94	0.09	16,16,16,16	0
57	MG	2a	1683	1/1	0.94	0.10	57,57,57,57	0
57	MG	1a	1669	1/1	0.94	0.19	50,50,50,50	0
57	MG	1A	3780	1/1	0.94	0.09	14,14,14,14	0
57	MG	2A	3033	1/1	0.94	0.09	63,63,63,63	0
57	MG	2A	3500	1/1	0.94	0.12	47,47,47,47	0
57	MG	1A	3002	1/1	0.94	0.09	42,42,42,42	0
57	MG	2A	3035	1/1	0.94	0.12	31,31,31,31	0
57	MG	2A	3505	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3226	1/1	0.94	0.08	24,24,24,24	0
57	MG	2A	3039	1/1	0.94	0.17	22,22,22,22	0
57	MG	2a	1699	1/1	0.94	0.16	41,41,41,41	0
57	MG	2a	1700	1/1	0.94	0.10	48,48,48,48	0
57	MG	1A	3400	1/1	0.94	0.07	13,13,13,13	0
57	MG	1A	3401	1/1	0.94	0.09	24,24,24,24	0
57	MG	2A	3511	1/1	0.94	0.12	58,58,58,58	0
57	MG	2A	3048	1/1	0.94	0.20	54,54,54,54	0
57	MG	1A	3011	1/1	0.94	0.08	31,31,31,31	0
57	MG	1A	3791	1/1	0.94	0.07	48,48,48,48	0
57	MG	1A	3116	1/1	0.94	0.28	42,42,42,42	0
57	MG	2A	3282	1/1	0.94	0.10	42,42,42,42	0
57	MG	1A	3021	1/1	0.94	0.07	24,24,24,24	0
57	MG	1A	3174	1/1	0.94	0.20	41,41,41,41	0
57	MG	1A	3640	1/1	0.94	0.06	25,25,25,25	0
57	MG	2A	3289	1/1	0.94	0.07	32,32,32,32	0
57	MG	1A	3641	1/1	0.94	0.15	26,26,26,26	0
57	MG	2a	1721	1/1	0.94	0.14	45,45,45,45	0
57	MG	1B	205	1/1	0.94	0.10	47,47,47,47	0
57	MG	1A	3514	1/1	0.94	0.11	32,32,32,32	0
57	MG	2A	3062	1/1	0.94	0.13	38,38,38,38	0
57	MG	1A	3645	1/1	0.94	0.11	35,35,35,35	0
57	MG	1a	1692	1/1	0.94	0.24	46,46,46,46	0
57	MG	1A	3411	1/1	0.94	0.06	12,12,12,12	0
57	MG	1A	3176	1/1	0.94	0.13	33,33,33,33	0
57	MG	2A	3069	1/1	0.94	0.14	44,44,44,44	0
57	MG	1a	1695	1/1	0.94	0.33	49,49,49,49	0
57	MG	2A	3072	1/1	0.94	0.09	48,48,48,48	0
57	MG	2A	3541	1/1	0.94	0.12	53,53,53,53	0
57	MG	1B	215	1/1	0.94	0.08	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	2A	3544	1/1	0.94	0.17	51,51,51,51	0
57	MG	1D	304	1/1	0.94	0.21	25,25,25,25	0
57	MG	2A	3076	1/1	0.94	0.14	48,48,48,48	0
57	MG	2a	1740	1/1	0.94	0.14	46,46,46,46	0
57	MG	1A	3653	1/1	0.94	0.15	34,34,34,34	0
57	MG	1a	1700	1/1	0.94	0.14	47,47,47,47	0
57	MG	2A	3081	1/1	0.94	0.10	39,39,39,39	0
57	MG	2A	3553	1/1	0.94	0.08	25,25,25,25	0
57	MG	2A	3082	1/1	0.94	0.12	37,37,37,37	0
57	MG	1A	3655	1/1	0.94	0.09	47,47,47,47	0
57	MG	1A	3060	1/1	0.94	0.06	23,23,23,23	0
57	MG	2A	3321	1/1	0.94	0.17	50,50,50,50	0
57	MG	1A	3185	1/1	0.94	0.13	25,25,25,25	0
57	MG	1F	301	1/1	0.94	0.09	34,34,34,34	0
57	MG	2A	3091	1/1	0.94	0.06	40,40,40,40	0
57	MG	1F	302	1/1	0.94	0.10	21,21,21,21	0
57	MG	2A	3569	1/1	0.94	0.10	38,38,38,38	0
57	MG	2a	1757	1/1	0.94	0.16	49,49,49,49	0
57	MG	1A	3425	1/1	0.94	0.13	22,22,22,22	0
57	MG	2A	3331	1/1	0.94	0.10	30,30,30,30	0
57	MG	1a	1710	1/1	0.94	0.20	48,48,48,48	0
57	MG	1A	3349	1/1	0.94	0.08	10,10,10,10	0
57	MG	2A	3335	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3338	1/1	0.94	0.09	34,34,34,34	0
57	MG	1A	3122	1/1	0.94	0.15	33,33,33,33	0
57	MG	2A	3580	1/1	0.94	0.13	46,46,46,46	0
57	MG	1G	203	1/1	0.94	0.07	51,51,51,51	0
57	MG	2a	1768	1/1	0.94	0.07	46,46,46,46	0
57	MG	2A	3342	1/1	0.94	0.07	27,27,27,27	0
57	MG	2d	302	1/1	0.94	0.17	48,48,48,48	0
57	MG	2A	3110	1/1	0.94	0.13	72,72,72,72	0
57	MG	2e	203	1/1	0.94	0.16	43,43,43,43	0
57	MG	2A	3586	1/1	0.94	0.06	59,59,59,59	0
57	MG	2j	201	1/1	0.94	0.14	53,53,53,53	0
57	MG	2A	3111	1/1	0.94	0.15	34,34,34,34	0
57	MG	1A	3529	1/1	0.94	0.09	17,17,17,17	0
57	MG	1A	3351	1/1	0.94	0.04	10,10,10,10	0
57	MG	2A	3351	1/1	0.94	0.08	47,47,47,47	0
57	MG	1A	3188	1/1	0.94	0.07	33,33,33,33	0
57	MG	1A	3123	1/1	0.94	0.09	45,45,45,45	0
57	MG	1a	1723	1/1	0.94	0.16	24,24,24,24	0
57	MG	1a	1725	1/1	0.94	0.13	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	1a	1726	1/1	0.94	0.23	55,55,55,55	0
57	MG	1A	3677	1/1	0.94	0.12	22,22,22,22	0
57	MG	2A	3362	1/1	0.94	0.19	50,50,50,50	0
57	MG	1Q	204	1/1	0.94	0.07	31,31,31,31	0
57	MG	2A	3608	1/1	0.94	0.08	43,43,43,43	0
58	ZN	24	501	1/1	0.94	0.18	137,137,137,137	0
57	MG	1A	3128	1/1	0.95	0.05	26,26,26,26	0
57	MG	1A	3048	1/1	0.95	0.29	36,36,36,36	0
57	MG	1A	3033	1/1	0.95	0.14	16,16,16,16	0
57	MG	2A	3168	1/1	0.95	0.12	40,40,40,40	0
57	MG	1A	3733	1/1	0.95	0.06	33,33,33,33	0
57	MG	1A	3318	1/1	0.95	0.06	8,8,8,8	0
57	MG	1A	3319	1/1	0.95	0.11	29,29,29,29	0
57	MG	1a	1624	1/1	0.95	0.21	56,56,56,56	0
57	MG	2B	203	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3393	1/1	0.95	0.15	42,42,42,42	0
57	MG	1A	3478	1/1	0.95	0.08	32,32,32,32	0
57	MG	2A	3177	1/1	0.95	0.17	40,40,40,40	0
57	MG	1a	1778	1/1	0.95	0.18	45,45,45,45	0
57	MG	1a	1779	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3479	1/1	0.95	0.10	35,35,35,35	0
57	MG	2B	210	1/1	0.95	0.23	52,52,52,52	0
57	MG	1A	3596	1/1	0.95	0.07	24,24,24,24	0
57	MG	2A	3185	1/1	0.95	0.23	43,43,43,43	0
57	MG	1A	3229	1/1	0.95	0.09	38,38,38,38	0
57	MG	1A	3481	1/1	0.95	0.09	18,18,18,18	0
57	MG	2A	3190	1/1	0.95	0.19	34,34,34,34	0
57	MG	1A	3746	1/1	0.95	0.07	37,37,37,37	0
57	MG	2A	3192	1/1	0.95	0.09	24,24,24,24	0
57	MG	2F	302	1/1	0.95	0.04	26,26,26,26	0
57	MG	1A	3321	1/1	0.95	0.07	19,19,19,19	0
57	MG	1A	3026	1/1	0.95	0.16	27,27,27,27	0
57	MG	1A	3179	1/1	0.95	0.12	37,37,37,37	0
57	MG	1a	1639	1/1	0.95	0.15	34,34,34,34	0
57	MG	1A	3602	1/1	0.95	0.08	19,19,19,19	0
57	MG	1A	3325	1/1	0.95	0.09	28,28,28,28	0
57	MG	2Q	203	1/1	0.95	0.18	44,44,44,44	0
57	MG	1a	1642	1/1	0.95	0.20	55,55,55,55	0
57	MG	1A	3488	1/1	0.95	0.12	33,33,33,33	0
57	MG	2V	202	1/1	0.95	0.23	45,45,45,45	0
57	MG	2X	101	1/1	0.95	0.10	42,42,42,42	0
57	MG	2A	3424	1/1	0.95	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	3610	1/1	0.95	0.40	21,21,21,21	0
57	MG	2A	3427	1/1	0.95	0.10	30,30,30,30	0
57	MG	2A	3428	1/1	0.95	0.16	51,51,51,51	0
57	MG	1A	3182	1/1	0.95	0.29	35,35,35,35	0
57	MG	1A	3239	1/1	0.95	0.20	24,24,24,24	0
57	MG	1A	3184	1/1	0.95	0.07	27,27,27,27	0
57	MG	1A	3762	1/1	0.95	0.11	33,33,33,33	0
57	MG	2A	3435	1/1	0.95	0.12	37,37,37,37	0
57	MG	1A	3405	1/1	0.95	0.07	33,33,33,33	0
57	MG	1A	3406	1/1	0.95	0.07	26,26,26,26	0
57	MG	1A	3623	1/1	0.95	0.14	23,23,23,23	0
57	MG	2A	3215	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3625	1/1	0.95	0.07	32,32,32,32	0
57	MG	2A	3217	1/1	0.95	0.06	35,35,35,35	0
57	MG	2A	3001	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3501	1/1	0.95	0.05	25,25,25,25	0
57	MG	2A	3220	1/1	0.95	0.10	42,42,42,42	0
57	MG	2a	1619	1/1	0.95	0.09	32,32,32,32	0
57	MG	1A	3502	1/1	0.95	0.08	44,44,44,44	0
57	MG	2A	3005	1/1	0.95	0.20	40,40,40,40	0
57	MG	1A	3775	1/1	0.95	0.09	34,34,34,34	0
57	MG	2A	3009	1/1	0.95	0.09	42,42,42,42	0
57	MG	2A	3010	1/1	0.95	0.13	31,31,31,31	0
57	MG	1A	3068	1/1	0.95	0.21	41,41,41,41	0
57	MG	2A	3459	1/1	0.95	0.06	66,66,66,66	0
57	MG	2A	3460	1/1	0.95	0.17	60,60,60,60	0
57	MG	1A	3508	1/1	0.95	0.10	20,20,20,20	0
57	MG	1A	3778	1/1	0.95	0.07	57,57,57,57	0
57	MG	1A	3332	1/1	0.95	0.10	37,37,37,37	0
57	MG	2A	3234	1/1	0.95	0.11	45,45,45,45	0
57	MG	1A	3103	1/1	0.95	0.07	34,34,34,34	0
57	MG	1a	1665	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3634	1/1	0.95	0.08	49,49,49,49	0
57	MG	1A	3248	1/1	0.95	0.07	24,24,24,24	0
57	MG	2a	1638	1/1	0.95	0.17	48,48,48,48	0
57	MG	1A	3249	1/1	0.95	0.05	30,30,30,30	0
57	MG	1a	1672	1/1	0.95	0.10	36,36,36,36	0
57	MG	1a	1673	1/1	0.95	0.10	52,52,52,52	0
57	MG	1A	3136	1/1	0.95	0.12	27,27,27,27	0
57	MG	2A	3036	1/1	0.95	0.14	47,47,47,47	0
57	MG	2a	1647	1/1	0.95	0.28	44,44,44,44	0
57	MG	2A	3248	1/1	0.95	0.14	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	3344	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3347	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3642	1/1	0.95	0.10	30,30,30,30	0
57	MG	2a	1652	1/1	0.95	0.19	50,50,50,50	0
57	MG	2A	3481	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	3254	1/1	0.95	0.06	21,21,21,21	0
57	MG	2A	3047	1/1	0.95	0.15	57,57,57,57	0
57	MG	1A	3644	1/1	0.95	0.07	41,41,41,41	0
57	MG	2a	1658	1/1	0.95	0.34	53,53,53,53	0
57	MG	1A	3139	1/1	0.95	0.16	22,22,22,22	0
57	MG	2A	3257	1/1	0.95	0.05	40,40,40,40	0
57	MG	1A	3523	1/1	0.95	0.07	37,37,37,37	0
57	MG	2A	3259	1/1	0.95	0.09	48,48,48,48	0
57	MG	1a	1683	1/1	0.95	0.18	45,45,45,45	0
57	MG	1A	3140	1/1	0.95	0.09	32,32,32,32	0
57	MG	1B	207	1/1	0.95	0.07	22,22,22,22	0
57	MG	1A	3651	1/1	0.95	0.08	32,32,32,32	0
57	MG	2A	3056	1/1	0.95	0.13	26,26,26,26	0
57	MG	1A	3141	1/1	0.95	0.06	23,23,23,23	0
57	MG	1A	3654	1/1	0.95	0.10	44,44,44,44	0
57	MG	2a	1671	1/1	0.95	0.28	49,49,49,49	0
57	MG	2a	1672	1/1	0.95	0.11	43,43,43,43	0
57	MG	1A	3436	1/1	0.95	0.12	42,42,42,42	0
57	MG	2A	3501	1/1	0.95	0.08	53,53,53,53	0
57	MG	2A	3061	1/1	0.95	0.10	56,56,56,56	0
57	MG	1A	3658	1/1	0.95	0.12	34,34,34,34	0
57	MG	1D	306	1/1	0.95	0.08	23,23,23,23	0
57	MG	2A	3506	1/1	0.95	0.12	44,44,44,44	0
57	MG	2a	1681	1/1	0.95	0.21	49,49,49,49	0
57	MG	1D	307	1/1	0.95	0.14	31,31,31,31	0
57	MG	1A	3530	1/1	0.95	0.09	12,12,12,12	0
57	MG	1A	3533	1/1	0.95	0.14	30,30,30,30	0
57	MG	1a	1697	1/1	0.95	0.05	36,36,36,36	0
57	MG	1A	3195	1/1	0.95	0.13	33,33,33,33	0
57	MG	2a	1687	1/1	0.95	0.23	44,44,44,44	0
57	MG	2A	3512	1/1	0.95	0.10	39,39,39,39	0
57	MG	1A	3148	1/1	0.95	0.38	34,34,34,34	0
57	MG	2A	3288	1/1	0.95	0.10	42,42,42,42	0
57	MG	2a	1693	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3440	1/1	0.95	0.05	23,23,23,23	0
57	MG	2a	1696	1/1	0.95	0.21	42,42,42,42	0
57	MG	1A	3668	1/1	0.95	0.06	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	3669	1/1	0.95	0.13	41,41,41,41	0
57	MG	1A	3052	1/1	0.95	0.12	20,20,20,20	0
57	MG	2A	3522	1/1	0.95	0.06	49,49,49,49	0
57	MG	2A	3078	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3106	1/1	0.95	0.19	31,31,31,31	0
57	MG	2A	3080	1/1	0.95	0.12	33,33,33,33	0
57	MG	2A	3298	1/1	0.95	0.14	52,52,52,52	0
57	MG	2a	1706	1/1	0.95	0.19	59,59,59,59	0
57	MG	1A	3152	1/1	0.95	0.22	27,27,27,27	0
57	MG	1N	201	1/1	0.95	0.16	25,25,25,25	0
57	MG	1A	3154	1/1	0.95	0.08	26,26,26,26	0
57	MG	2a	1712	1/1	0.95	0.17	54,54,54,54	0
57	MG	2A	3303	1/1	0.95	0.11	20,20,20,20	0
57	MG	1A	3675	1/1	0.95	0.05	24,24,24,24	0
57	MG	2A	3085	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3072	1/1	0.95	0.18	40,40,40,40	0
57	MG	1O	201	1/1	0.95	0.10	31,31,31,31	0
57	MG	2A	3088	1/1	0.95	0.14	38,38,38,38	0
57	MG	2a	1720	1/1	0.95	0.13	40,40,40,40	0
57	MG	2A	3089	1/1	0.95	0.12	54,54,54,54	0
57	MG	1P	203	1/1	0.95	0.13	27,27,27,27	0
57	MG	2a	1724	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3093	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3451	1/1	0.95	0.06	34,34,34,34	0
57	MG	2A	3317	1/1	0.95	0.11	35,35,35,35	0
57	MG	1A	3004	1/1	0.95	0.08	14,14,14,14	0
57	MG	1A	3551	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3681	1/1	0.95	0.18	40,40,40,40	0
57	MG	2A	3323	1/1	0.95	0.08	48,48,48,48	0
57	MG	1A	3557	1/1	0.95	0.04	24,24,24,24	0
57	MG	1A	3208	1/1	0.95	0.10	25,25,25,25	0
57	MG	2A	3105	1/1	0.95	0.28	60,60,60,60	0
57	MG	2A	3328	1/1	0.95	0.17	42,42,42,42	0
57	MG	2A	3109	1/1	0.95	0.12	38,38,38,38	0
57	MG	1U	202	1/1	0.95	0.23	32,32,32,32	0
57	MG	1A	3160	1/1	0.95	0.10	32,32,32,32	0
57	MG	2A	3332	1/1	0.95	0.11	30,30,30,30	0
57	MG	1U	205	1/1	0.95	0.16	39,39,39,39	0
57	MG	1V	205	1/1	0.95	0.05	37,37,37,37	0
57	MG	1A	3560	1/1	0.95	0.07	17,17,17,17	0
57	MG	1A	3689	1/1	0.95	0.12	20,20,20,20	0
57	MG	1A	3692	1/1	0.95	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3213	1/1	0.95	0.10	28,28,28,28	0
57	MG	1Z	301	1/1	0.95	0.08	34,34,34,34	0
57	MG	1A	3697	1/1	0.95	0.10	24,24,24,24	0
57	MG	1A	3217	1/1	0.95	0.13	44,44,44,44	0
57	MG	2A	3124	1/1	0.95	0.22	53,53,53,53	0
57	MG	1A	3700	1/1	0.95	0.05	38,38,38,38	0
57	MG	2A	3350	1/1	0.95	0.16	48,48,48,48	0
57	MG	2A	3584	1/1	0.95	0.09	67,67,67,67	0
57	MG	1A	3306	1/1	0.95	0.06	24,24,24,24	0
57	MG	2A	3352	1/1	0.95	0.13	53,53,53,53	0
57	MG	1A	3565	1/1	0.95	0.07	12,12,12,12	0
57	MG	1A	3566	1/1	0.95	0.07	64,64,64,64	0
57	MG	1A	3375	1/1	0.95	0.05	12,12,12,12	0
57	MG	1A	3572	1/1	0.95	0.14	37,37,37,37	0
57	MG	1A	3461	1/1	0.95	0.06	33,33,33,33	0
57	MG	17	103	1/1	0.95	0.20	24,24,24,24	0
57	MG	2A	3139	1/1	0.95	0.15	43,43,43,43	0
57	MG	1A	3125	1/1	0.95	0.12	27,27,27,27	0
57	MG	2A	3367	1/1	0.95	0.14	30,30,30,30	0
57	MG	2A	3142	1/1	0.95	0.31	42,42,42,42	0
57	MG	1a	1753	1/1	0.95	0.14	54,54,54,54	0
57	MG	2A	3371	1/1	0.95	0.07	58,58,58,58	0
57	MG	2e	202	1/1	0.95	0.06	54,54,54,54	0
57	MG	1a	1754	1/1	0.95	0.14	64,64,64,64	0
57	MG	1A	3578	1/1	0.95	0.06	14,14,14,14	0
57	MG	1A	3079	1/1	0.95	0.08	38,38,38,38	0
57	MG	2A	3375	1/1	0.95	0.12	47,47,47,47	0
57	MG	1a	1757	1/1	0.95	0.15	42,42,42,42	0
57	MG	2A	3380	1/1	0.95	0.12	50,50,50,50	0
57	MG	2t	201	1/1	0.95	0.12	48,48,48,48	0
57	MG	19	102	1/1	0.95	0.09	44,44,44,44	0
57	MG	2A	3616	1/1	0.95	0.06	50,50,50,50	0
57	MG	1A	3381	1/1	0.95	0.08	19,19,19,19	0
57	MG	1A	3719	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3581	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3047	1/1	0.95	0.07	18,18,18,18	0
57	MG	1A	3222	1/1	0.95	0.11	44,44,44,44	0
57	MG	2A	3160	1/1	0.95	0.23	44,44,44,44	0
57	MG	2A	3389	1/1	0.95	0.09	36,36,36,36	0
57	MG	1a	1609	1/1	0.95	0.15	50,50,50,50	0
57	MG	1A	3170	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3100	1/1	0.96	0.15	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	2A	3128	1/1	0.96	0.48	58,58,58,58	0
57	MG	1A	3686	1/1	0.96	0.14	11,11,11,11	0
57	MG	1A	3567	1/1	0.96	0.08	32,32,32,32	0
57	MG	2A	3617	1/1	0.96	0.07	38,38,38,38	0
57	MG	2A	3131	1/1	0.96	0.23	49,49,49,49	0
57	MG	1A	3069	1/1	0.96	0.21	48,48,48,48	0
57	MG	2A	3620	1/1	0.96	0.23	42,42,42,42	0
57	MG	1A	3690	1/1	0.96	0.11	46,46,46,46	0
57	MG	2A	3622	1/1	0.96	0.06	39,39,39,39	0
57	MG	2A	3136	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3691	1/1	0.96	0.11	22,22,22,22	0
57	MG	1A	3459	1/1	0.96	0.07	5,5,5,5	0
57	MG	1A	3014	1/1	0.96	0.08	17,17,17,17	0
57	MG	2A	3627	1/1	0.96	0.15	51,51,51,51	0
57	MG	2A	3628	1/1	0.96	0.09	41,41,41,41	0
57	MG	2A	3629	1/1	0.96	0.04	43,43,43,43	0
57	MG	1V	202	1/1	0.96	0.06	33,33,33,33	0
57	MG	1a	1741	1/1	0.96	0.06	42,42,42,42	0
57	MG	2A	3378	1/1	0.96	0.09	31,31,31,31	0
57	MG	1A	3694	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3696	1/1	0.96	0.05	34,34,34,34	0
57	MG	2A	3637	1/1	0.96	0.15	61,61,61,61	0
57	MG	1A	3369	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	3698	1/1	0.96	0.08	33,33,33,33	0
57	MG	1A	3371	1/1	0.96	0.05	33,33,33,33	0
57	MG	2A	3149	1/1	0.96	0.05	36,36,36,36	0
57	MG	1a	1748	1/1	0.96	0.05	57,57,57,57	0
57	MG	1X	102	1/1	0.96	0.07	18,18,18,18	0
57	MG	2A	3152	1/1	0.96	0.23	43,43,43,43	0
57	MG	1a	1750	1/1	0.96	0.05	29,29,29,29	0
57	MG	1A	3039	1/1	0.96	0.22	24,24,24,24	0
57	MG	10	101	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3105	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3465	1/1	0.96	0.06	45,45,45,45	0
57	MG	11	101	1/1	0.96	0.18	32,32,32,32	0
57	MG	1A	3042	1/1	0.96	0.08	16,16,16,16	0
57	MG	2D	301	1/1	0.96	0.11	45,45,45,45	0
57	MG	1A	3074	1/1	0.96	0.18	34,34,34,34	0
57	MG	11	104	1/1	0.96	0.09	32,32,32,32	0
57	MG	2D	307	1/1	0.96	0.08	54,54,54,54	0
57	MG	1A	3468	1/1	0.96	0.07	39,39,39,39	0
57	MG	12	102	1/1	0.96	0.04	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	1A	3709	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3227	1/1	0.96	0.07	21,21,21,21	0
57	MG	2E	305	1/1	0.96	0.08	33,33,33,33	0
57	MG	1A	3380	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3713	1/1	0.96	0.12	41,41,41,41	0
57	MG	16	101	1/1	0.96	0.10	38,38,38,38	0
57	MG	1A	3108	1/1	0.96	0.14	16,16,16,16	0
57	MG	2A	3176	1/1	0.96	0.13	48,48,48,48	0
57	MG	2O	201	1/1	0.96	0.11	40,40,40,40	0
57	MG	2P	201	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3077	1/1	0.96	0.09	41,41,41,41	0
57	MG	1A	3028	1/1	0.96	0.25	31,31,31,31	0
57	MG	2Q	202	1/1	0.96	0.12	45,45,45,45	0
57	MG	1A	3718	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3081	1/1	0.96	0.13	22,22,22,22	0
57	MG	1A	3592	1/1	0.96	0.03	27,27,27,27	0
57	MG	2U	201	1/1	0.96	0.22	48,48,48,48	0
57	MG	2A	3184	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3313	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3594	1/1	0.96	0.12	14,14,14,14	0
57	MG	2Y	201	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3386	1/1	0.96	0.10	22,22,22,22	0
57	MG	1A	3727	1/1	0.96	0.11	43,43,43,43	0
57	MG	1a	1607	1/1	0.96	0.11	15,15,15,15	0
57	MG	29	101	1/1	0.96	0.14	52,52,52,52	0
57	MG	1a	1780	1/1	0.96	0.06	55,55,55,55	0
57	MG	1A	3238	1/1	0.96	0.29	25,25,25,25	0
57	MG	2a	1604	1/1	0.96	0.15	43,43,43,43	0
57	MG	1a	1610	1/1	0.96	0.13	30,30,30,30	0
57	MG	2a	1606	1/1	0.96	0.16	38,38,38,38	0
57	MG	2A	3425	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	3083	1/1	0.96	0.28	33,33,33,33	0
57	MG	1a	1785	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3146	1/1	0.96	0.11	31,31,31,31	0
57	MG	2a	1611	1/1	0.96	0.14	55,55,55,55	0
57	MG	1a	1613	1/1	0.96	0.12	32,32,32,32	0
57	MG	1A	3731	1/1	0.96	0.06	26,26,26,26	0
57	MG	1a	1615	1/1	0.96	0.04	44,44,44,44	0
57	MG	2A	3433	1/1	0.96	0.10	37,37,37,37	0
57	MG	1A	3317	1/1	0.96	0.08	41,41,41,41	0
57	MG	1a	1617	1/1	0.96	0.10	36,36,36,36	0
57	MG	1A	3241	1/1	0.96	0.04	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1619	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3242	1/1	0.96	0.16	22,22,22,22	0
57	MG	2A	3439	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3243	1/1	0.96	0.07	27,27,27,27	0
57	MG	2A	3441	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3397	1/1	0.96	0.07	15,15,15,15	0
57	MG	2A	3210	1/1	0.96	0.10	33,33,33,33	0
57	MG	1A	3740	1/1	0.96	0.11	46,46,46,46	0
57	MG	2A	3213	1/1	0.96	0.12	25,25,25,25	0
57	MG	2a	1628	1/1	0.96	0.05	34,34,34,34	0
57	MG	2A	3214	1/1	0.96	0.05	39,39,39,39	0
57	MG	1A	3604	1/1	0.96	0.10	15,15,15,15	0
57	MG	2A	3449	1/1	0.96	0.15	44,44,44,44	0
57	MG	1x	101	1/1	0.96	0.10	36,36,36,36	0
57	MG	1A	3605	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3743	1/1	0.96	0.14	13,13,13,13	0
57	MG	1A	3245	1/1	0.96	0.05	21,21,21,21	0
57	MG	2A	3456	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3608	1/1	0.96	0.09	38,38,38,38	0
57	MG	2a	1639	1/1	0.96	0.22	49,49,49,49	0
57	MG	2a	1640	1/1	0.96	0.14	37,37,37,37	0
57	MG	2a	1641	1/1	0.96	0.13	60,60,60,60	0
57	MG	1A	3085	1/1	0.96	0.07	7,7,7,7	0
57	MG	1A	3611	1/1	0.96	0.17	48,48,48,48	0
57	MG	1A	3749	1/1	0.96	0.13	58,58,58,58	0
57	MG	2A	3462	1/1	0.96	0.17	51,51,51,51	0
57	MG	1a	1636	1/1	0.96	0.14	25,25,25,25	0
57	MG	1A	3612	1/1	0.96	0.15	36,36,36,36	0
57	MG	1A	3492	1/1	0.96	0.10	34,34,34,34	0
57	MG	2A	3229	1/1	0.96	0.12	35,35,35,35	0
57	MG	2A	3467	1/1	0.96	0.19	39,39,39,39	0
57	MG	1A	3010	1/1	0.96	0.06	26,26,26,26	0
57	MG	1A	3754	1/1	0.96	0.07	29,29,29,29	0
57	MG	1A	3495	1/1	0.96	0.04	23,23,23,23	0
57	MG	2A	3011	1/1	0.96	0.05	34,34,34,34	0
57	MG	1a	1643	1/1	0.96	0.09	52,52,52,52	0
57	MG	2A	3013	1/1	0.96	0.05	40,40,40,40	0
57	MG	2A	3474	1/1	0.96	0.10	51,51,51,51	0
57	MG	1a	1645	1/1	0.96	0.07	61,61,61,61	0
57	MG	2A	3016	1/1	0.96	0.11	45,45,45,45	0
57	MG	1A	3617	1/1	0.96	0.08	16,16,16,16	0
57	MG	2A	3240	1/1	0.96	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	2A	3019	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3242	1/1	0.96	0.08	34,34,34,34	0
57	MG	2a	1665	1/1	0.96	0.23	53,53,53,53	0
57	MG	1A	3087	1/1	0.96	0.24	39,39,39,39	0
57	MG	1A	3619	1/1	0.96	0.14	33,33,33,33	0
57	MG	1A	3151	1/1	0.96	0.17	16,16,16,16	0
57	MG	2A	3485	1/1	0.96	0.11	45,45,45,45	0
57	MG	1A	3621	1/1	0.96	0.12	33,33,33,33	0
57	MG	1A	3622	1/1	0.96	0.12	26,26,26,26	0
57	MG	2A	3027	1/1	0.96	0.17	34,34,34,34	0
57	MG	2A	3028	1/1	0.96	0.12	36,36,36,36	0
57	MG	2A	3031	1/1	0.96	0.11	39,39,39,39	0
57	MG	1A	3088	1/1	0.96	0.05	20,20,20,20	0
57	MG	1A	3328	1/1	0.96	0.07	23,23,23,23	0
57	MG	2a	1678	1/1	0.96	0.09	43,43,43,43	0
57	MG	1A	3505	1/1	0.96	0.06	26,26,26,26	0
57	MG	1A	3253	1/1	0.96	0.07	23,23,23,23	0
57	MG	1A	3507	1/1	0.96	0.06	49,49,49,49	0
57	MG	1A	3407	1/1	0.96	0.15	51,51,51,51	0
57	MG	2A	3262	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3770	1/1	0.96	0.07	29,29,29,29	0
57	MG	1A	3771	1/1	0.96	0.07	40,40,40,40	0
57	MG	2A	3266	1/1	0.96	0.15	30,30,30,30	0
57	MG	2A	3267	1/1	0.96	0.08	30,30,30,30	0
57	MG	2A	3044	1/1	0.96	0.11	56,56,56,56	0
57	MG	2A	3045	1/1	0.96	0.24	48,48,48,48	0
57	MG	1A	3774	1/1	0.96	0.07	24,24,24,24	0
57	MG	1A	3118	1/1	0.96	0.15	33,33,33,33	0
57	MG	1A	3090	1/1	0.96	0.07	15,15,15,15	0
57	MG	1A	3259	1/1	0.96	0.13	36,36,36,36	0
57	MG	1A	3413	1/1	0.96	0.05	15,15,15,15	0
57	MG	1a	1666	1/1	0.96	0.08	49,49,49,49	0
57	MG	1a	1667	1/1	0.96	0.14	50,50,50,50	0
57	MG	1A	3260	1/1	0.96	0.12	23,23,23,23	0
57	MG	1A	3418	1/1	0.96	0.07	13,13,13,13	0
57	MG	2A	3055	1/1	0.96	0.19	51,51,51,51	0
57	MG	2A	3518	1/1	0.96	0.07	45,45,45,45	0
57	MG	2a	1704	1/1	0.96	0.15	48,48,48,48	0
57	MG	2A	3519	1/1	0.96	0.06	54,54,54,54	0
57	MG	2A	3283	1/1	0.96	0.07	43,43,43,43	0
57	MG	2a	1707	1/1	0.96	0.14	47,47,47,47	0
57	MG	1A	3419	1/1	0.96	0.07	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1709	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3157	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3523	1/1	0.96	0.11	35,35,35,35	0
57	MG	1A	3341	1/1	0.96	0.11	39,39,39,39	0
57	MG	1A	3342	1/1	0.96	0.06	12,12,12,12	0
57	MG	2A	3526	1/1	0.96	0.11	68,68,68,68	0
57	MG	1a	1675	1/1	0.96	0.09	29,29,29,29	0
57	MG	1A	3789	1/1	0.96	0.12	39,39,39,39	0
57	MG	2A	3291	1/1	0.96	0.05	41,41,41,41	0
57	MG	2A	3530	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3063	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3790	1/1	0.96	0.11	43,43,43,43	0
57	MG	2a	1722	1/1	0.96	0.10	58,58,58,58	0
57	MG	2A	3065	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3158	1/1	0.96	0.12	20,20,20,20	0
57	MG	1A	3792	1/1	0.96	0.10	11,11,11,11	0
57	MG	1A	3265	1/1	0.96	0.18	34,34,34,34	0
57	MG	1A	3345	1/1	0.96	0.05	13,13,13,13	0
57	MG	1A	3647	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3430	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3649	1/1	0.96	0.13	35,35,35,35	0
57	MG	2a	1731	1/1	0.96	0.10	49,49,49,49	0
57	MG	2A	3542	1/1	0.96	0.22	51,51,51,51	0
57	MG	2A	3304	1/1	0.96	0.07	37,37,37,37	0
57	MG	1B	204	1/1	0.96	0.10	28,28,28,28	0
57	MG	2A	3075	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3266	1/1	0.96	0.08	25,25,25,25	0
57	MG	1A	3348	1/1	0.96	0.04	30,30,30,30	0
57	MG	2A	3549	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3537	1/1	0.96	0.07	13,13,13,13	0
57	MG	1A	3267	1/1	0.96	0.16	14,14,14,14	0
57	MG	1A	3017	1/1	0.96	0.05	20,20,20,20	0
57	MG	2a	1742	1/1	0.96	0.12	48,48,48,48	0
57	MG	1B	211	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3025	1/1	0.96	0.20	30,30,30,30	0
57	MG	2A	3316	1/1	0.96	0.10	34,34,34,34	0
57	MG	1A	3094	1/1	0.96	0.10	18,18,18,18	0
57	MG	2A	3560	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3318	1/1	0.96	0.07	39,39,39,39	0
57	MG	1B	216	1/1	0.96	0.10	35,35,35,35	0
57	MG	2A	3564	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3565	1/1	0.96	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	1B	219	1/1	0.96	0.10	40,40,40,40	0
57	MG	2A	3567	1/1	0.96	0.08	29,29,29,29	0
57	MG	1A	3662	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3663	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	3441	1/1	0.96	0.06	24,24,24,24	0
57	MG	1A	3442	1/1	0.96	0.04	7,7,7,7	0
57	MG	1A	3444	1/1	0.96	0.12	12,12,12,12	0
57	MG	1A	3548	1/1	0.96	0.12	17,17,17,17	0
57	MG	1E	306	1/1	0.96	0.08	15,15,15,15	0
57	MG	1E	307	1/1	0.96	0.05	42,42,42,42	0
57	MG	1E	308	1/1	0.96	0.08	23,23,23,23	0
57	MG	1a	1708	1/1	0.96	0.07	33,33,33,33	0
57	MG	1A	3272	1/1	0.96	0.05	48,48,48,48	0
57	MG	2A	3582	1/1	0.96	0.05	42,42,42,42	0
57	MG	1a	1711	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3166	1/1	0.96	0.05	25,25,25,25	0
57	MG	2A	3337	1/1	0.96	0.08	47,47,47,47	0
57	MG	2A	3108	1/1	0.96	0.26	42,42,42,42	0
57	MG	1a	1713	1/1	0.96	0.07	52,52,52,52	0
57	MG	1A	3671	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3447	1/1	0.96	0.07	22,22,22,22	0
57	MG	2A	3343	1/1	0.96	0.04	20,20,20,20	0
57	MG	1A	3552	1/1	0.96	0.07	39,39,39,39	0
57	MG	2A	3594	1/1	0.96	0.06	50,50,50,50	0
57	MG	1A	3556	1/1	0.96	0.06	14,14,14,14	0
57	MG	1A	3356	1/1	0.96	0.06	27,27,27,27	0
57	MG	2A	3598	1/1	0.96	0.10	34,34,34,34	0
57	MG	2A	3347	1/1	0.96	0.11	21,21,21,21	0
57	MG	1A	3277	1/1	0.96	0.15	21,21,21,21	0
57	MG	1a	1722	1/1	0.96	0.10	28,28,28,28	0
57	MG	1A	3280	1/1	0.96	0.15	25,25,25,25	0
57	MG	1A	3167	1/1	0.96	0.08	20,20,20,20	0
57	MG	1A	3284	1/1	0.96	0.06	16,16,16,16	0
57	MG	1A	3362	1/1	0.96	0.11	29,29,29,29	0
57	MG	1A	3285	1/1	0.96	0.06	26,26,26,26	0
58	ZN	2Y	202	1/1	0.96	0.06	99,99,99,99	0
57	MG	1A	3008	1/1	0.96	0.13	17,17,17,17	0
58	ZN	2n	501	1/1	0.96	0.06	94,94,94,94	0
57	MG	2A	3255	1/1	0.97	0.07	34,34,34,34	0
57	MG	2A	3457	1/1	0.97	0.13	31,31,31,31	0
57	MG	1A	3422	1/1	0.97	0.04	16,16,16,16	0
57	MG	1A	3512	1/1	0.97	0.05	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1709	1/1	0.97	0.06	29,29,29,29	0
57	MG	1U	206	1/1	0.97	0.11	24,24,24,24	0
57	MG	1A	3725	1/1	0.97	0.25	18,18,18,18	0
57	MG	2A	3263	1/1	0.97	0.08	24,24,24,24	0
57	MG	2R	201	1/1	0.97	0.13	26,26,26,26	0
57	MG	1V	203	1/1	0.97	0.10	22,22,22,22	0
57	MG	2A	3071	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3726	1/1	0.97	0.15	25,25,25,25	0
57	MG	2V	201	1/1	0.97	0.11	55,55,55,55	0
57	MG	1a	1714	1/1	0.97	0.09	37,37,37,37	0
57	MG	2W	201	1/1	0.97	0.13	54,54,54,54	0
57	MG	1a	1715	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3616	1/1	0.97	0.07	44,44,44,44	0
57	MG	1A	3423	1/1	0.97	0.08	15,15,15,15	0
57	MG	1W	204	1/1	0.97	0.06	17,17,17,17	0
57	MG	1A	3279	1/1	0.97	0.22	31,31,31,31	0
57	MG	23	101	1/1	0.97	0.11	42,42,42,42	0
57	MG	1A	3089	1/1	0.97	0.11	30,30,30,30	0
57	MG	28	101	1/1	0.97	0.14	55,55,55,55	0
57	MG	1A	3516	1/1	0.97	0.14	26,26,26,26	0
57	MG	2A	3276	1/1	0.97	0.05	25,25,25,25	0
57	MG	1A	3732	1/1	0.97	0.12	37,37,37,37	0
57	MG	1A	3187	1/1	0.97	0.08	25,25,25,25	0
57	MG	1A	3282	1/1	0.97	0.18	29,29,29,29	0
57	MG	1A	3283	1/1	0.97	0.17	35,35,35,35	0
57	MG	10	104	1/1	0.97	0.07	42,42,42,42	0
57	MG	10	105	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3119	1/1	0.97	0.13	15,15,15,15	0
57	MG	1A	3189	1/1	0.97	0.18	14,14,14,14	0
57	MG	2A	3484	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3434	1/1	0.97	0.04	8,8,8,8	0
57	MG	1A	3527	1/1	0.97	0.08	36,36,36,36	0
57	MG	1A	3233	1/1	0.97	0.23	30,30,30,30	0
57	MG	1A	3120	1/1	0.97	0.06	9,9,9,9	0
57	MG	1A	3137	1/1	0.97	0.16	22,22,22,22	0
57	MG	2A	3096	1/1	0.97	0.06	36,36,36,36	0
57	MG	2A	3097	1/1	0.97	0.06	44,44,44,44	0
57	MG	2A	3294	1/1	0.97	0.04	39,39,39,39	0
57	MG	2A	3100	1/1	0.97	0.12	25,25,25,25	0
57	MG	1A	3633	1/1	0.97	0.22	25,25,25,25	0
57	MG	1A	3236	1/1	0.97	0.12	16,16,16,16	0
57	MG	1A	3360	1/1	0.97	0.04	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3636	1/1	0.97	0.08	35,35,35,35	0
57	MG	1A	3535	1/1	0.97	0.11	29,29,29,29	0
57	MG	1a	1743	1/1	0.97	0.06	30,30,30,30	0
57	MG	2A	3502	1/1	0.97	0.04	50,50,50,50	0
57	MG	2A	3302	1/1	0.97	0.06	49,49,49,49	0
57	MG	17	105	1/1	0.97	0.16	31,31,31,31	0
57	MG	1A	3536	1/1	0.97	0.05	30,30,30,30	0
57	MG	2a	1631	1/1	0.97	0.21	42,42,42,42	0
57	MG	1A	3237	1/1	0.97	0.20	24,24,24,24	0
57	MG	1A	3293	1/1	0.97	0.15	34,34,34,34	0
57	MG	19	101	1/1	0.97	0.15	34,34,34,34	0
57	MG	2A	3309	1/1	0.97	0.12	26,26,26,26	0
57	MG	1A	3363	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3138	1/1	0.97	0.04	15,15,15,15	0
57	MG	1A	3193	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3301	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3302	1/1	0.97	0.48	21,21,21,21	0
57	MG	1A	3544	1/1	0.97	0.08	14,14,14,14	0
57	MG	1A	3545	1/1	0.97	0.10	14,14,14,14	0
57	MG	1A	3303	1/1	0.97	0.05	14,14,14,14	0
57	MG	1A	3650	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3305	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3766	1/1	0.97	0.04	29,29,29,29	0
57	MG	1a	1760	1/1	0.97	0.08	22,22,22,22	0
57	MG	1A	3652	1/1	0.97	0.11	40,40,40,40	0
57	MG	2A	3324	1/1	0.97	0.12	56,56,56,56	0
57	MG	1A	3370	1/1	0.97	0.11	17,17,17,17	0
57	MG	1A	3162	1/1	0.97	0.08	51,51,51,51	0
57	MG	1A	3307	1/1	0.97	0.06	33,33,33,33	0
57	MG	2A	3135	1/1	0.97	0.15	42,42,42,42	0
57	MG	1A	3656	1/1	0.97	0.08	20,20,20,20	0
57	MG	1A	3773	1/1	0.97	0.08	11,11,11,11	0
57	MG	1A	3657	1/1	0.97	0.06	21,21,21,21	0
57	MG	2a	1657	1/1	0.97	0.15	45,45,45,45	0
57	MG	1A	3373	1/1	0.97	0.06	18,18,18,18	0
57	MG	1A	3553	1/1	0.97	0.10	12,12,12,12	0
57	MG	2A	3141	1/1	0.97	0.10	25,25,25,25	0
57	MG	1a	1622	1/1	0.97	0.04	42,42,42,42	0
57	MG	2A	3336	1/1	0.97	0.05	37,37,37,37	0
57	MG	1a	1623	1/1	0.97	0.24	41,41,41,41	0
57	MG	1A	3660	1/1	0.97	0.04	29,29,29,29	0
57	MG	1A	3163	1/1	0.97	0.10	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3779	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3165	1/1	0.97	0.10	24,24,24,24	0
57	MG	1a	1628	1/1	0.97	0.29	49,49,49,49	0
57	MG	1A	3781	1/1	0.97	0.06	32,32,32,32	0
57	MG	1A	3376	1/1	0.97	0.05	13,13,13,13	0
57	MG	1A	3063	1/1	0.97	0.13	31,31,31,31	0
57	MG	2A	3154	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3244	1/1	0.97	0.05	28,28,28,28	0
57	MG	1a	1783	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3199	1/1	0.97	0.12	17,17,17,17	0
57	MG	2A	3552	1/1	0.97	0.18	23,23,23,23	0
57	MG	1A	3076	1/1	0.97	0.07	40,40,40,40	0
57	MG	2A	3554	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3787	1/1	0.97	0.15	29,29,29,29	0
57	MG	2A	3354	1/1	0.97	0.12	35,35,35,35	0
57	MG	1a	1637	1/1	0.97	0.08	34,34,34,34	0
57	MG	1A	3788	1/1	0.97	0.07	16,16,16,16	0
57	MG	1A	3202	1/1	0.97	0.12	28,28,28,28	0
57	MG	1A	3564	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3203	1/1	0.97	0.17	40,40,40,40	0
57	MG	1A	3037	1/1	0.97	0.16	20,20,20,20	0
57	MG	2a	1688	1/1	0.97	0.17	50,50,50,50	0
57	MG	2A	3363	1/1	0.97	0.05	35,35,35,35	0
57	MG	2a	1690	1/1	0.97	0.19	57,57,57,57	0
57	MG	1A	3142	1/1	0.97	0.10	36,36,36,36	0
57	MG	2A	3170	1/1	0.97	0.11	52,52,52,52	0
57	MG	1a	1644	1/1	0.97	0.29	59,59,59,59	0
57	MG	2A	3369	1/1	0.97	0.08	50,50,50,50	0
57	MG	1A	3252	1/1	0.97	0.05	28,28,28,28	0
57	MG	2A	3571	1/1	0.97	0.04	40,40,40,40	0
57	MG	1A	3570	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3676	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3145	1/1	0.97	0.21	27,27,27,27	0
57	MG	1a	1649	1/1	0.97	0.20	41,41,41,41	0
57	MG	2A	3576	1/1	0.97	0.10	32,32,32,32	0
57	MG	1A	3388	1/1	0.97	0.10	42,42,42,42	0
57	MG	1A	3389	1/1	0.97	0.09	26,26,26,26	0
57	MG	2A	3579	1/1	0.97	0.10	49,49,49,49	0
57	MG	2A	3377	1/1	0.97	0.10	35,35,35,35	0
57	MG	1A	3207	1/1	0.97	0.04	30,30,30,30	0
57	MG	2A	3379	1/1	0.97	0.10	51,51,51,51	0
57	MG	2A	3181	1/1	0.97	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1x	105	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3171	1/1	0.97	0.12	19,19,19,19	0
57	MG	1x	107	1/1	0.97	0.05	49,49,49,49	0
57	MG	2A	3588	1/1	0.97	0.09	42,42,42,42	0
57	MG	1A	3256	1/1	0.97	0.07	21,21,21,21	0
57	MG	1x	109	1/1	0.97	0.10	34,34,34,34	0
57	MG	1A	3257	1/1	0.97	0.07	27,27,27,27	0
57	MG	2A	3188	1/1	0.97	0.10	34,34,34,34	0
57	MG	2a	1718	1/1	0.97	0.06	55,55,55,55	0
57	MG	1A	3324	1/1	0.97	0.05	42,42,42,42	0
57	MG	1B	212	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3395	1/1	0.97	0.07	47,47,47,47	0
57	MG	1B	214	1/1	0.97	0.05	29,29,29,29	0
57	MG	2A	3006	1/1	0.97	0.12	48,48,48,48	0
57	MG	1A	3687	1/1	0.97	0.11	33,33,33,33	0
57	MG	1A	3258	1/1	0.97	0.12	32,32,32,32	0
57	MG	1B	218	1/1	0.97	0.04	42,42,42,42	0
57	MG	2A	3602	1/1	0.97	0.08	28,28,28,28	0
57	MG	2A	3604	1/1	0.97	0.24	34,34,34,34	0
57	MG	2A	3605	1/1	0.97	0.06	46,46,46,46	0
57	MG	2A	3397	1/1	0.97	0.08	58,58,58,58	0
57	MG	1A	3209	1/1	0.97	0.19	24,24,24,24	0
57	MG	1B	220	1/1	0.97	0.07	26,26,26,26	0
57	MG	2A	3201	1/1	0.97	0.09	39,39,39,39	0
57	MG	1D	302	1/1	0.97	0.19	33,33,33,33	0
57	MG	1D	303	1/1	0.97	0.05	15,15,15,15	0
57	MG	2A	3015	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	3211	1/1	0.97	0.06	22,22,22,22	0
57	MG	2A	3017	1/1	0.97	0.14	38,38,38,38	0
57	MG	2A	3615	1/1	0.97	0.08	54,54,54,54	0
57	MG	1A	3483	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3110	1/1	0.97	0.11	33,33,33,33	0
57	MG	1a	1670	1/1	0.97	0.19	35,35,35,35	0
57	MG	1A	3066	1/1	0.97	0.13	18,18,18,18	0
57	MG	2a	1744	1/1	0.97	0.10	65,65,65,65	0
57	MG	1A	3264	1/1	0.97	0.30	31,31,31,31	0
57	MG	1A	3215	1/1	0.97	0.17	22,22,22,22	0
57	MG	2A	3025	1/1	0.97	0.14	49,49,49,49	0
57	MG	2a	1748	1/1	0.97	0.11	39,39,39,39	0
57	MG	1A	3175	1/1	0.97	0.09	28,28,28,28	0
57	MG	1A	3334	1/1	0.97	0.06	32,32,32,32	0
57	MG	1A	3053	1/1	0.97	0.04	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	2A	3030	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3054	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3702	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3494	1/1	0.97	0.09	38,38,38,38	0
57	MG	1F	303	1/1	0.97	0.27	33,33,33,33	0
57	MG	2A	3421	1/1	0.97	0.09	27,27,27,27	0
57	MG	2A	3632	1/1	0.97	0.10	26,26,26,26	0
57	MG	1F	305	1/1	0.97	0.06	33,33,33,33	0
57	MG	2A	3224	1/1	0.97	0.12	38,38,38,38	0
57	MG	1A	3339	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3496	1/1	0.97	0.06	20,20,20,20	0
57	MG	1A	3497	1/1	0.97	0.03	10,10,10,10	0
57	MG	2A	3040	1/1	0.97	0.23	40,40,40,40	0
57	MG	2A	3042	1/1	0.97	0.15	32,32,32,32	0
57	MG	1G	202	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3340	1/1	0.97	0.09	37,37,37,37	0
57	MG	1A	3056	1/1	0.97	0.08	29,29,29,29	0
57	MG	1A	3044	1/1	0.97	0.13	17,17,17,17	0
57	MG	1a	1689	1/1	0.97	0.04	29,29,29,29	0
57	MG	1A	3414	1/1	0.97	0.06	14,14,14,14	0
57	MG	1a	1691	1/1	0.97	0.20	49,49,49,49	0
57	MG	1A	3504	1/1	0.97	0.04	29,29,29,29	0
57	MG	1A	3606	1/1	0.97	0.04	18,18,18,18	0
57	MG	1P	201	1/1	0.97	0.07	17,17,17,17	0
57	MG	1A	3271	1/1	0.97	0.09	17,17,17,17	0
57	MG	1A	3183	1/1	0.97	0.31	23,23,23,23	0
57	MG	2D	303	1/1	0.97	0.10	38,38,38,38	0
57	MG	2A	3245	1/1	0.97	0.12	20,20,20,20	0
57	MG	1A	3717	1/1	0.97	0.13	22,22,22,22	0
57	MG	1A	3009	1/1	0.97	0.05	7,7,7,7	0
57	MG	1A	3346	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3040	1/1	0.97	0.05	36,36,36,36	0
57	MG	1R	201	1/1	0.97	0.12	44,44,44,44	0
57	MG	1R	202	1/1	0.97	0.21	33,33,33,33	0
57	MG	2x	107	1/1	0.97	0.06	68,68,68,68	0
57	MG	1A	3510	1/1	0.97	0.20	29,29,29,29	0
57	MG	2A	3453	1/1	0.97	0.11	25,25,25,25	0
57	MG	1U	201	1/1	0.97	0.13	27,27,27,27	0
57	MG	2F	304	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3722	1/1	0.97	0.19	21,21,21,21	0
57	MG	2F	306	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3424	1/1	0.98	0.03	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3261	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3097	1/1	0.98	0.15	29,29,29,29	0
57	MG	2A	3587	1/1	0.98	0.05	43,43,43,43	0
57	MG	2A	3038	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3427	1/1	0.98	0.04	15,15,15,15	0
57	MG	1A	3569	1/1	0.98	0.07	52,52,52,52	0
57	MG	2A	3041	1/1	0.98	0.06	34,34,34,34	0
57	MG	2A	3166	1/1	0.98	0.17	39,39,39,39	0
57	MG	1A	3734	1/1	0.98	0.05	28,28,28,28	0
57	MG	1A	3023	1/1	0.98	0.09	34,34,34,34	0
57	MG	2A	3595	1/1	0.98	0.12	65,65,65,65	0
57	MG	2A	3447	1/1	0.98	0.14	59,59,59,59	0
57	MG	1A	3571	1/1	0.98	0.06	32,32,32,32	0
57	MG	1A	3221	1/1	0.98	0.07	27,27,27,27	0
57	MG	2A	3450	1/1	0.98	0.07	39,39,39,39	0
57	MG	1F	304	1/1	0.98	0.21	18,18,18,18	0
57	MG	2A	3306	1/1	0.98	0.15	33,33,33,33	0
57	MG	1A	3573	1/1	0.98	0.06	35,35,35,35	0
57	MG	1A	3574	1/1	0.98	0.05	31,31,31,31	0
57	MG	1A	3575	1/1	0.98	0.03	35,35,35,35	0
57	MG	1A	3012	1/1	0.98	0.04	16,16,16,16	0
57	MG	1A	3102	1/1	0.98	0.16	28,28,28,28	0
57	MG	1A	3013	1/1	0.98	0.09	17,17,17,17	0
57	MG	1A	3153	1/1	0.98	0.15	21,21,21,21	0
57	MG	1A	3435	1/1	0.98	0.03	21,21,21,21	0
57	MG	1A	3747	1/1	0.98	0.07	17,17,17,17	0
57	MG	1A	3503	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3080	1/1	0.98	0.08	16,16,16,16	0
57	MG	1A	3155	1/1	0.98	0.27	28,28,28,28	0
57	MG	1P	202	1/1	0.98	0.17	16,16,16,16	0
57	MG	2A	3060	1/1	0.98	0.07	48,48,48,48	0
57	MG	1A	3035	1/1	0.98	0.13	19,19,19,19	0
57	MG	1A	3585	1/1	0.98	0.05	8,8,8,8	0
57	MG	2A	3189	1/1	0.98	0.14	60,60,60,60	0
57	MG	1A	3753	1/1	0.98	0.10	48,48,48,48	0
57	MG	1Q	202	1/1	0.98	0.11	22,22,22,22	0
57	MG	1Q	203	1/1	0.98	0.09	18,18,18,18	0
57	MG	1A	3082	1/1	0.98	0.11	9,9,9,9	0
57	MG	1A	3667	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3379	1/1	0.98	0.09	45,45,45,45	0
57	MG	2A	3196	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3274	1/1	0.98	0.18	25,25,25,25	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	0.98	0.10	14,14,14,14	0
57	MG	1a	1766	1/1	0.98	0.12	42,42,42,42	0
57	MG	1A	3275	1/1	0.98	0.14	26,26,26,26	0
57	MG	1A	3231	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3003	1/1	0.98	0.07	16,16,16,16	0
57	MG	1A	3278	1/1	0.98	0.11	22,22,22,22	0
57	MG	1A	3084	1/1	0.98	0.14	17,17,17,17	0
57	MG	2A	3635	1/1	0.98	0.06	32,32,32,32	0
57	MG	1A	3194	1/1	0.98	0.10	25,25,25,25	0
57	MG	2a	1694	1/1	0.98	0.06	31,31,31,31	0
57	MG	2A	3341	1/1	0.98	0.12	24,24,24,24	0
57	MG	1U	207	1/1	0.98	0.12	22,22,22,22	0
57	MG	1A	3517	1/1	0.98	0.05	21,21,21,21	0
57	MG	1A	3518	1/1	0.98	0.06	26,26,26,26	0
57	MG	1A	3131	1/1	0.98	0.07	19,19,19,19	0
57	MG	1A	3065	1/1	0.98	0.11	27,27,27,27	0
57	MG	2A	3211	1/1	0.98	0.21	29,29,29,29	0
57	MG	1A	3335	1/1	0.98	0.06	17,17,17,17	0
57	MG	2A	3349	1/1	0.98	0.11	39,39,39,39	0
57	MG	1W	203	1/1	0.98	0.21	27,27,27,27	0
57	MG	1A	3038	1/1	0.98	0.18	19,19,19,19	0
57	MG	2A	3498	1/1	0.98	0.03	32,32,32,32	0
57	MG	1A	3772	1/1	0.98	0.03	15,15,15,15	0
57	MG	1A	3005	1/1	0.98	0.07	34,34,34,34	0
57	MG	1A	3135	1/1	0.98	0.18	18,18,18,18	0
57	MG	1A	3685	1/1	0.98	0.04	37,37,37,37	0
57	MG	2A	3090	1/1	0.98	0.17	32,32,32,32	0
57	MG	1A	3200	1/1	0.98	0.07	17,17,17,17	0
57	MG	2D	305	1/1	0.98	0.08	32,32,32,32	0
57	MG	2A	3092	1/1	0.98	0.07	54,54,54,54	0
57	MG	1A	3016	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	3458	1/1	0.98	0.07	17,17,17,17	0
57	MG	1A	3041	1/1	0.98	0.07	23,23,23,23	0
57	MG	2E	302	1/1	0.98	0.14	37,37,37,37	0
57	MG	1A	3531	1/1	0.98	0.07	32,32,32,32	0
57	MG	2A	3226	1/1	0.98	0.08	44,44,44,44	0
57	MG	1A	3532	1/1	0.98	0.07	31,31,31,31	0
57	MG	2F	301	1/1	0.98	0.07	33,33,33,33	0
57	MG	2A	3098	1/1	0.98	0.06	36,36,36,36	0
57	MG	2A	3099	1/1	0.98	0.08	53,53,53,53	0
57	MG	1A	3289	1/1	0.98	0.16	7,7,7,7	0
57	MG	1A	3022	1/1	0.98	0.05	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3291	1/1	0.98	0.09	22,22,22,22	0
57	MG	2A	3233	1/1	0.98	0.05	50,50,50,50	0
57	MG	1A	3695	1/1	0.98	0.05	43,43,43,43	0
57	MG	1A	3055	1/1	0.98	0.06	14,14,14,14	0
57	MG	1A	3092	1/1	0.98	0.13	35,35,35,35	0
57	MG	2A	3106	1/1	0.98	0.08	40,40,40,40	0
57	MG	2A	3107	1/1	0.98	0.15	38,38,38,38	0
57	MG	1w	402	1/1	0.98	0.19	34,34,34,34	0
57	MG	1A	3294	1/1	0.98	0.09	37,37,37,37	0
57	MG	1A	3402	1/1	0.98	0.10	22,22,22,22	0
57	MG	15	102	1/1	0.98	0.14	33,33,33,33	0
57	MG	2A	3243	1/1	0.98	0.06	23,23,23,23	0
57	MG	1A	3296	1/1	0.98	0.08	24,24,24,24	0
57	MG	1A	3701	1/1	0.98	0.09	30,30,30,30	0
57	MG	17	102	1/1	0.98	0.22	24,24,24,24	0
57	MG	1A	3297	1/1	0.98	0.07	26,26,26,26	0
57	MG	1A	3043	1/1	0.98	0.07	23,23,23,23	0
57	MG	2X	102	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3470	1/1	0.98	0.10	25,25,25,25	0
57	MG	2A	3119	1/1	0.98	0.14	19,19,19,19	0
57	MG	2A	3120	1/1	0.98	0.08	46,46,46,46	0
57	MG	1A	3705	1/1	0.98	0.05	26,26,26,26	0
57	MG	1A	3299	1/1	0.98	0.06	33,33,33,33	0
57	MG	18	102	1/1	0.98	0.12	22,22,22,22	0
57	MG	1A	3057	1/1	0.98	0.07	9,9,9,9	0
57	MG	1A	3624	1/1	0.98	0.04	32,32,32,32	0
57	MG	2a	1601	1/1	0.98	0.16	35,35,35,35	0
57	MG	1A	3143	1/1	0.98	0.14	32,32,32,32	0
57	MG	1A	3547	1/1	0.98	0.05	16,16,16,16	0
57	MG	1A	3409	1/1	0.98	0.08	20,20,20,20	0
57	MG	2A	3260	1/1	0.98	0.04	20,20,20,20	0
57	MG	2A	3261	1/1	0.98	0.07	41,41,41,41	0
57	MG	1B	208	1/1	0.98	0.03	38,38,38,38	0
57	MG	1A	3712	1/1	0.98	0.04	29,29,29,29	0
57	MG	1a	1606	1/1	0.98	0.20	34,34,34,34	0
57	MG	2A	3133	1/1	0.98	0.10	17,17,17,17	0
57	MG	1A	3144	1/1	0.98	0.19	17,17,17,17	0
57	MG	1a	1608	1/1	0.98	0.12	49,49,49,49	0
57	MG	1A	3629	1/1	0.98	0.06	61,61,61,61	0
57	MG	1A	3210	1/1	0.98	0.13	14,14,14,14	0
57	MG	1A	3304	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3095	1/1	0.98	0.17	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	3075	1/1	0.98	0.12	22,22,22,22	0
57	MG	2A	3561	1/1	0.98	0.13	31,31,31,31	0
57	MG	1A	3554	1/1	0.98	0.08	11,11,11,11	0
57	MG	2A	3274	1/1	0.98	0.09	26,26,26,26	0
57	MG	1A	3416	1/1	0.98	0.07	19,19,19,19	0
57	MG	1A	3417	1/1	0.98	0.06	12,12,12,12	0
57	MG	1A	3178	1/1	0.98	0.25	24,24,24,24	0
57	MG	1A	3214	1/1	0.98	0.04	23,23,23,23	0
57	MG	1A	3147	1/1	0.98	0.11	19,19,19,19	0
57	MG	2A	3422	1/1	0.98	0.10	49,49,49,49	0
57	MG	2A	3280	1/1	0.98	0.14	31,31,31,31	0
57	MG	1a	1724	1/1	0.98	0.06	25,25,25,25	0
57	MG	2A	3148	1/1	0.98	0.06	27,27,27,27	0
57	MG	1A	3216	1/1	0.98	0.04	26,26,26,26	0
57	MG	1A	3180	1/1	0.98	0.13	15,15,15,15	0
57	MG	1A	3181	1/1	0.98	0.03	19,19,19,19	0
57	MG	1D	308	1/1	0.98	0.06	24,24,24,24	0
57	MG	2A	3287	1/1	0.98	0.08	35,35,35,35	0
57	MG	2A	3431	1/1	0.98	0.05	43,43,43,43	0
57	MG	2A	3153	1/1	0.98	0.11	29,29,29,29	0
57	MG	1a	1729	1/1	0.98	0.15	53,53,53,53	0
58	ZN	1n	102	1/1	0.98	0.04	85,85,85,85	0
57	MG	1E	301	1/1	0.98	0.26	25,25,25,25	0
57	MG	1A	3490	1/1	0.98	0.06	33,33,33,33	0
57	MG	2A	3157	1/1	0.98	0.08	22,22,22,22	0
59	SF4	1d	302	8/8	0.98	0.04	52,61,71,77	0
59	SF4	2d	303	8/8	0.98	0.04	49,56,67,71	0
57	MG	1A	3555	1/1	0.99	0.08	25,25,25,25	0
57	MG	1A	3232	1/1	0.99	0.13	22,22,22,22	0
57	MG	1A	3609	1/1	0.99	0.04	13,13,13,13	0
57	MG	1A	3637	1/1	0.99	0.10	23,23,23,23	0
57	MG	1B	217	1/1	0.99	0.04	41,41,41,41	0
57	MG	2A	3179	1/1	0.99	0.03	28,28,28,28	0
57	MG	2A	3355	1/1	0.99	0.10	26,26,26,26	0
57	MG	1A	3164	1/1	0.99	0.04	24,24,24,24	0
57	MG	1A	3078	1/1	0.99	0.07	22,22,22,22	0
57	MG	13	101	1/1	0.99	0.12	20,20,20,20	0
57	MG	2A	3359	1/1	0.99	0.11	50,50,50,50	0
57	MG	2A	3125	1/1	0.99	0.04	34,34,34,34	0
57	MG	2A	3488	1/1	0.99	0.04	39,39,39,39	0
57	MG	25	101	1/1	0.99	0.04	49,49,49,49	0
57	MG	1A	3058	1/1	0.99	0.07	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3557	1/1	0.99	0.03	45,45,45,45	0
57	MG	1D	301	1/1	0.99	0.04	26,26,26,26	0
57	MG	1a	1631	1/1	0.99	0.09	41,41,41,41	0
57	MG	2A	3364	1/1	0.99	0.07	34,34,34,34	0
57	MG	1A	3034	1/1	0.99	0.14	8,8,8,8	0
57	MG	1a	1777	1/1	0.99	0.06	50,50,50,50	0
57	MG	2a	1675	1/1	0.99	0.11	32,32,32,32	0
57	MG	1A	3024	1/1	0.99	0.04	14,14,14,14	0
57	MG	2A	3022	1/1	0.99	0.04	34,34,34,34	0
57	MG	15	103	1/1	0.99	0.15	19,19,19,19	0
57	MG	1A	3295	1/1	0.99	0.16	31,31,31,31	0
57	MG	1D	305	1/1	0.99	0.03	17,17,17,17	0
57	MG	17	101	1/1	0.99	0.03	23,23,23,23	0
57	MG	1a	1733	1/1	0.99	0.10	25,25,25,25	0
57	MG	1A	3757	1/1	0.99	0.13	29,29,29,29	0
57	MG	2A	3029	1/1	0.99	0.05	29,29,29,29	0
57	MG	1A	3251	1/1	0.99	0.05	25,25,25,25	0
57	MG	17	104	1/1	0.99	0.07	20,20,20,20	0
57	MG	1A	3098	1/1	0.99	0.04	21,21,21,21	0
57	MG	1A	3330	1/1	0.99	0.03	21,21,21,21	0
57	MG	1E	302	1/1	0.99	0.10	22,22,22,22	0
57	MG	1A	3099	1/1	0.99	0.09	21,21,21,21	0
57	MG	2a	1762	1/1	0.99	0.10	36,36,36,36	0
57	MG	1A	3061	1/1	0.99	0.09	32,32,32,32	0
57	MG	1U	203	1/1	0.99	0.04	21,21,21,21	0
57	MG	2A	3385	1/1	0.99	0.03	47,47,47,47	0
57	MG	2A	3322	1/1	0.99	0.07	19,19,19,19	0
57	MG	1A	3228	1/1	0.99	0.07	32,32,32,32	0
57	MG	1A	3794	1/1	0.99	0.05	15,15,15,15	0
57	MG	2A	3516	1/1	0.99	0.04	55,55,55,55	0
57	MG	2D	302	1/1	0.99	0.09	20,20,20,20	0
57	MG	1A	3036	1/1	0.99	0.15	21,21,21,21	0
57	MG	1A	3473	1/1	0.99	0.04	11,11,11,11	0
57	MG	1V	201	1/1	0.99	0.13	17,17,17,17	0
57	MG	1A	3736	1/1	0.99	0.05	14,14,14,14	0
57	MG	1A	3353	1/1	0.99	0.08	19,19,19,19	0
57	MG	1V	204	1/1	0.99	0.08	17,17,17,17	0
57	MG	1A	3498	1/1	0.99	0.06	8,8,8,8	0
57	MG	1A	3049	1/1	0.99	0.08	20,20,20,20	0
57	MG	1A	3412	1/1	0.99	0.07	8,8,8,8	0
57	MG	1a	1705	1/1	0.99	0.12	42,42,42,42	0
57	MG	1A	3524	1/1	0.99	0.02	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1F	306	1/1	0.99	0.08	19,19,19,19	0
57	MG	1F	307	1/1	0.99	0.09	17,17,17,17	0
57	MG	1F	308	1/1	0.99	0.10	17,17,17,17	0
57	MG	1A	3525	1/1	0.99	0.05	12,12,12,12	0
57	MG	2A	3165	1/1	0.99	0.15	28,28,28,28	0
57	MG	1A	3070	1/1	0.99	0.03	28,28,28,28	0
57	MG	1F	311	1/1	0.99	0.03	21,21,21,21	0
57	MG	2A	3603	1/1	0.99	0.05	29,29,29,29	0
58	ZN	1Y	501	1/1	0.99	0.03	51,51,51,51	0
57	MG	2A	3003	1/1	0.99	0.11	17,17,17,17	0
58	ZN	16	102	1/1	0.99	0.02	38,38,38,38	0
58	ZN	19	103	1/1	0.99	0.04	38,38,38,38	0
57	MG	2A	3536	1/1	0.99	0.04	52,52,52,52	0
57	MG	1A	3337	1/1	0.99	0.04	27,27,27,27	0
57	MG	1A	3273	1/1	0.99	0.24	24,24,24,24	0
58	ZN	26	102	1/1	0.99	0.03	56,56,56,56	0
58	ZN	29	102	1/1	0.99	0.03	58,58,58,58	0
57	MG	1A	3437	1/1	0.99	0.07	16,16,16,16	0
57	MG	2A	3115	1/1	0.99	0.04	32,32,32,32	0
57	MG	2A	3007	1/1	0.99	0.02	33,33,33,33	0
57	MG	1A	3484	1/1	1.00	0.03	10,10,10,10	0
58	ZN	25	102	1/1	1.00	0.04	51,51,51,51	0
58	ZN	15	105	1/1	1.00	0.03	24,24,24,24	0
57	MG	2A	3548	1/1	1.00	0.03	16,16,16,16	0
57	MG	1A	3172	1/1	1.00	0.05	9,9,9,9	0
57	MG	2A	3365	1/1	1.00	0.05	37,37,37,37	0
57	MG	1A	3433	1/1	1.00	0.04	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.