



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 11:38 AM EDT

PDB ID : 5HCQ / pdb_00005hcq
Title : Crystal structure of antimicrobial peptide Oncocin d15-19 bound to the *Thermus thermophilus* 70S ribosome
Authors : Gagnon, M.G.; Roy, R.N.; Lomakin, I.B.; Florin, T.; Mankin, A.S.; Steitz, T.A.
Deposited on : 2016-01-04
Resolution : 2.80 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

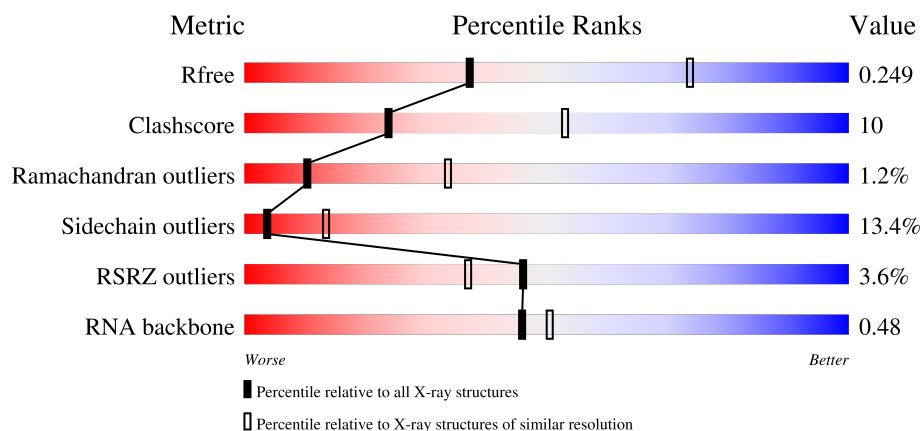
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



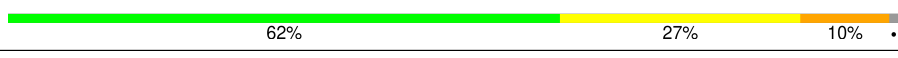
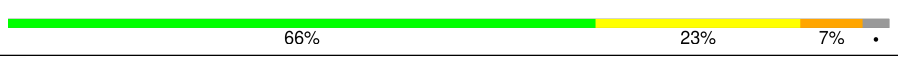
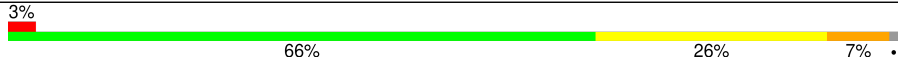
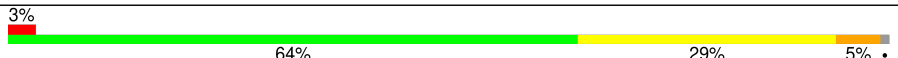
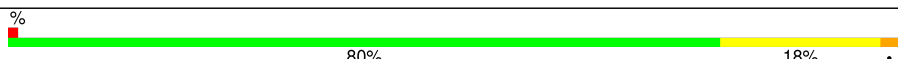
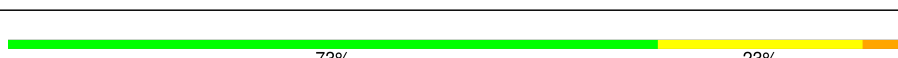
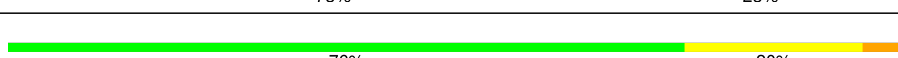
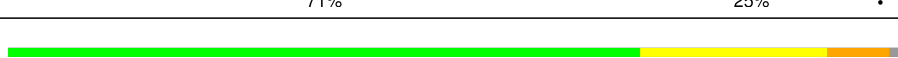
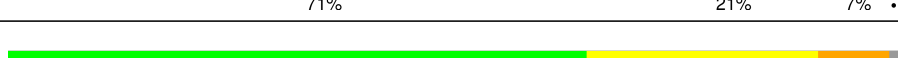
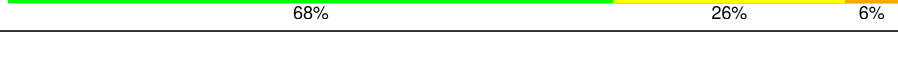
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	3% 64% 25% 5% 6%
1	2A	2915	54% 35% 7% .
2	1B	121	66% 31% ..
2	2B	121	3% 32% 49% 18% .

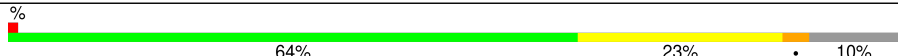
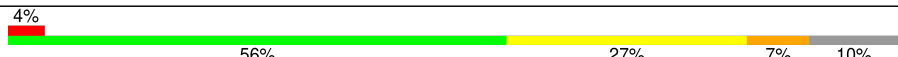
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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

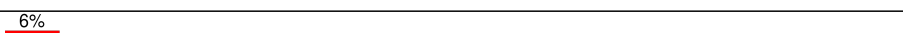
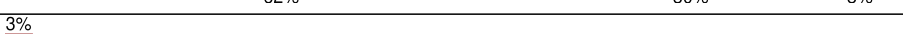
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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	

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Mol	Chain	Length	Quality of chain
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	
40	1i	128	

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Mol	Chain	Length	Quality of chain
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	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1x	77	
54	2x	77	
55	1z	14	
55	2z	14	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	1667	-	-	-	X
56	MG	2a	3034	-	-	-	X
56	MG	2a	3056	-	-	-	X
56	MG	2a	3220	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 288518 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	2746	Total	C	N	O	P	0	0	0
			59154	26327	11077	19005	2745			
1	2A	2790	Total	C	N	O	P	0	0	0
			60091	26746	11243	19313	2789			

- 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
			2572	1146	476	831	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			2142	1352	426	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
			1139	709	231	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
			750	488	135	126	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	186	Total	C	N	O	S	0	0	0
			1470	937	262	269	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1454	929	256	267	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			
22	20	75	Total	C	N	O	S	0	0	0
			598	370	127	100	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
			558	352	102	99	5			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1477	Total	C	N	O	P	0	0	0
			31750	14131	5883	10259	1477			
32	2a	1483	Total	C	N	O	P	0	0	0
			31877	14188	5905	10301	1483			

- 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
			1786	1136	321	325	4			
33	2b	231	Total	C	N	O	S	0	0	0
			1697	1079	292	321	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
			1480	932	281	266	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1412	883	269	259	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
			1618	1013	312	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1630	1022	321	280	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
			1095	695	203	193	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			817	516	146	152	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
			1183	732	232	213	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1167	728	220	213	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
			1074	681	202	189	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
			976	620	189	167			
40	2i	127	Total	C	N	O	0	0	0
			932	589	177	166			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			682	424	130	128			
41	2j	96	Total	C	N	O	0	0	0
			678	424	126	128			

- 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
			826	513	156	154	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			829	516	155	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
			920	579	181	159	1			
43	2l	122	Total	C	N	O	S	0	0	0
			918	576	182	159	1			

- 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	116	Total	C	N	O	S	0	0	0
			903	555	187	159	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
			482	306	100	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			459	291	93	71	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
			715	447	140	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
			671	424	133	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
			811	519	148	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	84	Total	C	N	O	S	0	0	0
			642	409	119	112	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
			712	435	152	123	2			
51	2t	96	Total	C	N	O	S	0	0	0
			731	449	156	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
			187	116	42	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			
53	2v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 54 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
54	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 55 is a protein called Oncocin d15-19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	12	Total	C	N	O	0	0	0
			101	67	19	15			
55	2z	12	Total	C	N	O	0	0	0
			101	67	19	15			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1051	Total	Mg	0	0
			1051	1051		
56	1B	26	Total	Mg	0	0
			26	26		
56	1D	17	Total	Mg	0	0
			17	17		
56	1E	10	Total	Mg	0	0
			10	10		
56	1F	7	Total	Mg	0	0
			7	7		
56	1G	3	Total	Mg	0	0
			3	3		
56	1H	4	Total	Mg	0	0
			4	4		
56	1N	8	Total	Mg	0	0
			8	8		
56	1O	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1P	5	Total 5	Mg 5	0	0
56	1Q	6	Total 6	Mg 6	0	0
56	1R	6	Total 6	Mg 6	0	0
56	1T	5	Total 5	Mg 5	0	0
56	1U	5	Total 5	Mg 5	0	0
56	1V	1	Total 1	Mg 1	0	0
56	1W	6	Total 6	Mg 6	0	0
56	1X	2	Total 2	Mg 2	0	0
56	1Y	1	Total 1	Mg 1	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	10	7	Total 7	Mg 7	0	0
56	11	1	Total 1	Mg 1	0	0
56	13	2	Total 2	Mg 2	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	4	Total 4	Mg 4	0	0
56	16	2	Total 2	Mg 2	0	0
56	17	4	Total 4	Mg 4	0	0
56	18	5	Total 5	Mg 5	0	0
56	19	3	Total 3	Mg 3	0	0
56	1a	306	Total 306	Mg 306	0	0
56	1b	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1c	1	Total 1	Mg 1	0	0
56	1d	2	Total 2	Mg 2	0	0
56	1e	4	Total 4	Mg 4	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1h	3	Total 3	Mg 3	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1l	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	1o	2	Total 2	Mg 2	0	0
56	1q	4	Total 4	Mg 4	0	0
56	1r	3	Total 3	Mg 3	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1x	11	Total 11	Mg 11	0	0
56	2A	583	Total 583	Mg 583	0	0
56	2B	10	Total 10	Mg 10	0	0
56	2D	4	Total 4	Mg 4	0	0
56	2E	7	Total 7	Mg 7	0	0
56	2F	2	Total 2	Mg 2	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	2O	3	Total 3	Mg 3	0	0

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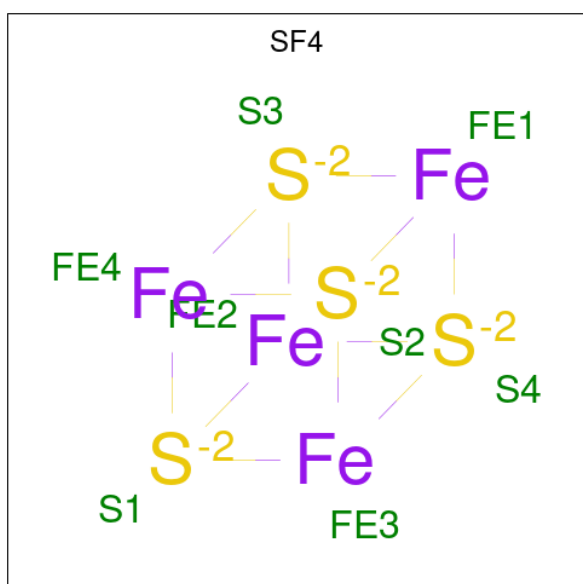
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2P	1	Total 1	Mg 1	0	0
56	2Q	5	Total 5	Mg 5	0	0
56	2R	1	Total 1	Mg 1	0	0
56	2U	2	Total 2	Mg 2	0	0
56	2V	1	Total 1	Mg 1	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	20	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	26	1	Total 1	Mg 1	0	0
56	28	1	Total 1	Mg 1	0	0
56	2a	244	Total 244	Mg 244	0	0
56	2d	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2k	2	Total 2	Mg 2	0	0
56	2l	3	Total 3	Mg 3	0	0
56	2n	2	Total 2	Mg 2	0	0
56	2p	1	Total 1	Mg 1	0	0
56	2q	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2x	6	Total 6	Mg 6	0	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		
57	14	1	Total	Zn	0	0
			1	1		
57	15	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		
57	19	1	Total	Zn	0	0
			1	1		
57	1n	1	Total	Zn	0	0
			1	1		
57	2Y	1	Total	Zn	0	0
			1	1		
57	24	1	Total	Zn	0	0
			1	1		
57	25	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total	Fe	S	0	0
			8	4	4		
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	2110	Total	O	0	0
			2110	2110		
59	1B	42	Total	O	0	0
			42	42		
59	1D	24	Total	O	0	0
			24	24		
59	1E	30	Total	O	0	0
			30	30		
59	1F	16	Total	O	0	0
			16	16		
59	1G	6	Total	O	0	0
			6	6		
59	1H	3	Total	O	0	0
			3	3		
59	1I	1	Total	O	0	0
			1	1		
59	1N	7	Total	O	0	0
			7	7		
59	1O	4	Total	O	0	0
			4	4		
59	1P	21	Total	O	0	0
			21	21		
59	1Q	11	Total	O	0	0
			11	11		
59	1R	16	Total	O	0	0
			16	16		
59	1S	2	Total	O	0	0
			2	2		
59	1T	7	Total	O	0	0
			7	7		
59	1U	14	Total	O	0	0
			14	14		
59	1V	4	Total	O	0	0
			4	4		
59	1W	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1X	4	Total 4	O 4	0	0
59	1Y	1	Total 1	O 1	0	0
59	1Z	4	Total 4	O 4	0	0
59	10	8	Total 8	O 8	0	0
59	11	7	Total 7	O 7	0	0
59	12	2	Total 2	O 2	0	0
59	13	4	Total 4	O 4	0	0
59	15	7	Total 7	O 7	0	0
59	16	5	Total 5	O 5	0	0
59	17	8	Total 8	O 8	0	0
59	18	9	Total 9	O 9	0	0
59	19	4	Total 4	O 4	0	0
59	1a	393	Total 393	O 393	0	0
59	1b	1	Total 1	O 1	0	0
59	1c	1	Total 1	O 1	0	0
59	1d	5	Total 5	O 5	0	0
59	1e	3	Total 3	O 3	0	0
59	1f	1	Total 1	O 1	0	0
59	1h	3	Total 3	O 3	0	0
59	1i	1	Total 1	O 1	0	0
59	1j	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1k	1	Total 1	O 1	0	0
59	1l	3	Total 3	O 3	0	0
59	1m	1	Total 1	O 1	0	0
59	1o	1	Total 1	O 1	0	0
59	1p	1	Total 1	O 1	0	0
59	1q	1	Total 1	O 1	0	0
59	1s	1	Total 1	O 1	0	0
59	1v	1	Total 1	O 1	0	0
59	1x	8	Total 8	O 8	0	0
59	1z	1	Total 1	O 1	0	0
59	2A	813	Total 813	O 813	0	0
59	2B	10	Total 10	O 10	0	0
59	2D	16	Total 16	O 16	0	0
59	2E	9	Total 9	O 9	0	0
59	2F	5	Total 5	O 5	0	0
59	2N	1	Total 1	O 1	0	0
59	2O	3	Total 3	O 3	0	0
59	2P	9	Total 9	O 9	0	0
59	2Q	2	Total 2	O 2	0	0
59	2R	3	Total 3	O 3	0	0
59	2T	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2U	3	Total 3	O 3	0	0
59	2W	1	Total 1	O 1	0	0
59	2X	2	Total 2	O 2	0	0
59	2Y	1	Total 1	O 1	0	0
59	2Z	4	Total 4	O 4	0	0
59	20	3	Total 3	O 3	0	0
59	21	1	Total 1	O 1	0	0
59	23	2	Total 2	O 2	0	0
59	26	1	Total 1	O 1	0	0
59	27	2	Total 2	O 2	0	0
59	28	2	Total 2	O 2	0	0
59	2a	321	Total 321	O 321	0	0
59	2d	1	Total 1	O 1	0	0
59	2e	1	Total 1	O 1	0	0
59	2i	2	Total 2	O 2	0	0
59	2j	1	Total 1	O 1	0	0
59	2l	1	Total 1	O 1	0	0
59	2m	3	Total 3	O 3	0	0
59	2p	1	Total 1	O 1	0	0
59	2q	1	Total 1	O 1	0	0
59	2t	4	Total 4	O 4	0	0

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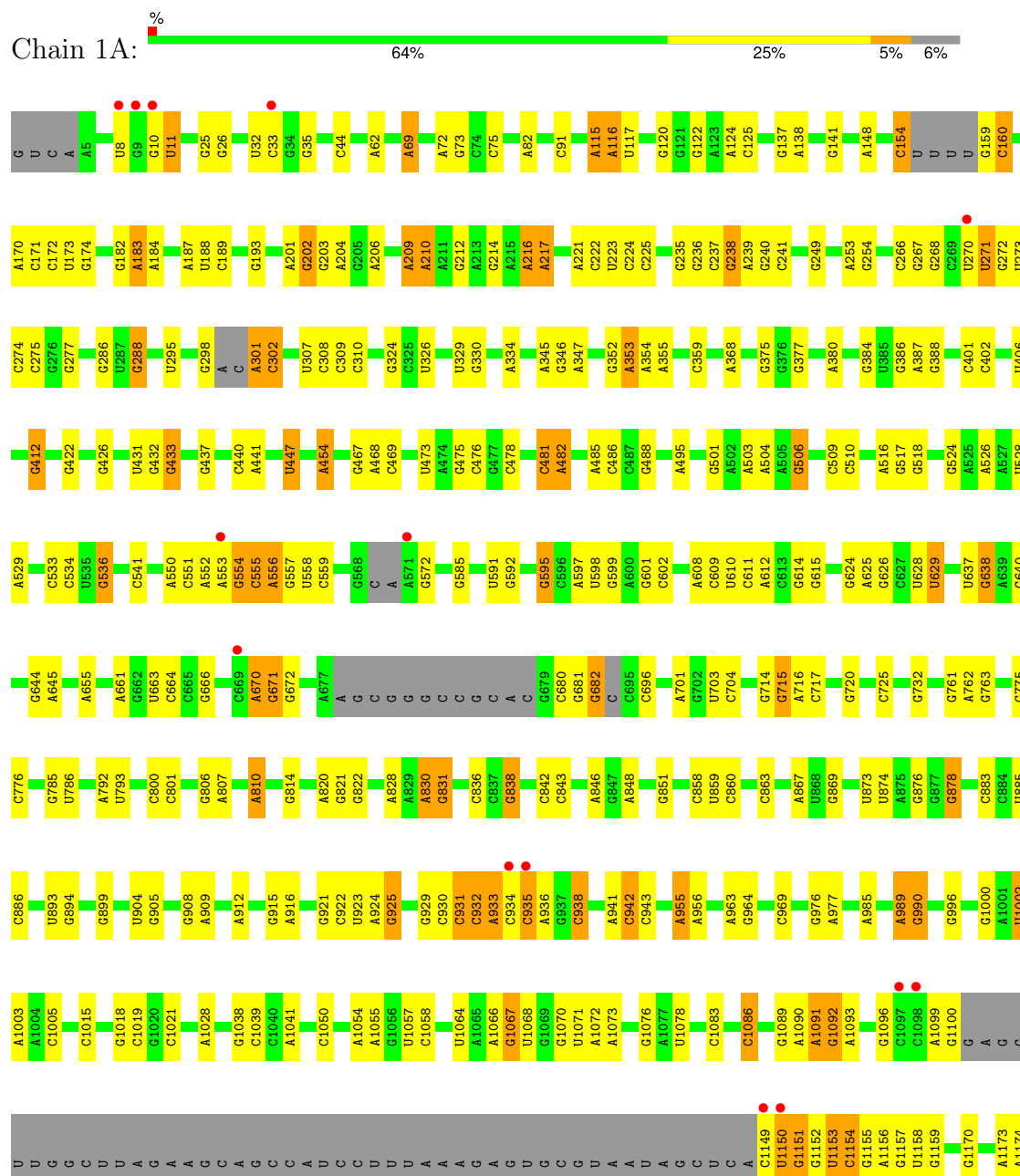
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2x	7	Total	O	0	0
			7	7		
59	2z	1	Total	O	0	0
			1	1		

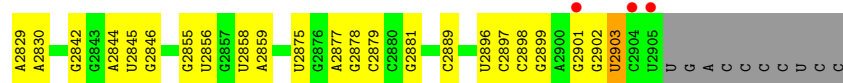
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

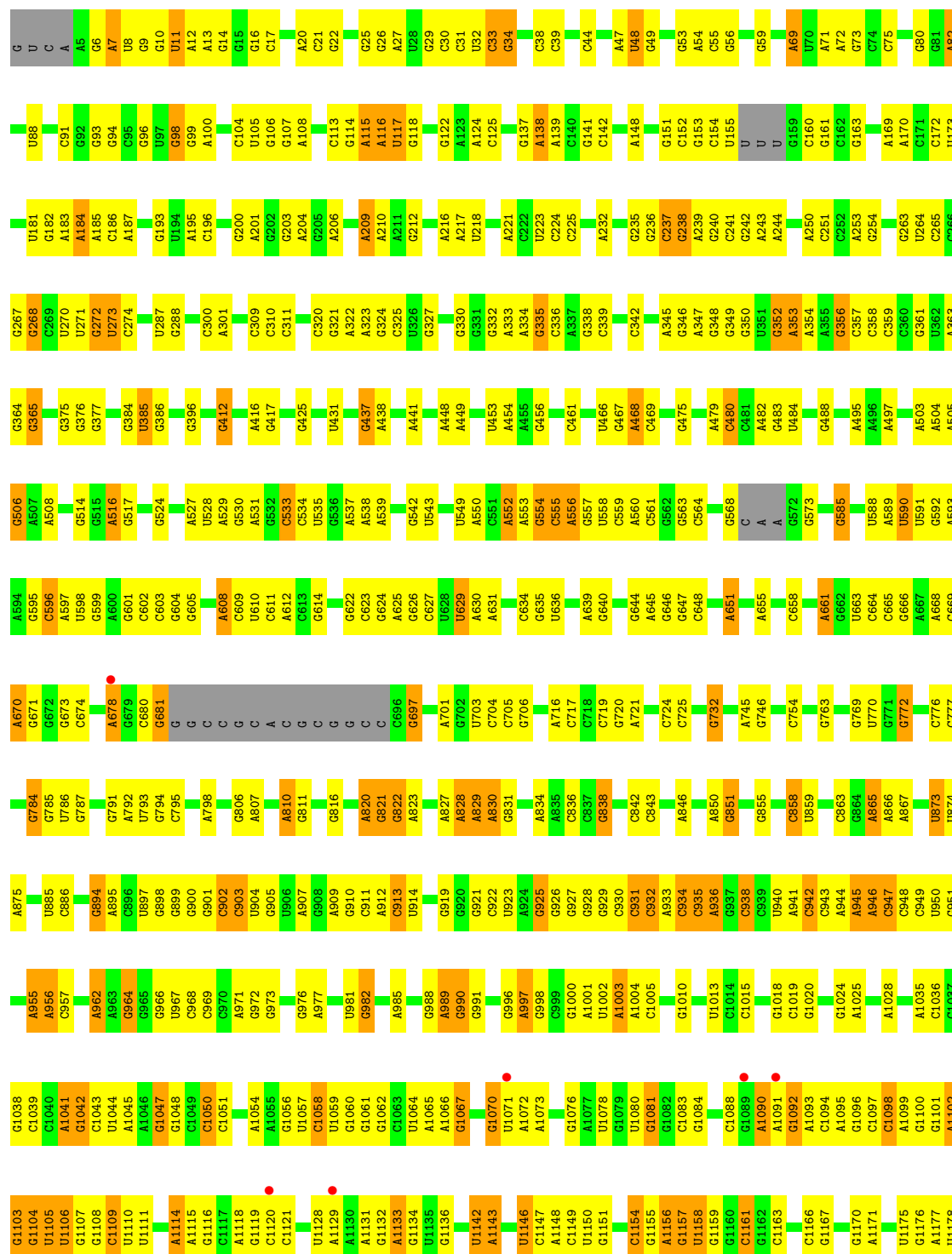
• Molecule 1: 23S Ribosomal RNA



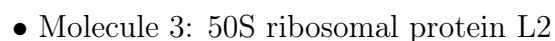
G2734	G2465	G2348	U2244	G	G2101	U1976	G1841	A1715	C1543				C1302	U1175
C2735	G2466	C2354	G2245	G	U2107	U1984	G1844	C1716	A1552	A1429			C1303	G1176
U2738	G2479	U2355	G2246	G	G2108	G1985	A1845	G1720	A1553	G1430			G1311	C1179
A2600	G2485	A2357	G2250	G	G2115	C1986	G1846	U1726	C1554	A1440			U1312	G1190
A2613	C2486	C2358	C2251	G	C2116	A1987	G1847		A1555	A1441			A1313	
A2745	U2487	U2359	A2252	A	U2117	C1988	G1858	C1732	U1565	U1450			G1316	G1183
A2753	C2488	C2360	G2253	A	G2121	C1989	A1859	G1733	G1566	U1451			A1317	C1184
C2621	A2489	C2361	U2254	G	U2122	A1990	C1868	U1734	U1570	U1452			U1318	G1186
U2622	G2493	G2364	U2255	C	U2123	A1992	G1869	A1735	G1570	C1453			A1187	
C2623	C2494	G2365	C2275	G	C2124	A1993	G1873	U1739	A1573	G1461			A1323	A1188
C2628		C2366		C	G					C1462				G1189
U2768	A2499	G2376	A2279	G	C	A2007	C1877	G1743	C1578	U1337			U1337	
A2770	U2502	G2388	A2280	G	C	G2013	A1877	A1744	G	C1338			C1338	C1198
C2771	U2502	A2389	G2281	U	C	U2014	G1888	A1746	A	U1345			U1345	G1199
C2772	C2509	G2390	U2283	G	C	U	A1889	A1747	C	G1466			A1346	A1200
G2773			A2284	A	G	G2018			G1583	G1467			A1347	
	G2513	G2394	A2285	A	C	G2019	A1897	G1763		C1473			G1348	G1209
A2776	A2514	G2395	C2286	U	C	G2020	A1898	U1764	A1588	G1474			G1354	U1210
G2778	G2515	G2396	G2287	A	U	G2021	A1899	G1765	C1589	U1476			G1355	C1211
	U2516	C2397	U2288	C	A	A2022	C1900	A1766	A1590	C1477				G1215
G2649	G2517	U2398	G2289	C	G	G2023	G1904	U1767	A1591	U1478			G1359	G1216
A2650		A2399	G2290	A	G	G2024		G1768	C1592	A1479			C1360	A1218
G2651	C2529	G2400	C2294	C	A									U1219
C2657	G2536	U2401	A2297	C	U	A2034	A1910	G1777	C1603	C1482			A1366	G1220
U2791			A2298	U	C	A2035		G1778	A1604				G1377	A1221
C2659	G2540	C2415	A2299	C	G	A2036	U1919		A1612	A1490			C1378	C1223
U2660		G2416	G2300	G	U	U2043	G1920	A1784	A1613	G1496			C1379	C1224
	A2544	U2417	U2302	G	G	G2044	A1921	G1786	A1614					
A2545		G2418	G2301	G	G		G1924		A1615	U1500			A1387	C1229
G2670		G2421	C2303	A	A	A2052	G1925	A1792	A1616	G1501			G1388	G1230
	G2554	C2428	U2307	C	G	G2053	G1926	G1793	A1617	G1389			G1231	G1231
U2694	G2555	A2429		C	C	A2054	G1927	G1794		G1507			G1390	U1232
U2695		U2430		U	C	C2060	G1928		U1624				G1391	
	G2560	G2315	G2307	C	U		C1929	A1803	A1625	C1513				G1285
C2800	G2561	A2316	G2315	U	U	A2063	A1934	A1810	A1626	C1514			U1397	
A2802	U2699	A2433	G2316	G	G	C2064	C1935	G1811	G1627				A1398	C1245
C2803	U2700	U2434	U2323	U	U	U1936	U1936	C1812		A1517			A1399	G1246
G2805	G2563	C2435		G	G		A1939	A1813	C1630	C1520			G1400	G1247
C2702	U2565	A2436	G2330	A	A	C2076	A1940		A1631	G1521			U1402	A1248
C2703	U2566		A2331	C	C	G2077	A1941	A1821	C1632	U1403			A1254	
A2704	A2575	G2440	A2332	C	C	A2081	A1942		C1633	G1403			G1262	
G2705	A2576	U2441	A2333	C	C	G2082	C1941		C1634	A1404			A1405	
	A2577	U2442	G2334	C	C	A2083	A1948	U1826	C1652	G1528			G1263	
U2713	C2576	A2443	C2335	C	C		A1949	C1827	A1653				A1264	
C2714	C2579	A2446	G2336	G	G	C2086	G1950	U1828	A1654	A1531			G1409	
			C2337	C	C	C2087	U1952		A1655	G1532			A1410	
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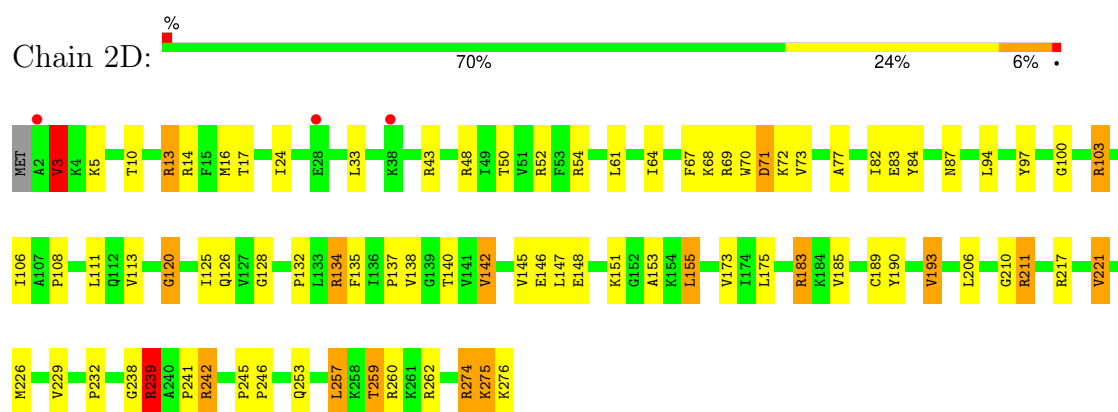


• Molecule 1: 23S Ribosomal RNA

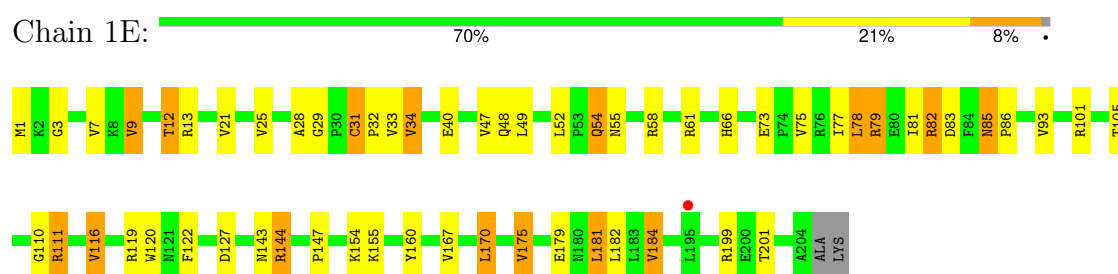


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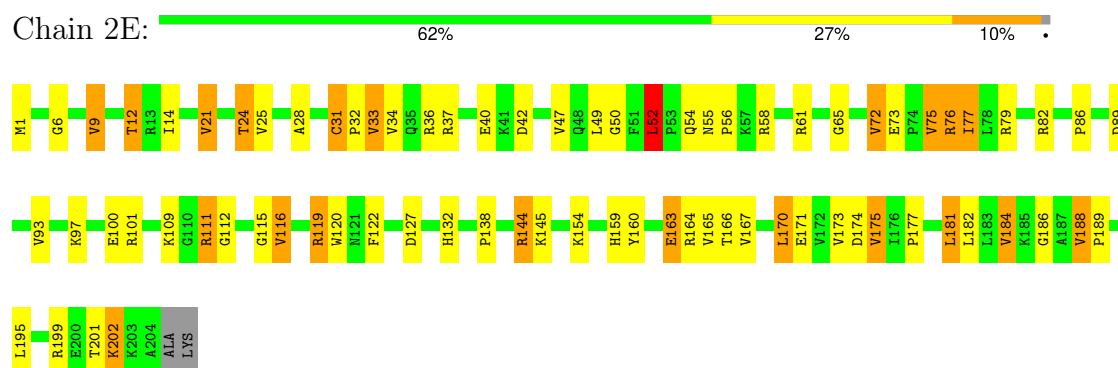




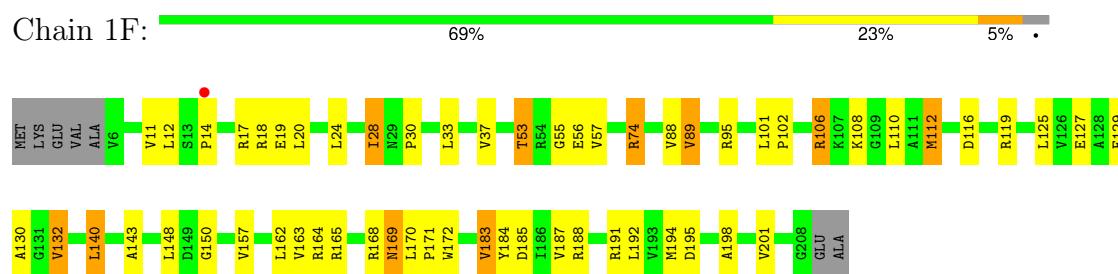
• Molecule 4: 50S ribosomal protein L3



• Molecule 4: 50S ribosomal protein L3

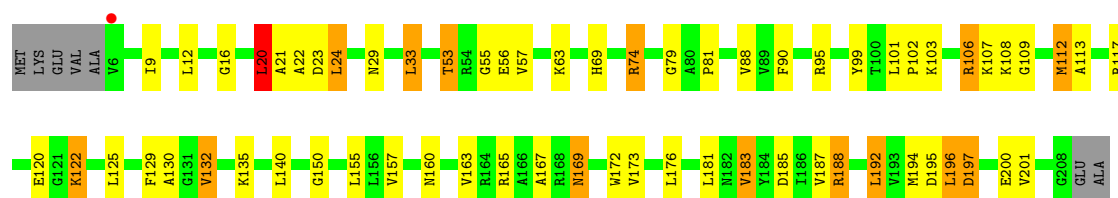


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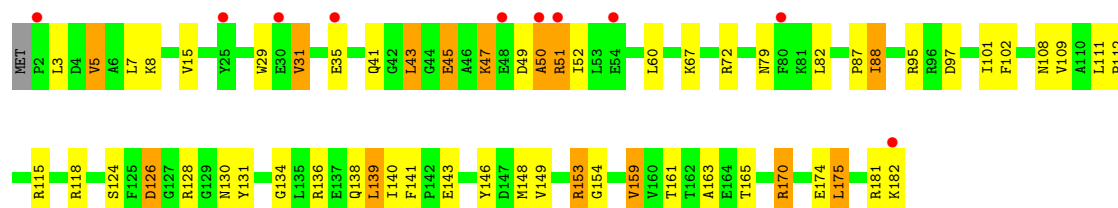


• Molecule 5: 50S ribosomal protein L4

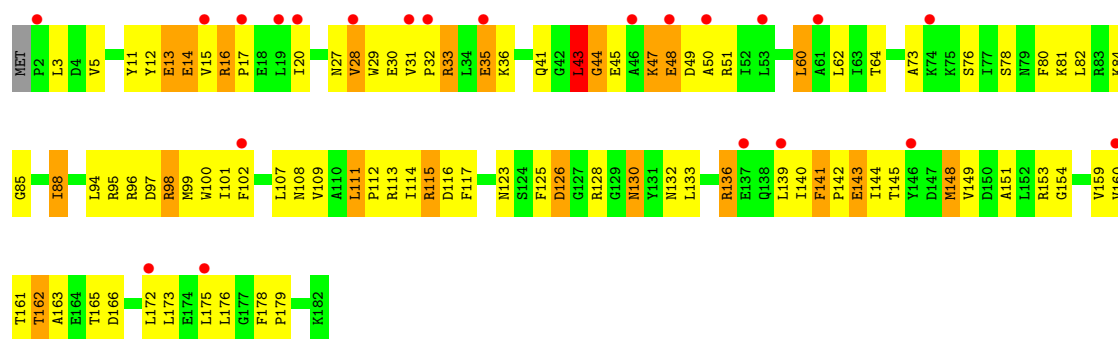




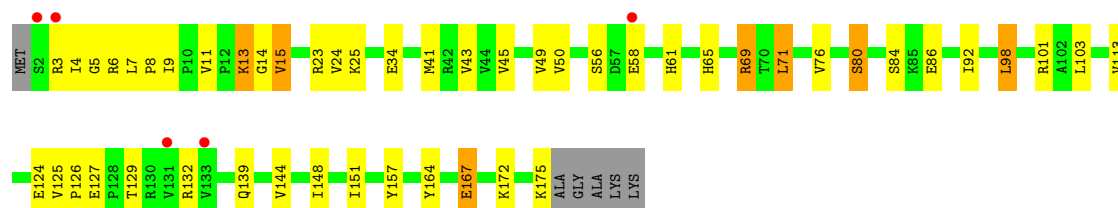
• Molecule 6: 50S ribosomal protein L5



• Molecule 6: 50S ribosomal protein L5

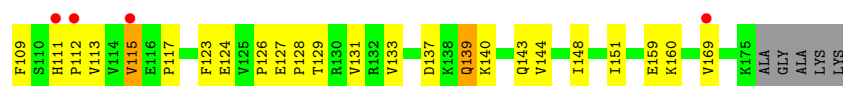


• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6





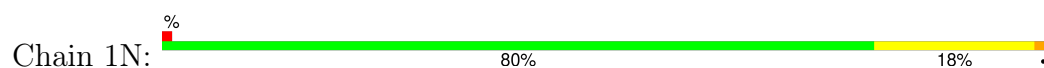
- Molecule 8: 50S ribosomal protein L9



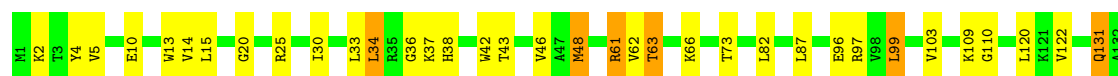
- Molecule 8: 50S ribosomal protein L9



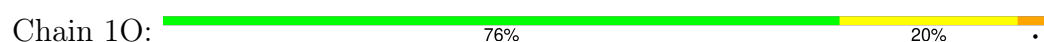
- Molecule 9: 50S ribosomal protein L13



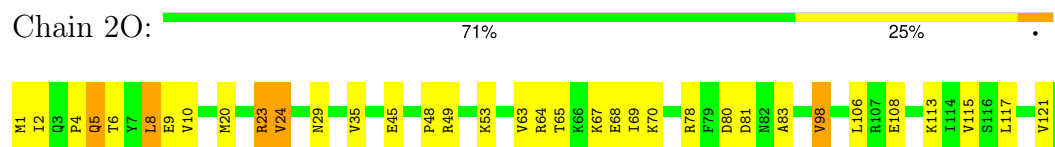
- Molecule 9: 50S ribosomal protein L13



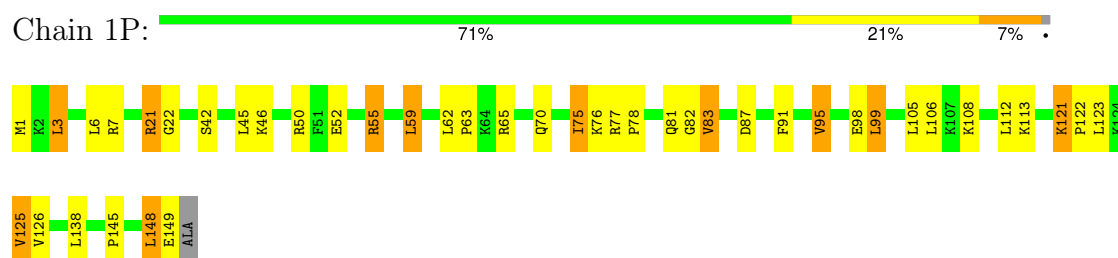
- Molecule 10: 50S ribosomal protein L14



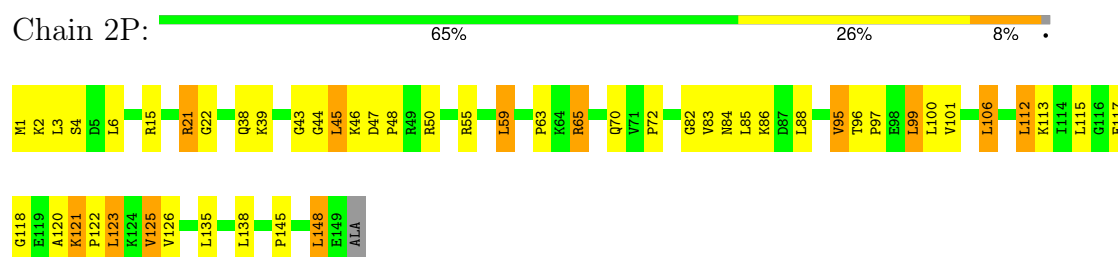
- Molecule 10: 50S ribosomal protein L14



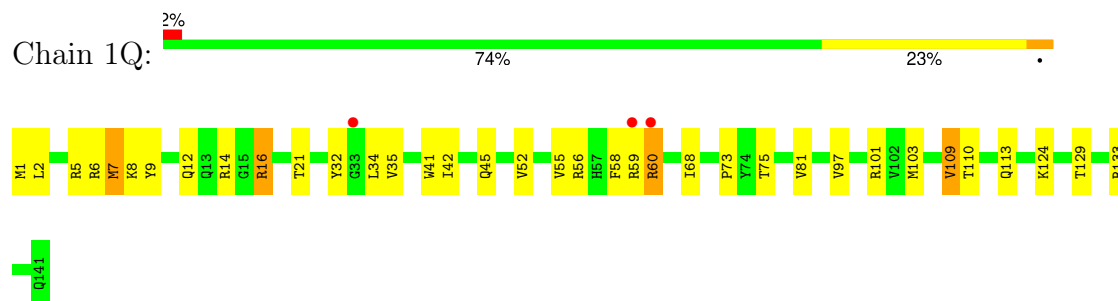
- Molecule 11: 50S ribosomal protein L15



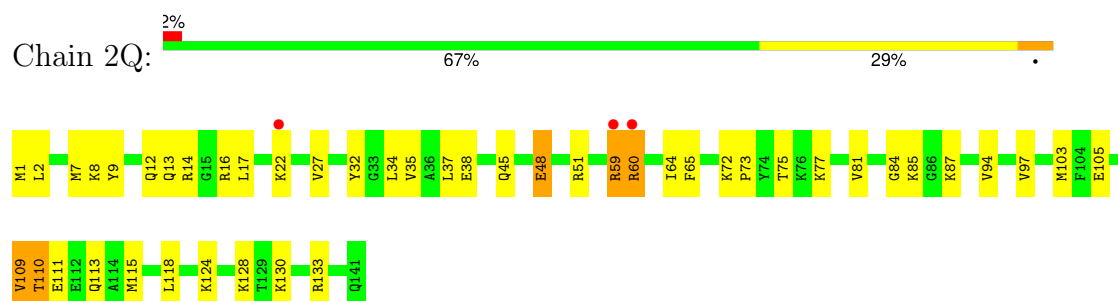
- Molecule 11: 50S ribosomal protein L15



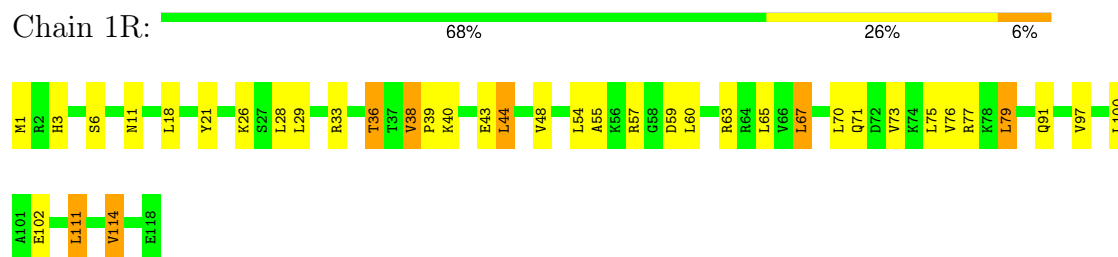
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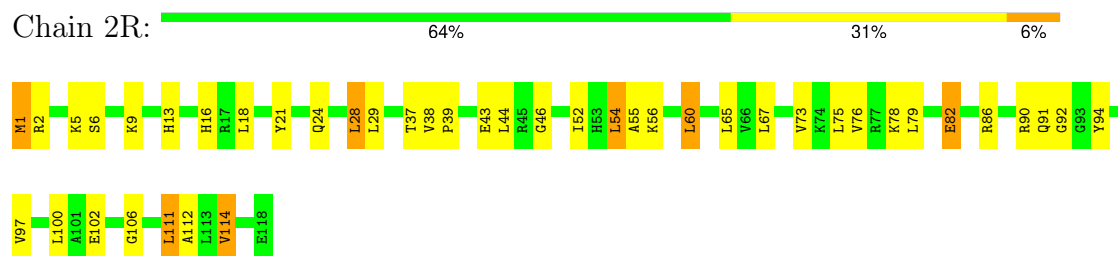
- Molecule 12: 50S ribosomal protein L16



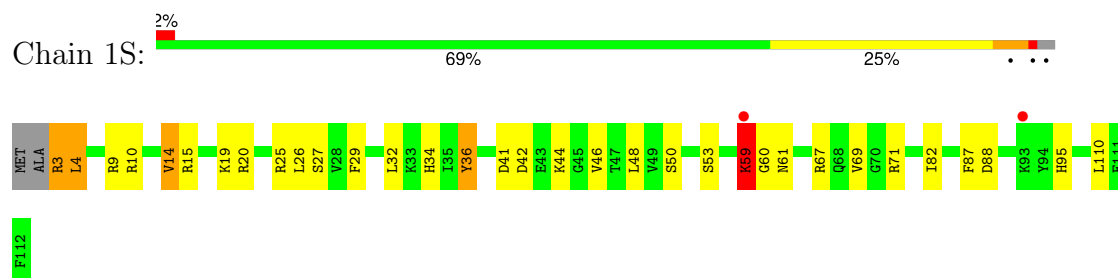
- Molecule 13: 50S ribosomal protein L17



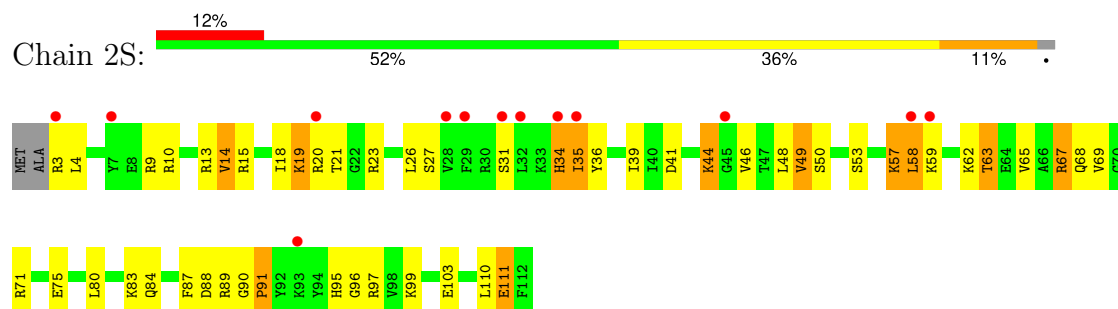
- Molecule 13: 50S ribosomal protein L17



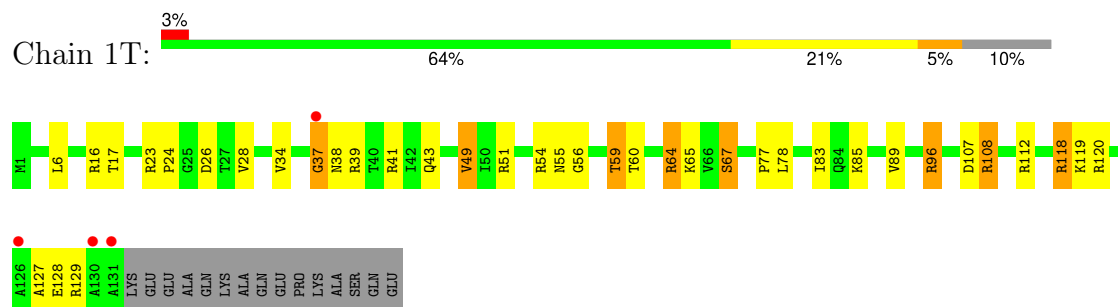
- Molecule 14: 50S ribosomal protein L18



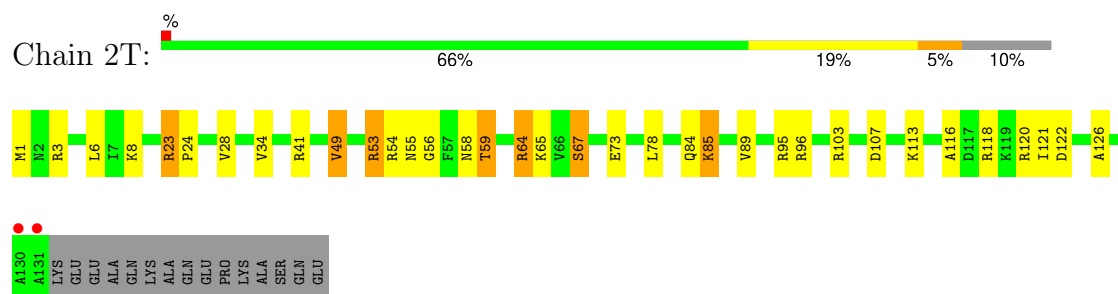
- Molecule 14: 50S ribosomal protein L18



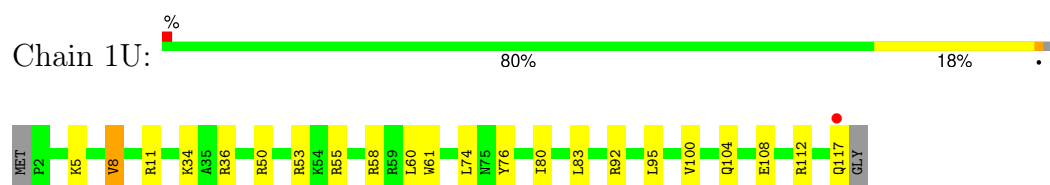
- Molecule 15: 50S ribosomal protein L19



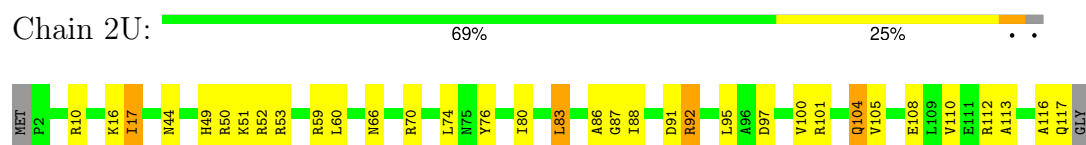
- Molecule 15: 50S ribosomal protein L19



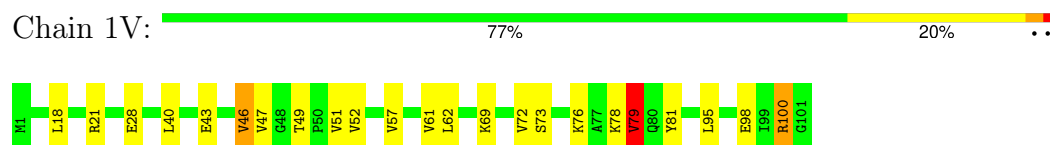
- Molecule 16: 50S ribosomal protein L20



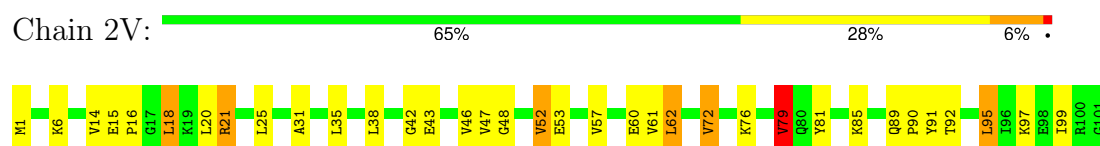
- Molecule 16: 50S ribosomal protein L20



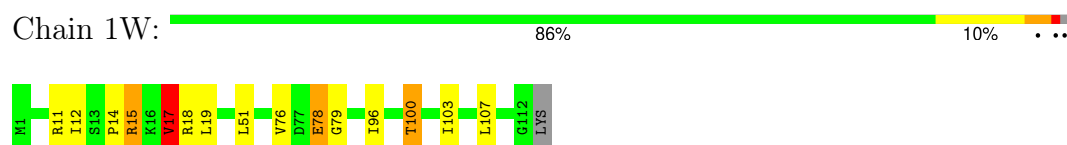
- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22

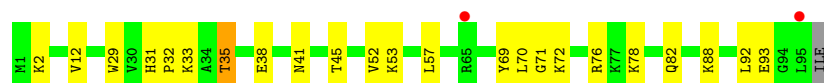
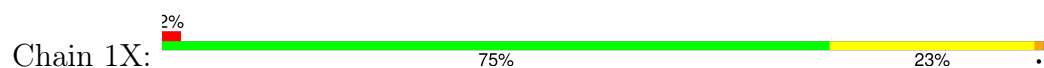


- Molecule 18: 50S ribosomal protein L22





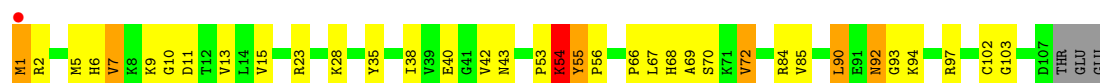
- Molecule 19: 50S ribosomal protein L23



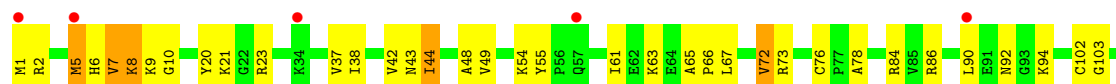
- Molecule 19: 50S ribosomal protein L23



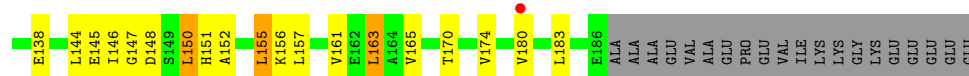
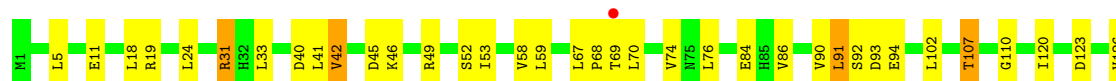
- Molecule 20: 50S ribosomal protein L24



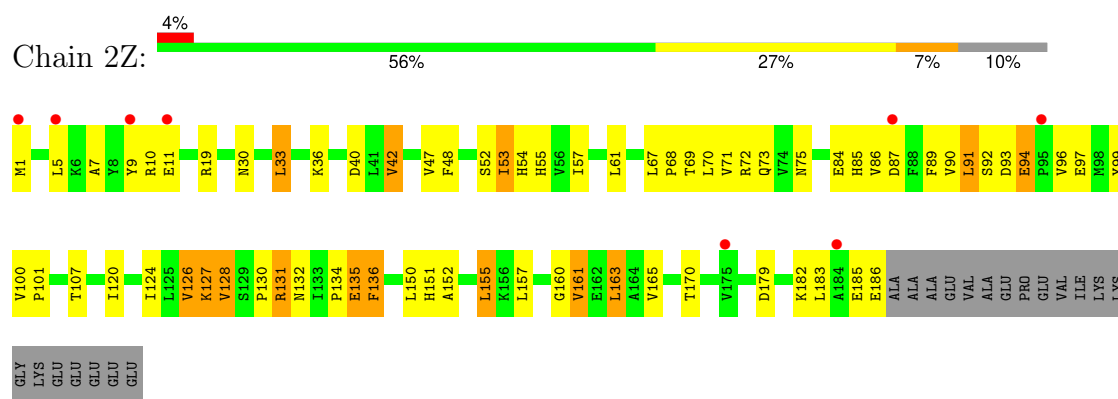
- Molecule 20: 50S ribosomal protein L24

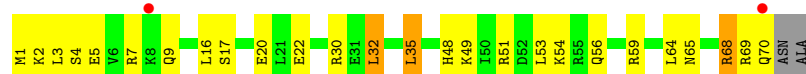


- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25

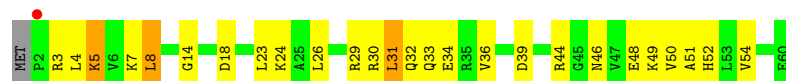




- Molecule 25: 50S ribosomal protein L30



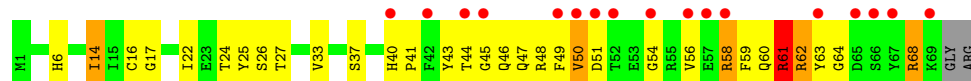
- Molecule 25: 50S ribosomal protein L30



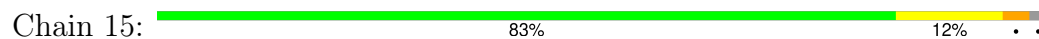
- Molecule 26: 50S ribosomal protein L31



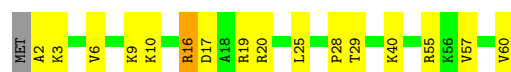
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

Chain 16:  74% 22% ..



- Molecule 28: 50S ribosomal protein L33

Chain 26:  69% 26% ..



- Molecule 29: 50S ribosomal protein L34

Chain 17:  4% 71% 22% ..



- Molecule 29: 50S ribosomal protein L34

Chain 27:  4% 61% 35% ..



- Molecule 30: 50S ribosomal protein L35

Chain 18:  68% 28% ..



- Molecule 30: 50S ribosomal protein L35

Chain 28:  55% 40% ..



- Molecule 31: 50S ribosomal protein L36

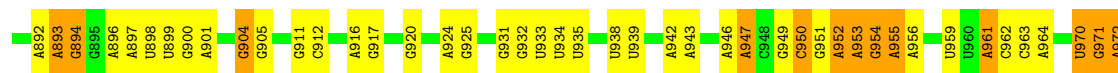
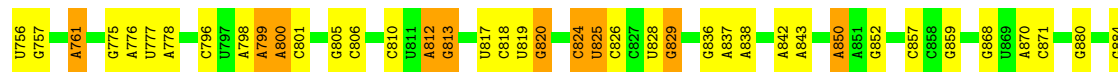
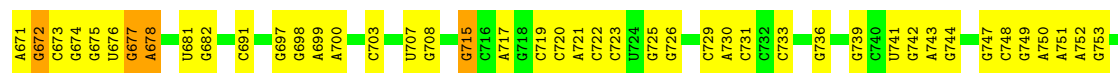
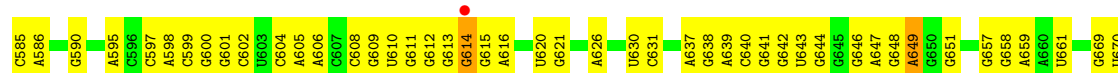
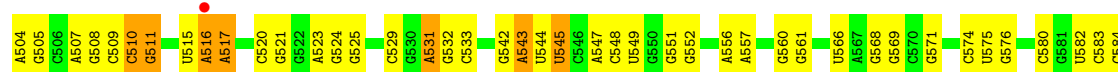
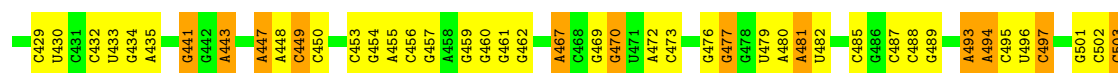
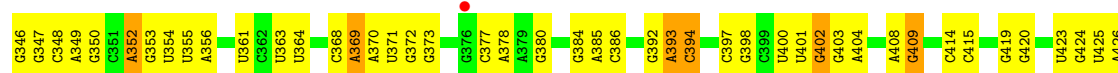
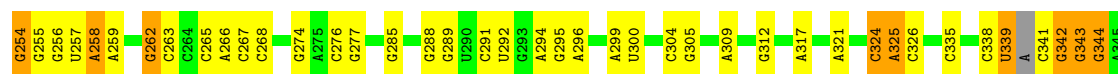
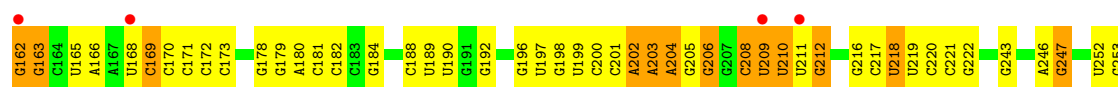
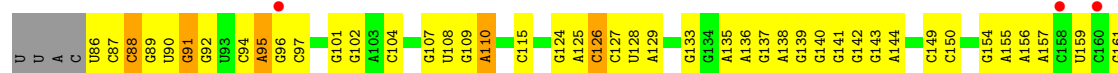
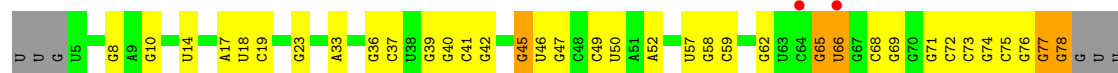
Chain 19:  5% 78% 19% .



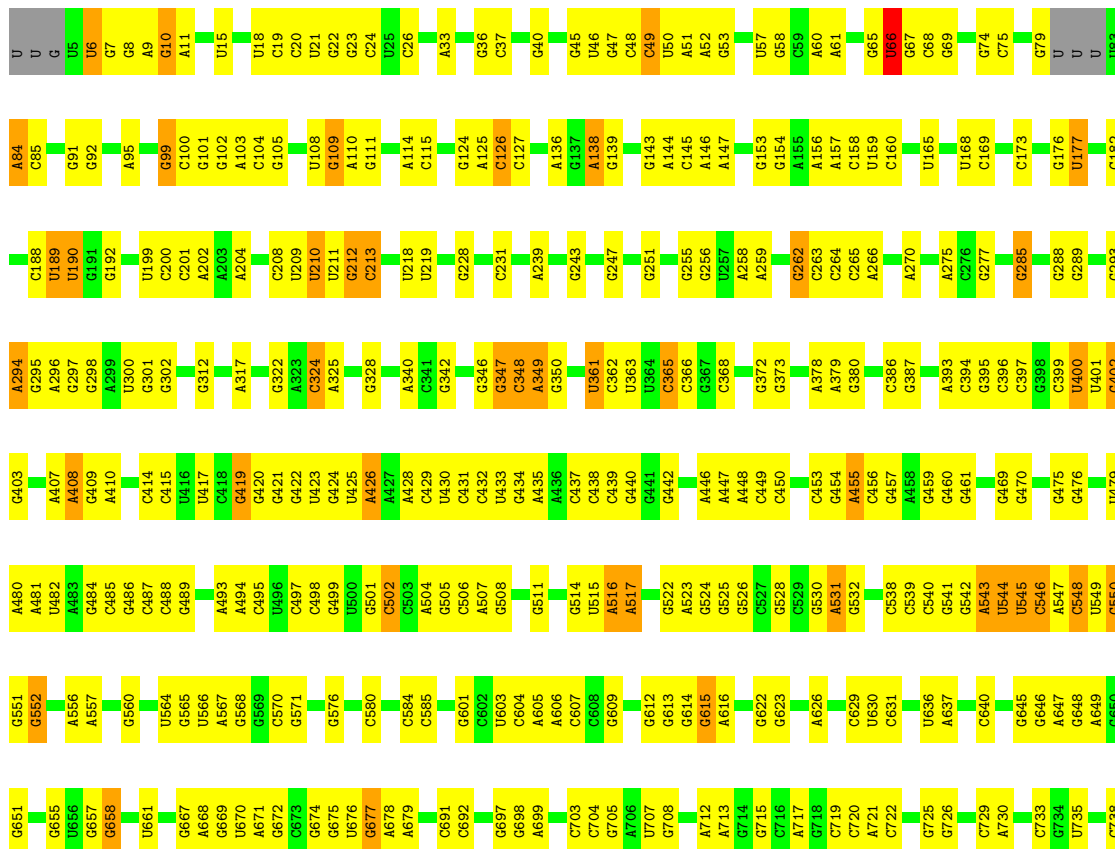
- Molecule 31: 50S ribosomal protein L36

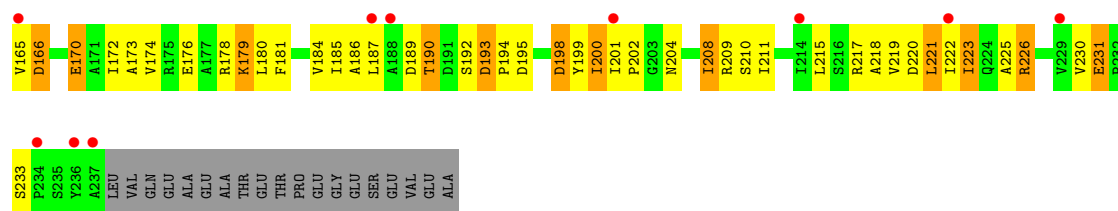


• Molecule 32: 16S Ribosomal RNA

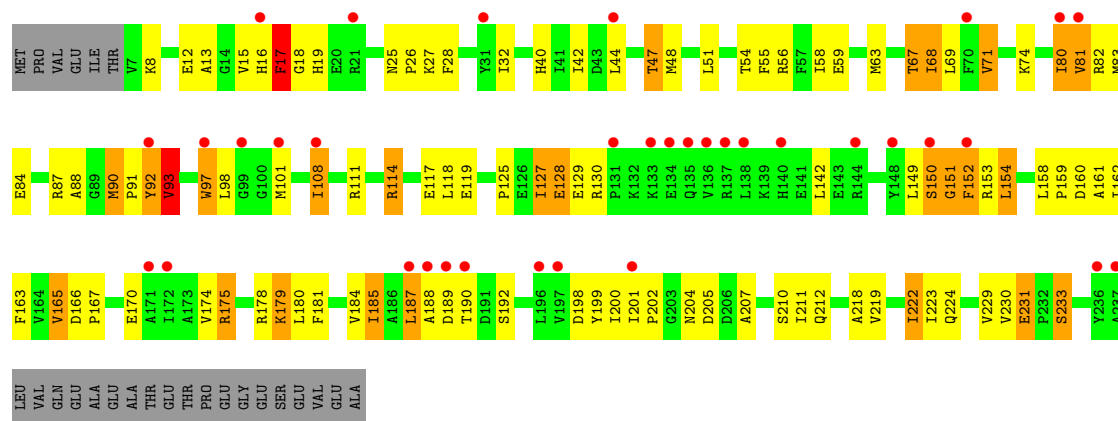


- Molecule 32: 16S Ribosomal RNA

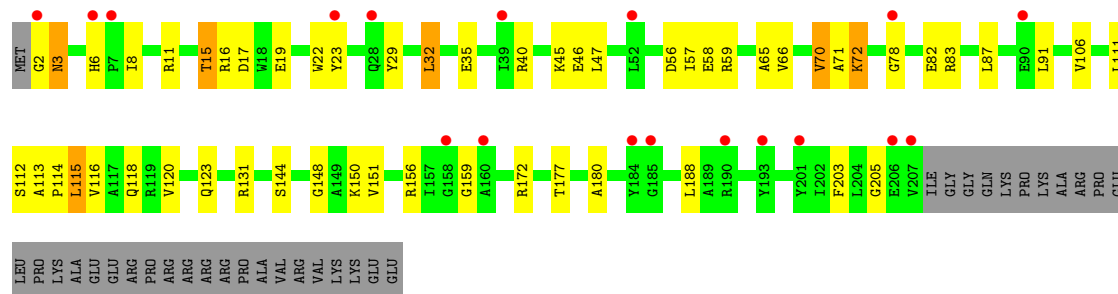




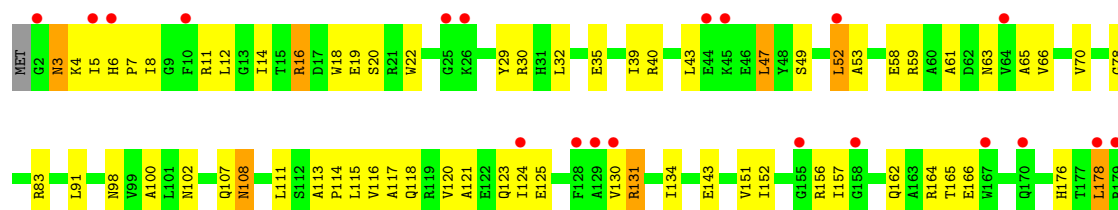
• Molecule 33: 30S ribosomal protein S2

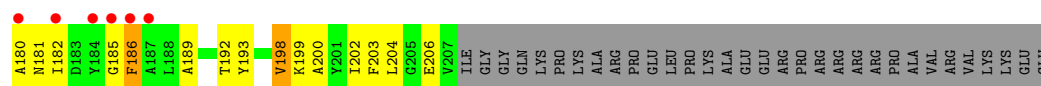


• Molecule 34: 30S ribosomal protein S3

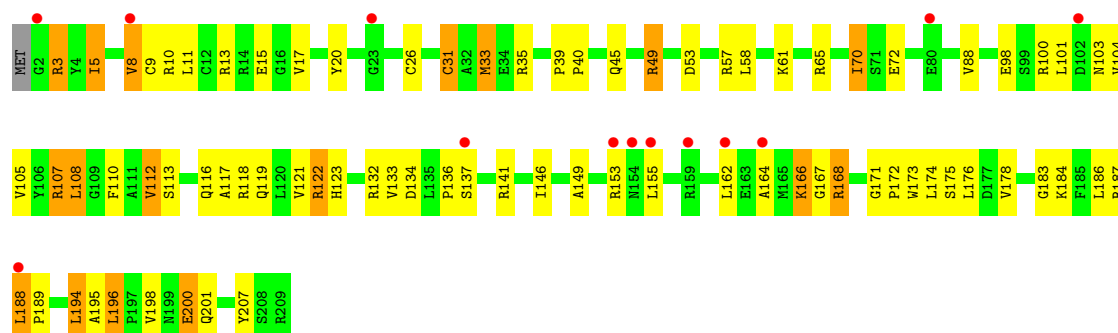


• Molecule 34: 30S ribosomal protein S3

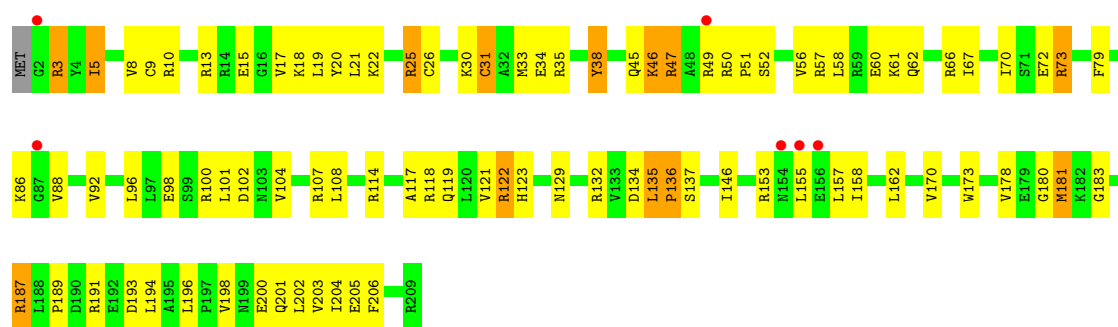




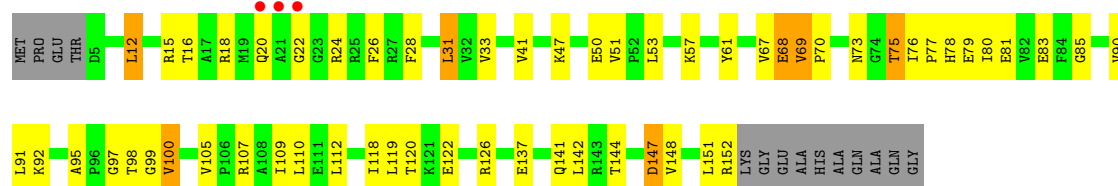
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

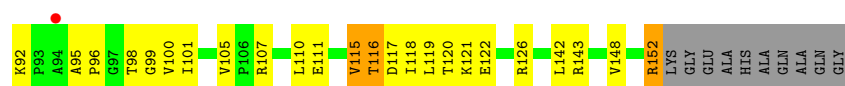


• Molecule 36: 30S ribosomal protein S5

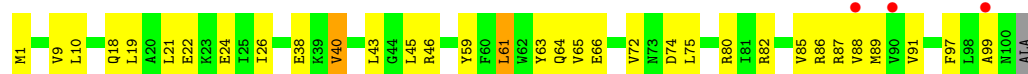


• Molecule 36: 30S ribosomal protein S5

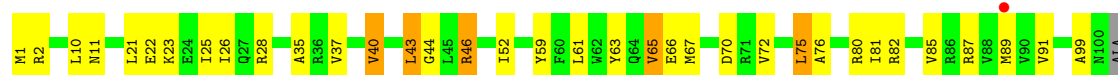




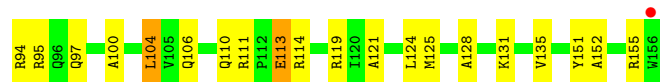
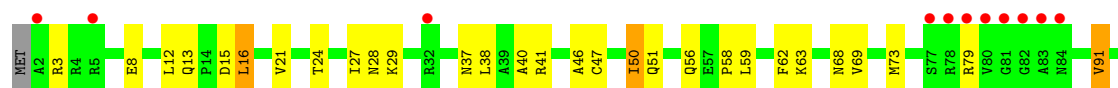
- Molecule 37: 30S ribosomal protein S6



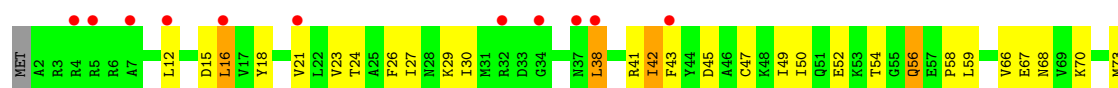
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



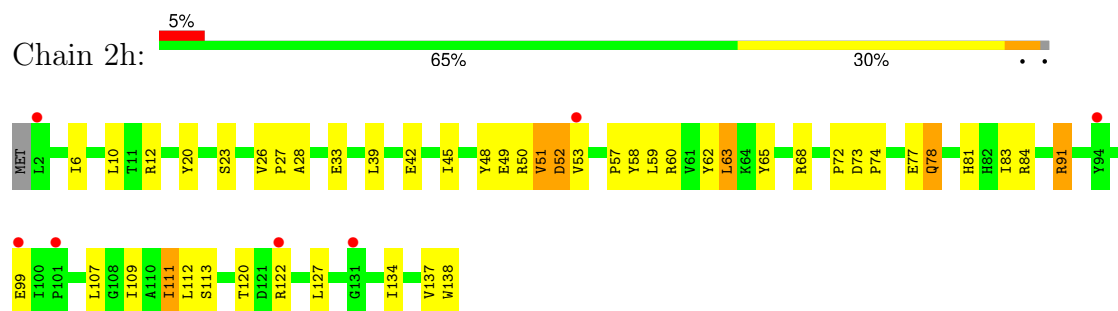
- Molecule 38: 30S ribosomal protein S7



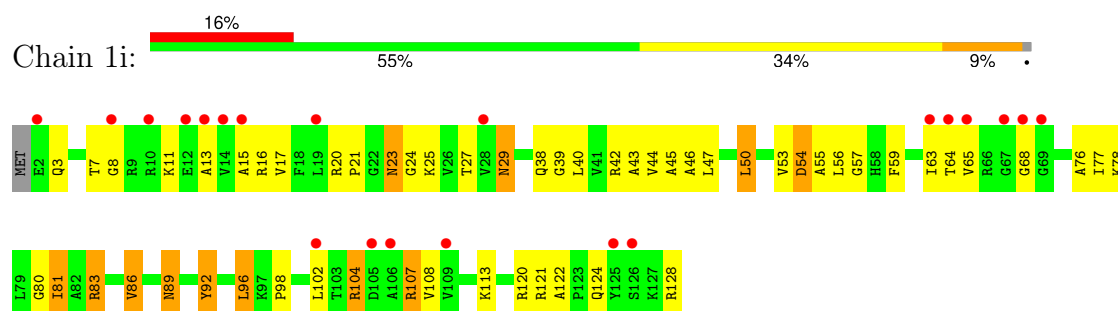
- Molecule 39: 30S ribosomal protein S8



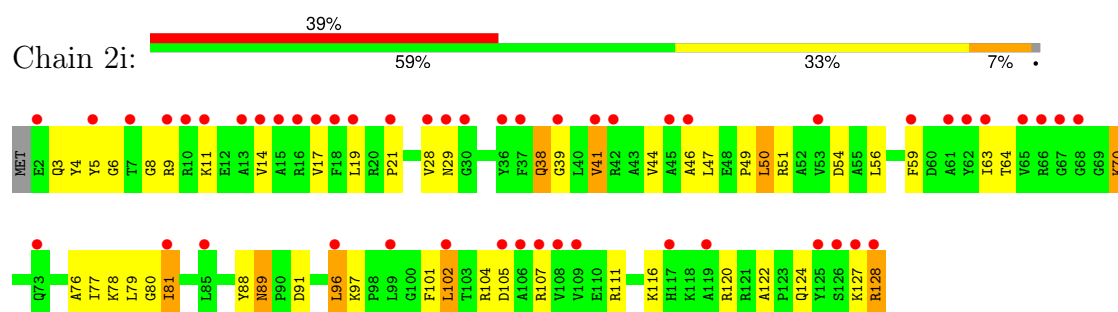
- Molecule 39: 30S ribosomal protein S8



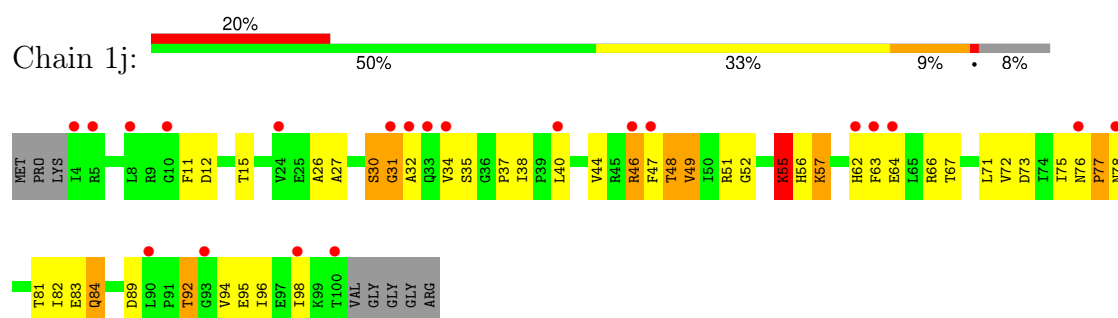
- Molecule 40: 30S ribosomal protein S9



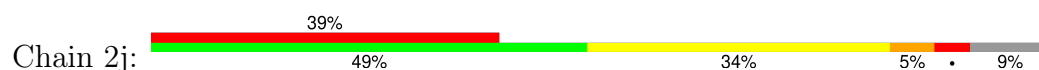
- Molecule 40: 30S ribosomal protein S9

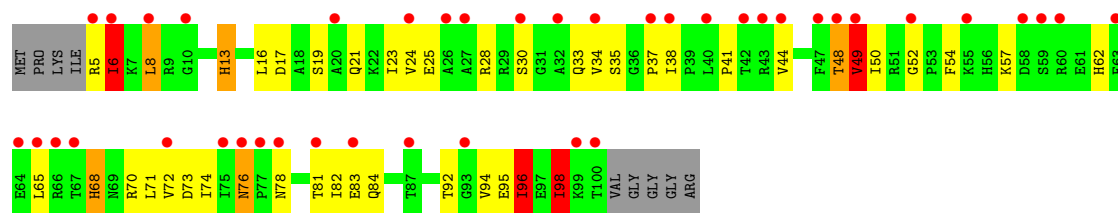


- Molecule 41: 30S ribosomal protein S10

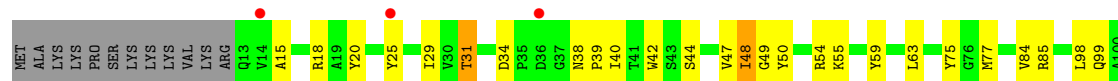


- Molecule 41: 30S ribosomal protein S10

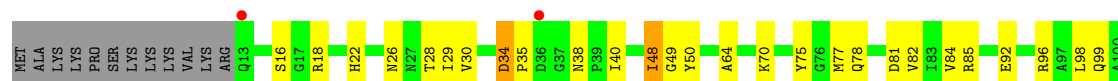




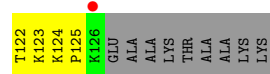
• Molecule 42: 30S ribosomal protein S11



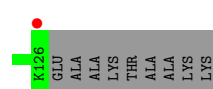
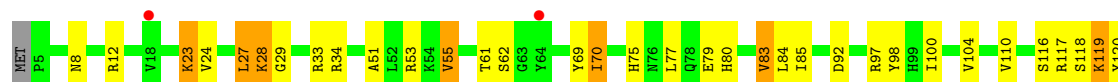
• Molecule 42: 30S ribosomal protein S11



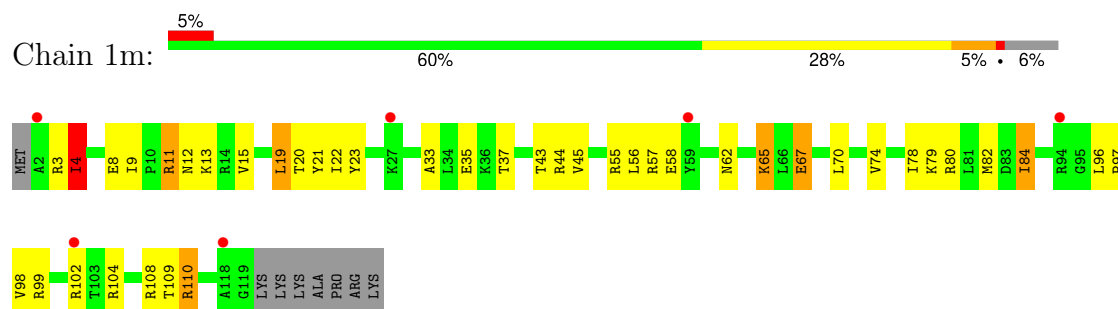
• Molecule 43: 30S ribosomal protein S12



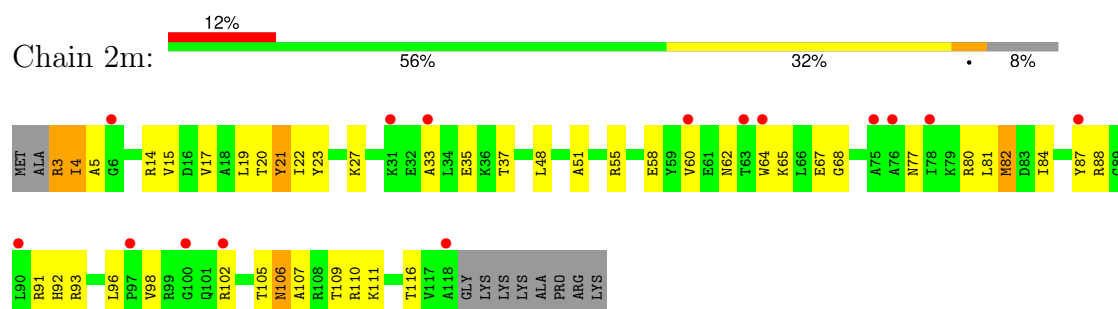
• Molecule 43: 30S ribosomal protein S12



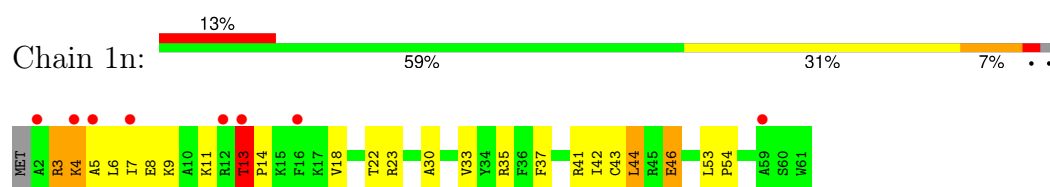
- Molecule 44: 30S ribosomal protein S13



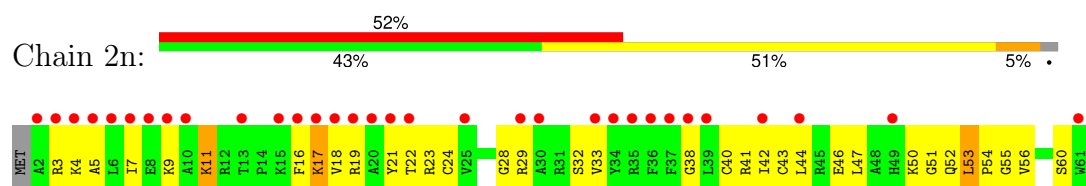
- Molecule 44: 30S ribosomal protein S13



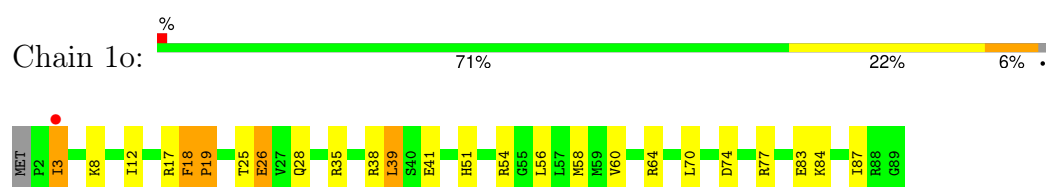
- Molecule 45: 30S ribosomal protein S14 type Z



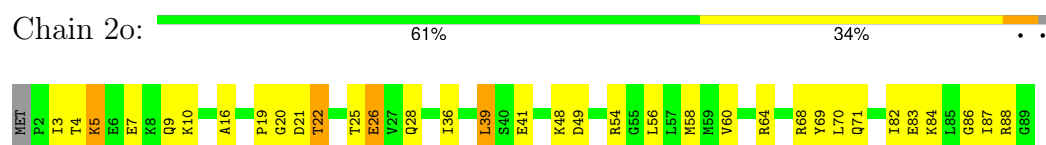
- Molecule 45: 30S ribosomal protein S14 type Z



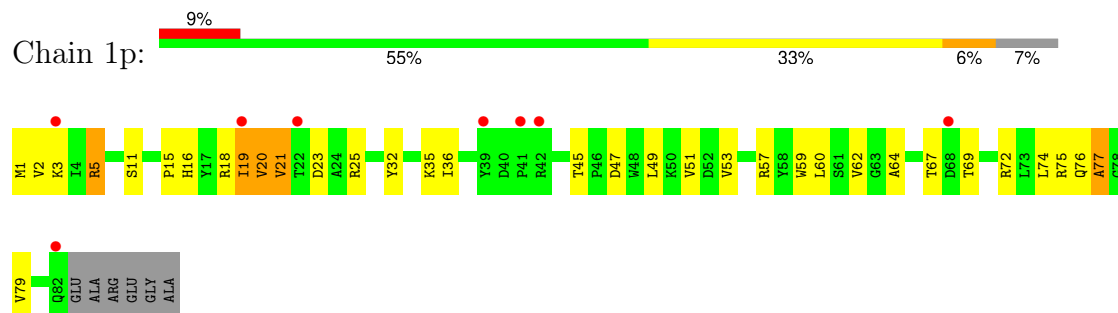
- Molecule 46: 30S ribosomal protein S15



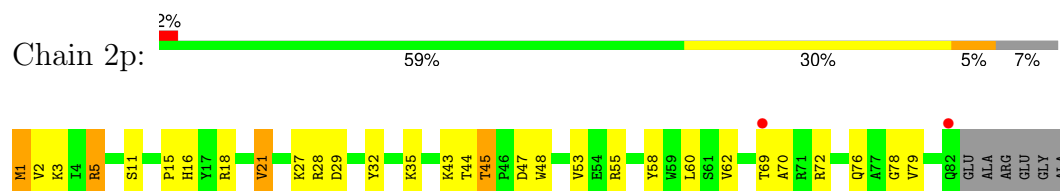
- Molecule 46: 30S ribosomal protein S15



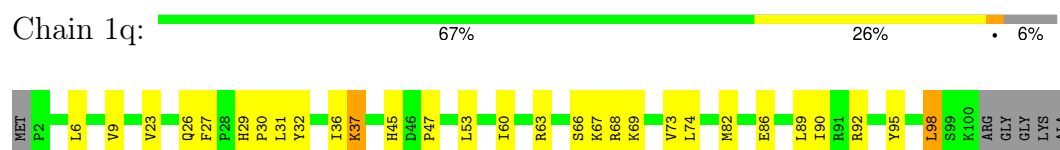
- Molecule 47: 30S ribosomal protein S16



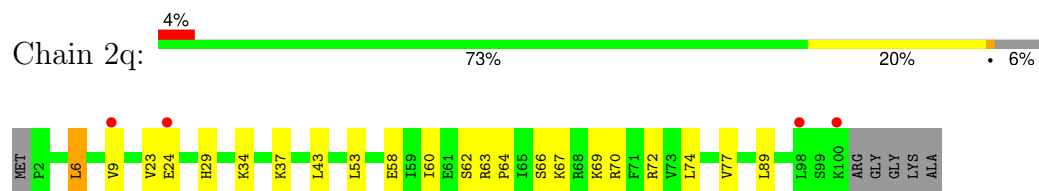
- Molecule 47: 30S ribosomal protein S16



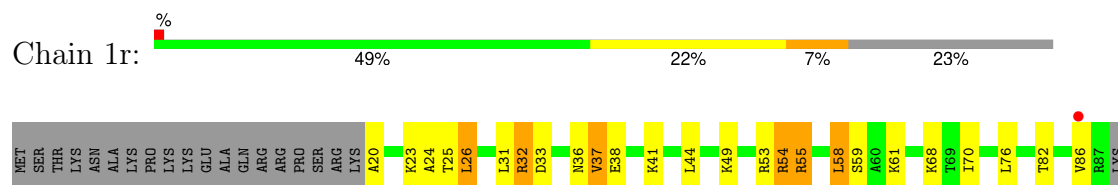
- Molecule 48: 30S ribosomal protein S17



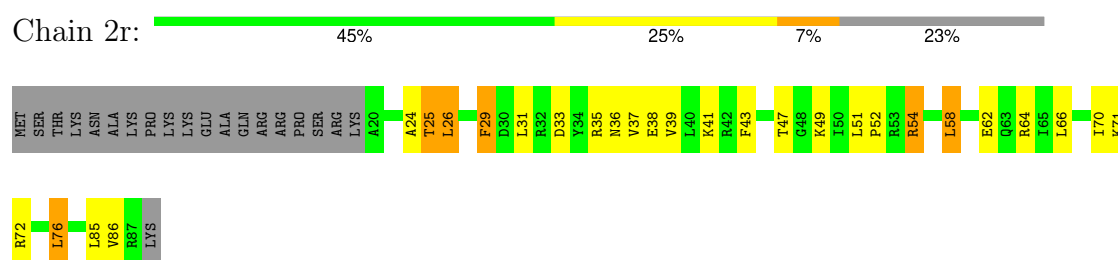
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18



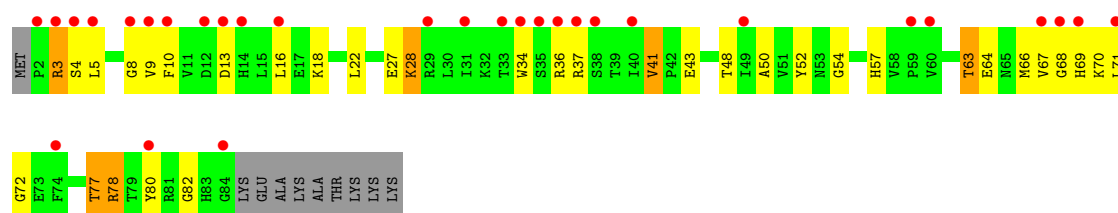
- Molecule 49: 30S ribosomal protein S18



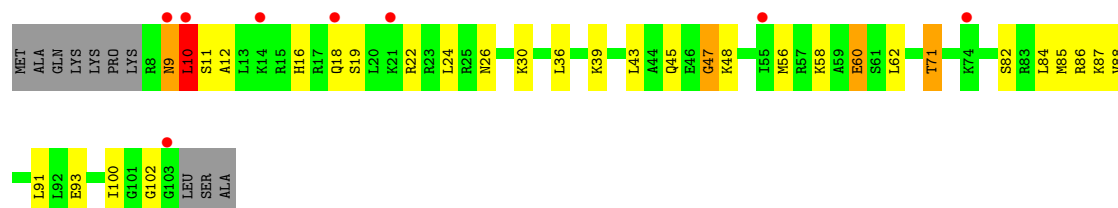
- Molecule 50: 30S ribosomal protein S19



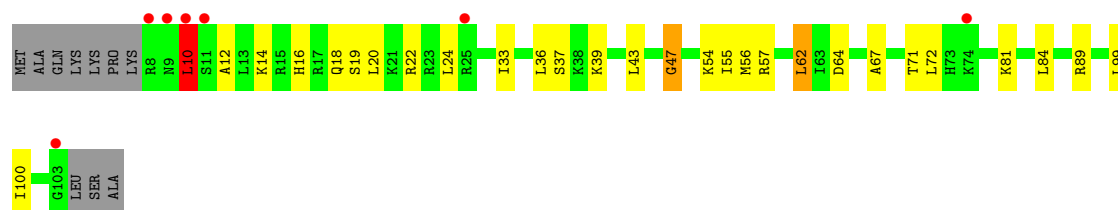
- Molecule 50: 30S ribosomal protein S19



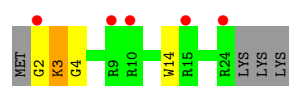
- Molecule 51: 30S ribosomal protein S20



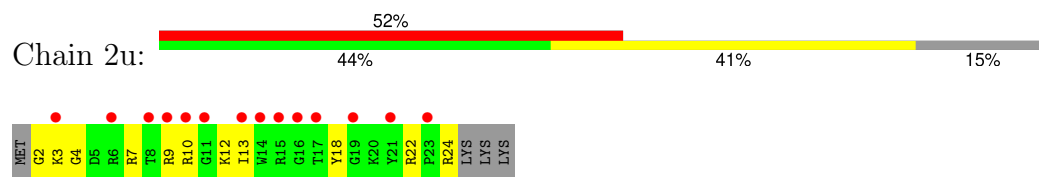
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



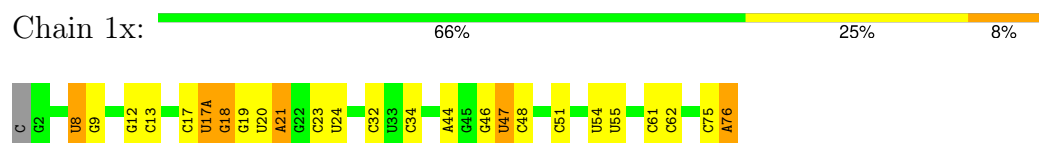
- Molecule 53: mRNA



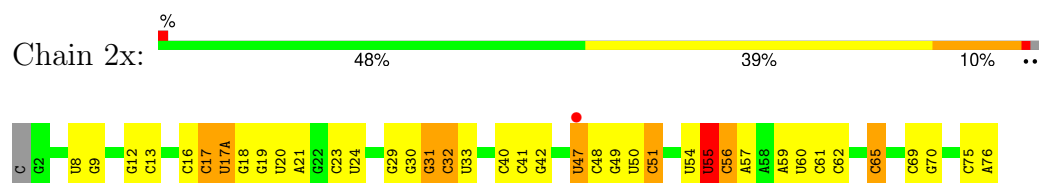
- Molecule 53: mRNA



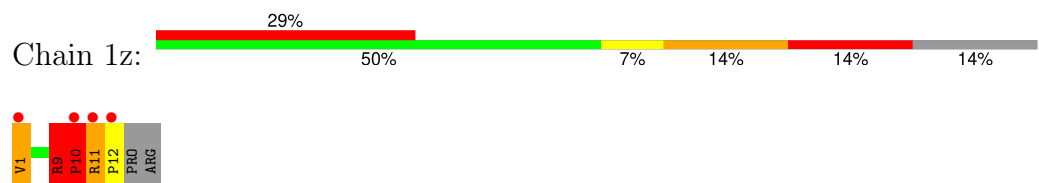
- Molecule 54: P-site tRNA



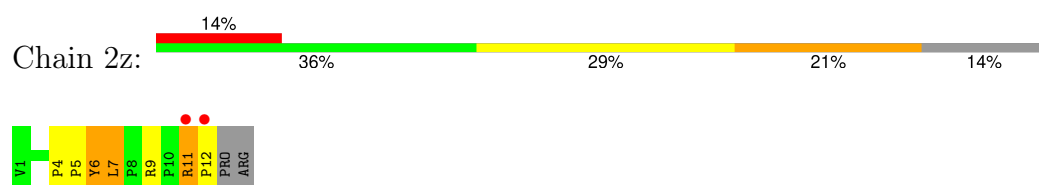
- Molecule 54: P-site tRNA



- Molecule 55: Oncocin d15-19



- Molecule 55: Oncocin d15-19



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.05Å 450.75Å 623.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 2.80 49.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.92-2.80) 99.6 (49.92-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.200 , 0.251 0.200 , 0.249	Depositor DCC
R_{free} test set	71597 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	288518	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: PSU, 5MC, SF4, 4SU, ZN, MG, 5MU

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	0.47	0/66249	0.58	4/103407 (0.0%)
1	2A	0.35	0/67298	0.56	1/105044 (0.0%)
2	1B	0.35	0/2877	0.50	0/4488
2	2B	0.42	0/2878	0.57	0/4490
3	1D	0.70	0/2186	0.96	0/2944
3	2D	0.58	0/2192	0.97	4/2951 (0.1%)
4	1E	0.72	0/1592	1.01	4/2149 (0.2%)
4	2E	0.60	0/1592	1.01	8/2149 (0.4%)
5	1F	0.70	0/1619	0.99	3/2193 (0.1%)
5	2F	0.51	0/1615	1.01	2/2188 (0.1%)
6	1G	0.55	0/1450	0.94	4/1959 (0.2%)
6	2G	0.56	0/1449	1.09	6/1958 (0.3%)
7	1H	0.63	0/1356	0.94	4/1834 (0.2%)
7	2H	0.55	0/1356	1.02	1/1834 (0.1%)
8	1I	0.53	0/1100	0.99	2/1501 (0.1%)
8	2I	0.50	0/1076	1.02	5/1471 (0.3%)
9	1N	0.69	0/1144	0.84	0/1543
9	2N	0.50	0/1144	0.92	2/1543 (0.1%)
10	1O	0.72	0/943	0.94	0/1269
10	2O	0.57	0/943	0.98	0/1269
11	1P	0.65	0/1156	0.93	2/1537 (0.1%)
11	2P	0.52	0/1152	1.03	5/1533 (0.3%)
12	1Q	0.70	0/1143	0.93	0/1527
12	2Q	0.55	0/1143	0.95	1/1527 (0.1%)
13	1R	0.77	1/982 (0.1%)	0.86	0/1312
13	2R	0.52	0/982	0.85	0/1312
14	1S	0.57	0/887	0.91	1/1180 (0.1%)
14	2S	0.61	0/880	1.05	5/1172 (0.4%)
15	1T	0.64	0/1105	0.94	0/1477
15	2T	0.50	0/1097	0.90	0/1468
16	1U	0.81	0/977	0.92	0/1301
16	2U	0.56	0/977	0.89	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	1V	0.68	0/782	0.91	0/1049
17	2V	0.58	0/782	0.91	1/1049 (0.1%)
18	1W	0.80	0/897	0.92	1/1205 (0.1%)
18	2W	0.62	0/897	0.94	1/1205 (0.1%)
19	1X	0.68	0/764	0.91	1/1025 (0.1%)
19	2X	0.57	0/764	0.95	1/1025 (0.1%)
20	1Y	0.66	0/819	0.97	2/1095 (0.2%)
20	2Y	0.51	0/819	0.98	0/1095
21	1Z	0.56	0/1502	0.98	3/2041 (0.1%)
21	2Z	0.54	0/1486	1.00	2/2022 (0.1%)
22	10	0.65	0/606	1.02	4/808 (0.5%)
22	20	0.47	0/606	0.97	4/808 (0.5%)
23	11	0.66	0/762	0.90	0/1014
23	21	0.58	0/762	0.91	0/1014
24	12	0.65	0/590	0.85	0/781
24	22	0.50	0/590	0.85	0/781
25	13	0.72	0/474	1.01	4/635 (0.6%)
25	23	0.50	0/469	0.93	0/630
26	14	0.52	0/571	1.03	3/768 (0.4%)
26	24	0.63	0/545	1.20	2/737 (0.3%)
27	15	0.76	0/469	0.95	0/635
27	25	0.59	0/469	0.93	0/635
28	16	0.63	0/460	0.82	0/613
28	26	0.57	0/456	0.87	0/608
29	17	0.76	0/426	0.89	1/561 (0.2%)
29	27	0.63	0/426	0.92	1/561 (0.2%)
30	18	0.71	0/525	0.91	1/691 (0.1%)
30	28	0.56	0/525	0.96	0/691
31	19	0.74	0/310	0.91	0/407
31	29	0.51	0/310	0.99	0/407
32	1a	0.31	0/35537	0.50	2/55456 (0.0%)
32	2a	0.28	0/35680	0.48	1/55681 (0.0%)
33	1b	0.51	0/1820	1.02	7/2468 (0.3%)
33	2b	1.65	8/1728 (0.5%)	1.17	12/2352 (0.5%)
34	1c	0.50	0/1504	0.90	2/2047 (0.1%)
34	2c	0.55	0/1435	0.99	0/1960
35	1d	0.52	0/1648	0.94	2/2222 (0.1%)
35	2d	0.48	0/1659	0.94	0/2230
36	1e	0.53	0/1145	1.02	6/1543 (0.4%)
36	2e	0.50	0/1111	1.09	10/1504 (0.7%)
37	1f	0.48	0/819	0.86	0/1111
37	2f	0.47	0/830	0.86	2/1125 (0.2%)
38	1g	0.46	0/1198	0.94	1/1613 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	2g	0.47	0/1185	0.91	0/1602
39	1h	0.46	0/1108	0.92	0/1494
39	2h	0.43	0/1094	0.91	2/1478 (0.1%)
40	1i	0.46	0/995	0.93	2/1339 (0.1%)
40	2i	0.54	0/949	0.94	1/1284 (0.1%)
41	1j	0.59	0/695	1.13	7/950 (0.7%)
41	2j	0.59	0/690	1.15	10/943 (1.1%)
42	1k	0.50	0/840	0.95	1/1138 (0.1%)
42	2k	0.46	0/844	0.93	4/1145 (0.3%)
43	1l	0.53	0/936	0.93	0/1263
43	2l	0.51	0/934	0.97	4/1262 (0.3%)
44	1m	0.46	0/933	0.93	1/1254 (0.1%)
44	2m	0.54	0/913	0.93	0/1230
45	1n	0.50	0/491	1.08	3/653 (0.5%)
45	2n	0.48	0/467	0.92	0/624
46	1o	0.49	0/726	0.94	2/970 (0.2%)
46	2o	0.44	0/739	0.89	0/985
47	1p	0.49	0/686	0.96	2/926 (0.2%)
47	2p	0.51	0/693	0.91	3/935 (0.3%)
48	1q	0.46	0/824	0.85	0/1105
48	2q	0.44	0/836	0.85	2/1117 (0.2%)
49	1r	0.49	0/560	0.89	0/746
49	2r	0.44	0/560	0.84	0/746
50	1s	0.49	0/657	1.04	6/890 (0.7%)
50	2s	0.52	0/661	1.02	1/893 (0.1%)
51	1t	0.46	0/714	1.04	1/948 (0.1%)
51	2t	0.47	0/733	0.93	0/969
52	1u	0.41	0/191	0.79	0/252
52	2u	0.49	0/203	1.03	2/266 (0.8%)
53	1v	0.42	0/122	0.76	0/188
53	2v	0.47	0/122	0.61	0/188
54	1x	0.37	0/1725	0.55	0/2689
54	2x	0.34	0/1725	0.54	0/2689
55	1z	1.16	1/106 (0.9%)	1.36	2/146 (1.4%)
55	2z	0.78	0/106	1.65	4/146 (2.7%)
All	All	0.46	10/306280 (0.0%)	0.68	201/458192 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	2F	0	1
19	1X	0	1
19	2X	0	1
20	1Y	0	1
34	2c	0	1
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	92	TYR	CD1-CE1	30.24	2.29	1.38
33	2b	92	TYR	CD2-CE2	26.56	2.18	1.38
33	2b	151	GLY	N-CA	23.94	1.80	1.45
33	2b	92	TYR	CE1-CZ	22.82	1.93	1.38
33	2b	92	TYR	CE2-CZ	22.55	1.92	1.38

The worst 5 of 201 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2b	150	SER	CA-C-N	17.99	156.68	121.41
33	2b	150	SER	C-N-CA	17.99	156.68	121.41
33	2b	151	GLY	N-CA-C	9.45	135.57	113.18
1	1A	2013	G	C2'-C3'-O3'	9.33	123.50	109.50
36	1e	105	VAL	CA-C-N	-9.12	110.42	119.64

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	1X	93	GLU	Peptide
20	1Y	54	LYS	Peptide
5	2F	20	LEU	Peptide
19	2X	93	GLU	Peptide
34	2c	186	PHE	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	59154	0	29828	522	0
1	2A	60091	0	30300	810	0
2	1B	2572	0	1306	31	0
2	2B	2573	0	1306	61	0
3	1D	2136	0	2218	51	0
3	2D	2142	0	2229	61	0
4	1E	1559	0	1618	35	0
4	2E	1559	0	1618	53	0
5	1F	1584	0	1625	33	0
5	2F	1580	0	1619	49	0
6	1G	1425	0	1443	35	0
6	2G	1424	0	1434	75	0
7	1H	1330	0	1407	26	0
7	2H	1330	0	1407	38	0
8	1I	1085	0	1114	25	0
8	2I	1061	0	1080	28	0
9	1N	1117	0	1184	14	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	16	0
10	2O	933	0	996	21	0
11	1P	1139	0	1223	32	0
11	2P	1135	0	1212	40	0
12	1Q	1122	0	1179	23	0
12	2Q	1122	0	1179	28	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	22	0
14	1S	877	0	938	28	0
14	2S	870	0	923	31	0
15	1T	1091	0	1151	25	0
15	2T	1083	0	1136	22	0
16	1U	959	0	1019	11	0
16	2U	959	0	1018	24	0
17	1V	771	0	830	9	0
17	2V	771	0	830	18	0
18	1W	886	0	940	8	0
18	2W	886	0	940	19	0
19	1X	750	0	814	16	0
19	2X	750	0	814	16	0
20	1Y	806	0	881	26	0
20	2Y	806	0	881	27	0
21	1Z	1470	0	1478	24	0
21	2Z	1454	0	1452	49	0
22	10	598	0	614	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	598	0	614	12	0
23	11	755	0	826	12	0
23	21	755	0	826	12	0
24	12	588	0	643	7	0
24	22	588	0	643	16	0
25	13	469	0	518	6	0
25	23	464	0	514	18	0
26	14	558	0	544	40	0
26	24	532	0	503	26	0
27	15	455	0	465	7	0
27	25	455	0	465	13	0
28	16	453	0	472	7	0
28	26	449	0	469	6	0
29	17	418	0	467	8	0
29	27	418	0	467	11	0
30	18	517	0	582	18	0
30	28	517	0	582	27	0
31	19	307	0	335	7	0
31	29	307	0	335	8	0
32	1a	31750	0	16028	528	0
32	2a	31877	0	16090	618	0
33	1b	1786	0	1744	81	0
33	2b	1697	0	1574	112	0
34	1c	1480	0	1400	39	0
34	2c	1412	0	1246	67	0
35	1d	1618	0	1579	60	0
35	2d	1630	0	1633	62	0
36	1e	1129	0	1184	33	0
36	2e	1095	0	1124	40	0
37	1f	806	0	793	18	0
37	2f	817	0	808	22	0
38	1g	1183	0	1165	26	0
38	2g	1167	0	1119	31	0
39	1h	1088	0	1126	34	0
39	2h	1074	0	1100	28	0
40	1i	976	0	973	39	0
40	2i	932	0	891	39	0
41	1j	682	0	598	32	0
41	2j	678	0	612	24	0
42	1k	826	0	829	21	0
42	2k	829	0	825	16	0
43	1l	920	0	958	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	918	0	947	31	0
44	1m	923	0	962	32	0
44	2m	903	0	923	41	0
45	1n	482	0	507	24	0
45	2n	459	0	467	40	0
46	1o	715	0	729	14	0
46	2o	728	0	760	23	0
47	1p	671	0	679	23	0
47	2p	677	0	686	21	0
48	1q	811	0	858	16	0
48	2q	823	0	891	14	0
49	1r	555	0	618	13	0
49	2r	555	0	618	21	0
50	1s	642	0	629	39	0
50	2s	646	0	644	31	0
51	1t	712	0	759	20	0
51	2t	731	0	807	18	0
52	1u	187	0	186	5	0
52	2u	199	0	208	9	0
53	1v	109	0	55	0	0
53	2v	109	0	55	2	0
54	1x	1625	0	829	12	0
54	2x	1625	0	829	20	0
55	1z	101	0	109	7	0
55	2z	101	0	109	4	0
56	10	7	0	0	0	0
56	11	1	0	0	0	0
56	13	2	0	0	0	0
56	14	1	0	0	0	0
56	15	4	0	0	0	0
56	16	2	0	0	0	0
56	17	4	0	0	0	0
56	18	5	0	0	0	0
56	19	3	0	0	0	0
56	1A	1051	0	0	0	0
56	1B	26	0	0	0	0
56	1D	17	0	0	0	0
56	1E	10	0	0	0	0
56	1F	7	0	0	0	0
56	1G	3	0	0	0	0
56	1H	4	0	0	0	0
56	1N	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1O	2	0	0	0	0
56	1P	5	0	0	0	0
56	1Q	6	0	0	0	0
56	1R	6	0	0	0	0
56	1T	5	0	0	0	0
56	1U	5	0	0	0	0
56	1V	1	0	0	0	0
56	1W	6	0	0	0	0
56	1X	2	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	306	0	0	0	0
56	1b	2	0	0	0	0
56	1c	1	0	0	0	0
56	1d	2	0	0	0	0
56	1e	4	0	0	0	0
56	1f	1	0	0	0	0
56	1h	3	0	0	0	0
56	1k	1	0	0	0	0
56	1l	1	0	0	0	0
56	1n	1	0	0	0	0
56	1o	2	0	0	0	0
56	1q	4	0	0	0	0
56	1r	3	0	0	0	0
56	1t	1	0	0	0	0
56	1x	11	0	0	0	0
56	20	1	0	0	0	0
56	25	1	0	0	0	0
56	26	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	583	0	0	0	0
56	2B	10	0	0	0	0
56	2D	4	0	0	0	0
56	2E	7	0	0	0	0
56	2F	2	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	3	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	5	0	0	0	0
56	2R	1	0	0	0	0
56	2U	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2V	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2a	244	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2k	2	0	0	0	0
56	2l	3	0	0	0	0
56	2n	2	0	0	0	0
56	2p	1	0	0	0	0
56	2q	1	0	0	0	0
56	2t	1	0	0	0	0
56	2x	6	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0
58	2d	8	0	0	0	0
59	10	8	0	0	0	0
59	11	7	0	0	0	0
59	12	2	0	0	0	0
59	13	4	0	0	0	0
59	15	7	0	0	1	0
59	16	5	0	0	1	0
59	17	8	0	0	0	0
59	18	9	0	0	0	0
59	19	4	0	0	2	0
59	1A	2110	0	0	85	0
59	1B	42	0	0	4	0
59	1D	24	0	0	0	0
59	1E	30	0	0	4	0
59	1F	16	0	0	1	0
59	1G	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1H	3	0	0	1	0
59	1I	1	0	0	0	0
59	1N	7	0	0	0	0
59	1O	4	0	0	0	0
59	1P	21	0	0	1	0
59	1Q	11	0	0	0	0
59	1R	16	0	0	4	0
59	1S	2	0	0	0	0
59	1T	7	0	0	1	0
59	1U	14	0	0	0	0
59	1V	4	0	0	1	0
59	1W	5	0	0	0	0
59	1X	4	0	0	0	0
59	1Y	1	0	0	0	0
59	1Z	4	0	0	0	0
59	1a	393	0	0	32	0
59	1b	1	0	0	0	0
59	1c	1	0	0	0	0
59	1d	5	0	0	0	0
59	1e	3	0	0	0	0
59	1f	1	0	0	0	0
59	1h	3	0	0	0	0
59	1i	1	0	0	0	0
59	1j	1	0	0	0	0
59	1k	1	0	0	1	0
59	1l	3	0	0	0	0
59	1m	1	0	0	0	0
59	1o	1	0	0	0	0
59	1p	1	0	0	0	0
59	1q	1	0	0	0	0
59	1s	1	0	0	1	0
59	1v	1	0	0	0	0
59	1x	8	0	0	1	0
59	1z	1	0	0	0	0
59	20	3	0	0	0	0
59	21	1	0	0	0	0
59	23	2	0	0	0	0
59	26	1	0	0	0	0
59	27	2	0	0	0	0
59	28	2	0	0	0	0
59	2A	813	0	0	62	0
59	2B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2D	16	0	0	1	0
59	2E	9	0	0	2	0
59	2F	5	0	0	0	0
59	2N	1	0	0	0	0
59	2O	3	0	0	0	0
59	2P	9	0	0	0	0
59	2Q	2	0	0	0	0
59	2R	3	0	0	0	0
59	2T	1	0	0	0	0
59	2U	3	0	0	0	0
59	2W	1	0	0	0	0
59	2X	2	0	0	0	0
59	2Y	1	0	0	1	0
59	2Z	4	0	0	2	0
59	2a	321	0	0	52	0
59	2d	1	0	0	0	0
59	2e	1	0	0	0	0
59	2i	2	0	0	0	0
59	2j	1	0	0	0	0
59	2l	1	0	0	0	0
59	2m	3	0	0	0	0
59	2p	1	0	0	0	0
59	2q	1	0	0	0	0
59	2t	4	0	0	0	0
59	2x	7	0	0	1	0
59	2z	1	0	0	0	0
All	All	288518	0	189963	4624	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 10.

The worst 5 of 4624 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)
33:2b:92:TYR:CD1	33:2b:92:TYR:CG	1.83	1.60
33:2b:92:TYR:CG	33:2b:92:TYR:CD2	1.81	1.60
33:2b:92:TYR:CZ	33:2b:92:TYR:CE2	1.92	1.56
33:2b:92:TYR:CZ	33:2b:92:TYR:CE1	1.93	1.52
33:2b:151:GLY:N	33:2b:151:GLY:CA	1.80	1.45

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	250 (92%)	21 (8%)	2 (1%)	18	47
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	55
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	55
5	1F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	24	55
5	2F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	24	55
6	1G	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	5	19
6	2G	179/182 (98%)	152 (85%)	22 (12%)	5 (3%)	4	14
7	1H	172/180 (96%)	158 (92%)	13 (8%)	1 (1%)	21	51
7	2H	172/180 (96%)	157 (91%)	13 (8%)	2 (1%)	10	34
8	1I	144/148 (97%)	119 (83%)	24 (17%)	1 (1%)	18	47
8	2I	144/148 (97%)	117 (81%)	26 (18%)	1 (1%)	18	47
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	18	47
10	1O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	44
10	2O	120/122 (98%)	116 (97%)	3 (2%)	1 (1%)	16	44
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	18	47
11	2P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	9	30
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	127 (91%)	10 (7%)	2 (1%)	9	30
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	14	41
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	1U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	38
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	38
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11	36
20	1Y	105/110 (96%)	91 (87%)	12 (11%)	2 (2%)	6	22
20	2Y	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	12	38
21	1Z	184/206 (89%)	170 (92%)	13 (7%)	1 (0%)	24	55
21	2Z	184/206 (89%)	166 (90%)	14 (8%)	4 (2%)	5	19
22	10	73/85 (86%)	69 (94%)	3 (4%)	1 (1%)	9	30
22	20	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	49 (73%)	9 (13%)	9 (13%)	0	0
26	24	67/71 (94%)	49 (73%)	12 (18%)	6 (9%)	0	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	0	1 (2%)	5	19
30	18	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	178 (78%)	42 (18%)	9 (4%)	2	8
33	2b	229/256 (90%)	183 (80%)	41 (18%)	5 (2%)	5	19
34	1c	204/239 (85%)	169 (83%)	33 (16%)	2 (1%)	12	38
34	2c	204/239 (85%)	167 (82%)	34 (17%)	3 (2%)	8	28
35	1d	206/209 (99%)	179 (87%)	25 (12%)	2 (1%)	12	38
35	2d	206/209 (99%)	182 (88%)	18 (9%)	6 (3%)	3	13
36	1e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	5	20
36	2e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	9	30
37	1f	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	12	38
37	2f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	12	38
38	1g	153/156 (98%)	136 (89%)	17 (11%)	0	100	100
38	2g	153/156 (98%)	134 (88%)	19 (12%)	0	100	100
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
40	1i	125/128 (98%)	105 (84%)	15 (12%)	5 (4%)	2	8
40	2i	125/128 (98%)	104 (83%)	14 (11%)	7 (6%)	1	4
41	1j	95/105 (90%)	77 (81%)	12 (13%)	6 (6%)	1	3
41	2j	94/105 (90%)	81 (86%)	11 (12%)	2 (2%)	5	20
42	1k	112/129 (87%)	97 (87%)	13 (12%)	2 (2%)	6	23
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	14	41
43	1l	120/132 (91%)	112 (93%)	8 (7%)	0	100	100
43	2l	120/132 (91%)	111 (92%)	9 (8%)	0	100	100
44	1m	116/126 (92%)	100 (86%)	13 (11%)	3 (3%)	4	15
44	2m	114/126 (90%)	96 (84%)	15 (13%)	3 (3%)	4	15
45	1n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	25
45	2n	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
46	1o	86/89 (97%)	75 (87%)	10 (12%)	1 (1%)	10	34
46	2o	86/89 (97%)	77 (90%)	7 (8%)	2 (2%)	5	18
47	1p	80/88 (91%)	67 (84%)	11 (14%)	2 (2%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	68 (85%)	12 (15%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12	38
48	2q	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
49	1r	66/88 (75%)	58 (88%)	6 (9%)	2 (3%)	3	12
49	2r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	8	28
50	1s	82/93 (88%)	70 (85%)	12 (15%)	0	100	100
50	2s	81/93 (87%)	67 (83%)	14 (17%)	0	100	100
51	1t	94/106 (89%)	81 (86%)	11 (12%)	2 (2%)	5	20
51	2t	94/106 (89%)	81 (86%)	10 (11%)	3 (3%)	3	11
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	6
52	2u	21/27 (78%)	17 (81%)	3 (14%)	1 (5%)	2	6
55	1z	10/14 (71%)	6 (60%)	1 (10%)	3 (30%)	0	0
55	2z	10/14 (71%)	8 (80%)	1 (10%)	1 (10%)	0	1
All	All	11430/12156 (94%)	10379 (91%)	909 (8%)	142 (1%)	10	34

5 of 142 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
6	1G	50	ALA
6	1G	51	ARG
6	1G	126	ASP
7	1H	126	PRO

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%)	188 (87%)	27 (13%)	4	15
3	2D	216/218 (99%)	186 (86%)	30 (14%)	3	12
4	1E	164/166 (99%)	139 (85%)	25 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	138 (84%)	26 (16%)	2	9
5	1F	160/166 (96%)	135 (84%)	25 (16%)	2	9
5	2F	159/166 (96%)	136 (86%)	23 (14%)	3	11
6	1G	143/156 (92%)	124 (87%)	19 (13%)	4	14
6	2G	142/156 (91%)	115 (81%)	27 (19%)	1	5
7	1H	144/148 (97%)	129 (90%)	15 (10%)	7	22
7	2H	144/148 (97%)	125 (87%)	19 (13%)	4	14
8	1I	110/124 (89%)	86 (78%)	24 (22%)	1	3
8	2I	104/124 (84%)	88 (85%)	16 (15%)	2	10
9	1N	118/119 (99%)	101 (86%)	17 (14%)	3	11
9	2N	118/119 (99%)	100 (85%)	18 (15%)	3	10
10	1O	100/100 (100%)	91 (91%)	9 (9%)	9	28
10	2O	100/100 (100%)	90 (90%)	10 (10%)	7	24
11	1P	116/116 (100%)	100 (86%)	16 (14%)	3	12
11	2P	115/116 (99%)	98 (85%)	17 (15%)	3	10
12	1Q	111/111 (100%)	99 (89%)	12 (11%)	6	21
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9	28
13	1R	101/101 (100%)	81 (80%)	20 (20%)	1	5
13	2R	101/101 (100%)	81 (80%)	20 (20%)	1	5
14	1S	87/88 (99%)	77 (88%)	10 (12%)	5	18
14	2S	85/88 (97%)	65 (76%)	20 (24%)	1	3
15	1T	115/127 (91%)	99 (86%)	16 (14%)	3	12
15	2T	113/127 (89%)	97 (86%)	16 (14%)	3	12
16	1U	93/94 (99%)	83 (89%)	10 (11%)	6	21
16	2U	93/94 (99%)	84 (90%)	9 (10%)	8	25
17	1V	80/82 (98%)	65 (81%)	15 (19%)	1	5
17	2V	80/82 (98%)	69 (86%)	11 (14%)	3	12
18	1W	90/92 (98%)	80 (89%)	10 (11%)	6	20
18	2W	90/92 (98%)	80 (89%)	10 (11%)	6	20
19	1X	77/78 (99%)	70 (91%)	7 (9%)	9	28
19	2X	77/78 (99%)	72 (94%)	5 (6%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	85/91 (93%)	76 (89%)	9 (11%)	6	22
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	10	33
21	1Z	159/179 (89%)	140 (88%)	19 (12%)	5	17
21	2Z	156/179 (87%)	139 (89%)	17 (11%)	6	21
22	10	60/67 (90%)	57 (95%)	3 (5%)	22	54
22	20	60/67 (90%)	57 (95%)	3 (5%)	22	54
23	11	80/83 (96%)	70 (88%)	10 (12%)	4	15
23	21	80/83 (96%)	68 (85%)	12 (15%)	3	10
24	12	65/67 (97%)	57 (88%)	8 (12%)	4	16
24	22	65/67 (97%)	57 (88%)	8 (12%)	4	16
25	13	51/52 (98%)	42 (82%)	9 (18%)	2	7
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	24
26	14	60/63 (95%)	51 (85%)	9 (15%)	3	10
26	24	53/63 (84%)	46 (87%)	7 (13%)	4	14
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	24
27	25	50/52 (96%)	44 (88%)	6 (12%)	5	17
28	16	51/52 (98%)	48 (94%)	3 (6%)	18	48
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	12
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	25
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	38
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	37
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	65
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	73
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	48
33	1b	177/220 (80%)	141 (80%)	36 (20%)	1	4
33	2b	158/220 (72%)	127 (80%)	31 (20%)	1	5
34	1c	127/188 (68%)	115 (91%)	12 (9%)	8	27
34	2c	108/188 (57%)	90 (83%)	18 (17%)	2	8
35	1d	161/181 (89%)	139 (86%)	22 (14%)	3	13
35	2d	164/181 (91%)	138 (84%)	26 (16%)	2	9
36	1e	113/123 (92%)	96 (85%)	17 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	106/123 (86%)	88 (83%)	18 (17%)	2	7
37	1f	83/90 (92%)	75 (90%)	8 (10%)	8	26
37	2f	86/90 (96%)	77 (90%)	9 (10%)	6	22
38	1g	111/127 (87%)	93 (84%)	18 (16%)	2	8
38	2g	107/127 (84%)	91 (85%)	16 (15%)	3	10
39	1h	114/119 (96%)	96 (84%)	18 (16%)	2	9
39	2h	111/119 (93%)	95 (86%)	16 (14%)	3	11
40	1i	89/99 (90%)	72 (81%)	17 (19%)	1	5
40	2i	80/99 (81%)	71 (89%)	9 (11%)	5	19
41	1j	60/92 (65%)	48 (80%)	12 (20%)	1	4
41	2j	62/92 (67%)	46 (74%)	16 (26%)	0	2
42	1k	82/99 (83%)	74 (90%)	8 (10%)	7	25
42	2k	82/99 (83%)	71 (87%)	11 (13%)	4	13
43	1l	95/109 (87%)	84 (88%)	11 (12%)	5	18
43	2l	94/109 (86%)	86 (92%)	8 (8%)	10	31
44	1m	90/101 (89%)	81 (90%)	9 (10%)	7	24
44	2m	87/101 (86%)	81 (93%)	6 (7%)	14	41
45	1n	47/50 (94%)	38 (81%)	9 (19%)	1	5
45	2n	43/50 (86%)	35 (81%)	8 (19%)	1	5
46	1o	75/80 (94%)	67 (89%)	8 (11%)	6	21
46	2o	78/80 (98%)	67 (86%)	11 (14%)	3	12
47	1p	67/74 (90%)	55 (82%)	12 (18%)	2	6
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	14
48	1q	91/97 (94%)	83 (91%)	8 (9%)	9	29
48	2q	94/97 (97%)	86 (92%)	8 (8%)	10	31
49	1r	59/77 (77%)	48 (81%)	11 (19%)	1	5
49	2r	59/77 (77%)	48 (81%)	11 (19%)	1	5
50	1s	65/80 (81%)	59 (91%)	6 (9%)	8	27
50	2s	67/80 (84%)	56 (84%)	11 (16%)	2	8
51	1t	66/82 (80%)	56 (85%)	10 (15%)	3	10
51	2t	71/82 (87%)	67 (94%)	4 (6%)	19	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	16/22 (73%)	16 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	50
55	1z	12/14 (86%)	11 (92%)	1 (8%)	10	32
55	2z	12/14 (86%)	11 (92%)	1 (8%)	10	32
All	All	9159/10094 (91%)	7931 (87%)	1228 (13%)	4	13

5 of 1228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	20	20	ARG
42	2k	84	VAL
26	24	14	ILE
22	20	10	THR
35	2d	70	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 160 such sidechains are listed below:

Mol	Chain	Res	Type
30	28	35	GLN
41	2j	56	HIS
33	2b	45	GLN
36	2e	141	GLN
43	2l	75	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2737/2915 (93%)	396 (14%)	28 (1%)
1	2A	2781/2915 (95%)	475 (17%)	26 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	119/121 (98%)	34 (28%)	2 (1%)
32	1a	1472/1521 (96%)	271 (18%)	0
32	2a	1479/1521 (97%)	282 (19%)	0
53	1v	4/24 (16%)	1 (25%)	0
53	2v	4/24 (16%)	1 (25%)	0
54	1x	75/77 (97%)	12 (16%)	0
54	2x	75/77 (97%)	15 (20%)	0
All	All	8865/9316 (95%)	1496 (16%)	56 (0%)

5 of 1496 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	32	U
1	1A	33	C
1	1A	35	G
1	1A	44	C

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	184	A
2	2B	45	A
1	2A	669	C
2	2B	42	C
1	2A	2013	G

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

8 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	$\# Z > 2$
54	5MU	2x	54	54	19,22,23	1.41	4 (21%)	27,32,35	1.90	6 (22%)
54	5MC	2x	32	54	19,22,23	1.62	2 (10%)	26,32,35	1.45	3 (11%)
54	PSU	2x	55	54	18,21,22	1.44	1 (5%)	21,30,33	2.00	3 (14%)
54	4SU	2x	8	54	18,21,22	1.88	5 (27%)	25,30,33	1.07	3 (12%)
54	5MC	1x	32	54	19,22,23	1.51	3 (15%)	26,32,35	1.29	2 (7%)
54	4SU	1x	8	54	18,21,22	2.17	5 (27%)	25,30,33	1.61	5 (20%)
54	5MU	1x	54	54	19,22,23	1.46	4 (21%)	27,32,35	1.95	6 (22%)
54	PSU	1x	55	54	18,21,22	1.28	2 (11%)	21,30,33	1.97	4 (19%)

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
54	5MU	2x	54	54	-	0/7/25/26	0/2/2/2
54	5MC	2x	32	54	-	1/7/25/26	0/2/2/2
54	PSU	2x	55	54	-	2/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/7/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/7/25/26	0/2/2/2
54	5MU	1x	54	54	-	0/7/25/26	0/2/2/2
54	PSU	1x	55	54	-	0/7/25/26	0/2/2/2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2x	32	5MC	C5-C4	5.45	1.48	1.44
54	1x	8	4SU	C4-N3	-5.42	1.32	1.37
54	1x	32	5MC	C5-C4	5.12	1.48	1.44
54	2x	55	PSU	C6-C5	4.48	1.40	1.35
54	1x	8	4SU	C4-S4	-4.44	1.60	1.68

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2x	55	PSU	N1-C2-N3	6.14	121.64	115.17
54	1x	55	PSU	N1-C2-N3	5.60	121.08	115.17
54	2x	54	5MU	N3-C2-N1	4.75	121.07	114.89
54	1x	8	4SU	C6-C5-C4	-4.74	115.84	119.95
54	1x	54	5MU	C5-C4-N3	4.69	119.40	115.32

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	2x	55	PSU	O4'-C4'-C5'-O5'
54	2x	55	PSU	C3'-C4'-C5'-O5'
54	2x	32	5MC	C2'-C1'-N1-C6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2x	32	5MC	1	0
54	2x	55	PSU	1	0
54	1x	8	4SU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2444 ligands modelled in this entry, 2442 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	$\# Z > 2$
58	SF4	1d	301	35	0,12,12	-	-	-		
58	SF4	2d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	1d	301	35	-	-	0/6/5/5
58	SF4	2d	501	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.

No monomer is involved in short contacts.

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	2746/2915 (94%)	-0.53	31 (1%) 78 70	23, 42, 86, 108	0
1	2A	2790/2915 (95%)	-0.42	16 (0%) 85 80	27, 47, 93, 110	0
2	1B	120/121 (99%)	-0.03	0 100 100	36, 64, 82, 95	0
2	2B	120/121 (99%)	0.65	4 (3%) 49 39	43, 70, 85, 96	0
3	1D	275/276 (99%)	-0.32	2 (0%) 84 77	21, 41, 57, 80	0
3	2D	275/276 (99%)	-0.31	3 (1%) 78 70	24, 43, 60, 80	0
4	1E	204/206 (99%)	-0.27	1 (0%) 87 82	20, 44, 67, 83	0
4	2E	204/206 (99%)	-0.19	0 100 100	24, 48, 69, 84	0
5	1F	203/210 (96%)	0.02	1 (0%) 87 82	23, 51, 77, 93	0
5	2F	203/210 (96%)	0.08	1 (0%) 87 82	27, 55, 79, 94	0
6	1G	181/182 (99%)	0.51	10 (5%) 30 23	52, 70, 83, 96	0
6	2G	181/182 (99%)	1.13	22 (12%) 8 6	58, 74, 85, 96	0
7	1H	174/180 (96%)	0.61	5 (2%) 53 43	49, 65, 77, 89	0
7	2H	174/180 (96%)	0.97	8 (4%) 37 29	55, 70, 81, 91	0
8	1I	146/148 (98%)	0.38	5 (3%) 48 39	48, 75, 85, 89	0
8	2I	146/148 (98%)	0.44	4 (2%) 56 46	51, 76, 86, 91	0
9	1N	140/140 (100%)	0.02	1 (0%) 84 77	33, 47, 69, 82	0
9	2N	140/140 (100%)	0.01	0 100 100	36, 52, 71, 84	0
10	1O	122/122 (100%)	-0.23	0 100 100	32, 44, 63, 71	0
10	2O	122/122 (100%)	-0.18	0 100 100	35, 47, 64, 72	0
11	1P	149/150 (99%)	0.07	0 100 100	24, 54, 76, 85	0
11	2P	149/150 (99%)	0.17	0 100 100	27, 58, 78, 88	0
12	1Q	141/141 (100%)	0.14	3 (2%) 63 54	33, 50, 66, 88	0
12	2Q	141/141 (100%)	0.22	3 (2%) 63 54	37, 54, 69, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.11	0 100 100	31, 40, 55, 66	0
13	2R	118/118 (100%)	-0.19	0 100 100	34, 44, 56, 69	0
14	1S	110/112 (98%)	0.32	2 (1%) 67 58	46, 63, 73, 77	0
14	2S	110/112 (98%)	1.13	13 (11%) 9 7	52, 67, 77, 80	0
15	1T	131/146 (89%)	0.07	4 (3%) 51 41	37, 50, 75, 86	0
15	2T	131/146 (89%)	0.03	2 (1%) 72 63	39, 53, 76, 85	0
16	1U	116/118 (98%)	-0.09	1 (0%) 81 74	28, 40, 56, 75	0
16	2U	116/118 (98%)	-0.00	0 100 100	32, 45, 62, 76	0
17	1V	101/101 (100%)	0.03	0 100 100	29, 49, 68, 80	0
17	2V	101/101 (100%)	0.15	0 100 100	32, 56, 73, 80	0
18	1W	112/113 (99%)	-0.30	0 100 100	27, 37, 57, 91	0
18	2W	112/113 (99%)	-0.26	1 (0%) 81 74	31, 40, 61, 91	0
19	1X	95/96 (98%)	0.10	2 (2%) 63 54	28, 47, 69, 80	0
19	2X	95/96 (98%)	0.32	3 (3%) 50 40	33, 51, 70, 81	0
20	1Y	107/110 (97%)	0.46	1 (0%) 81 74	45, 59, 78, 87	0
20	2Y	107/110 (97%)	0.74	6 (5%) 30 23	51, 63, 81, 90	0
21	1Z	186/206 (90%)	0.33	2 (1%) 78 70	52, 68, 83, 93	0
21	2Z	186/206 (90%)	0.79	8 (4%) 40 31	55, 72, 85, 94	0
22	10	75/85 (88%)	-0.44	0 100 100	16, 36, 52, 67	0
22	20	75/85 (88%)	0.58	3 (4%) 42 33	40, 64, 77, 80	0
23	11	97/98 (98%)	-0.07	1 (1%) 79 72	30, 48, 75, 79	0
23	21	97/98 (98%)	0.13	2 (2%) 63 54	34, 51, 76, 81	0
24	12	70/72 (97%)	0.42	4 (5%) 29 22	42, 59, 73, 82	0
24	22	70/72 (97%)	0.58	2 (2%) 53 43	47, 63, 76, 80	0
25	13	59/60 (98%)	0.17	0 100 100	32, 46, 67, 78	0
25	23	59/60 (98%)	0.19	1 (1%) 69 60	37, 51, 71, 82	0
26	14	69/71 (97%)	0.84	12 (17%) 4 3	63, 82, 95, 99	0
26	24	69/71 (97%)	1.39	17 (24%) 2 1	69, 85, 96, 100	0
27	15	59/60 (98%)	-0.45	0 100 100	22, 38, 57, 73	0
27	25	59/60 (98%)	-0.32	0 100 100	27, 42, 61, 74	0
28	16	53/54 (98%)	-0.22	0 100 100	37, 48, 66, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.06	0 100 100	40, 52, 63, 69	0
29	17	48/49 (97%)	-0.21	2 (4%) 40 32	26, 31, 65, 78	0
29	27	48/49 (97%)	-0.19	2 (4%) 40 32	29, 34, 65, 80	0
30	18	64/65 (98%)	-0.02	0 100 100	34, 41, 53, 61	0
30	28	64/65 (98%)	0.12	0 100 100	37, 45, 57, 64	0
31	19	37/37 (100%)	0.39	2 (5%) 31 24	40, 49, 69, 74	0
31	29	37/37 (100%)	0.74	2 (5%) 31 24	44, 54, 70, 76	0
32	1a	1477/1521 (97%)	0.05	28 (1%) 66 57	35, 71, 97, 112	0
32	2a	1483/1521 (97%)	0.24	26 (1%) 67 58	45, 79, 100, 110	0
33	1b	231/256 (90%)	0.93	24 (10%) 11 8	66, 83, 94, 100	0
33	2b	231/256 (90%)	1.18	35 (15%) 5 4	72, 89, 96, 104	0
34	1c	206/239 (86%)	0.93	18 (8%) 16 11	68, 83, 91, 96	0
34	2c	206/239 (86%)	1.22	26 (12%) 8 6	70, 85, 92, 95	0
35	1d	208/209 (99%)	0.85	13 (6%) 26 19	54, 76, 88, 96	0
35	2d	208/209 (99%)	0.67	6 (2%) 53 43	62, 75, 86, 92	0
36	1e	148/162 (91%)	0.24	3 (2%) 65 56	46, 66, 78, 89	0
36	2e	148/162 (91%)	0.57	4 (2%) 56 46	60, 75, 84, 92	0
37	1f	100/101 (99%)	0.43	3 (3%) 52 42	58, 74, 83, 90	0
37	2f	100/101 (99%)	0.27	1 (1%) 79 72	60, 74, 84, 88	0
38	1g	155/156 (99%)	0.66	12 (7%) 19 14	61, 79, 93, 97	0
38	2g	155/156 (99%)	0.87	21 (13%) 7 5	69, 80, 92, 97	0
39	1h	137/138 (99%)	0.32	0 100 100	54, 69, 79, 86	0
39	2h	137/138 (99%)	0.65	7 (5%) 33 25	65, 77, 86, 91	0
40	1i	127/128 (99%)	1.12	21 (16%) 4 3	64, 86, 93, 96	0
40	2i	127/128 (99%)	1.94	50 (39%) 1 0	64, 88, 95, 96	0
41	1j	97/105 (92%)	1.44	21 (21%) 2 2	63, 86, 95, 98	0
41	2j	96/105 (91%)	1.88	41 (42%) 0 0	76, 91, 99, 101	0
42	1k	114/129 (88%)	0.24	3 (2%) 57 47	40, 69, 83, 92	0
42	2k	114/129 (88%)	0.38	4 (3%) 47 38	53, 76, 86, 93	0
43	1l	122/132 (92%)	0.34	6 (4%) 35 27	46, 62, 73, 79	0
43	2l	122/132 (92%)	0.46	3 (2%) 58 48	56, 69, 78, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	118/126 (93%)	0.67	6 (5%) 33 25	65, 80, 87, 92	0
44	2m	116/126 (92%)	1.32	15 (12%) 7 6	70, 83, 89, 93	0
45	1n	60/61 (98%)	1.10	8 (13%) 7 5	63, 75, 88, 89	0
45	2n	60/61 (98%)	2.23	32 (53%) 0 0	76, 87, 92, 96	0
46	1o	88/89 (98%)	0.29	1 (1%) 78 70	51, 67, 82, 90	0
46	2o	88/89 (98%)	0.32	0 100 100	59, 73, 83, 89	0
47	1p	82/88 (93%)	1.07	8 (9%) 13 9	60, 78, 87, 93	0
47	2p	82/88 (93%)	0.71	2 (2%) 59 49	62, 70, 82, 91	0
48	1q	99/105 (94%)	0.41	0 100 100	51, 69, 80, 84	0
48	2q	99/105 (94%)	0.48	4 (4%) 42 33	59, 73, 83, 90	0
49	1r	68/88 (77%)	0.31	1 (1%) 72 63	58, 70, 84, 87	0
49	2r	68/88 (77%)	0.33	0 100 100	63, 73, 85, 90	0
50	1s	84/93 (90%)	0.91	6 (7%) 22 16	68, 81, 90, 95	0
50	2s	83/93 (89%)	1.78	30 (36%) 1 0	82, 91, 99, 104	0
51	1t	96/106 (90%)	0.81	8 (8%) 17 12	61, 75, 84, 93	0
51	2t	96/106 (90%)	0.59	7 (7%) 21 15	55, 73, 84, 88	0
52	1u	23/27 (85%)	1.44	5 (21%) 2 2	71, 78, 80, 84	0
52	2u	23/27 (85%)	2.26	14 (60%) 0 0	73, 80, 85, 86	0
53	1v	5/24 (20%)	1.06	1 (20%) 3 2	61, 64, 90, 97	0
53	2v	5/24 (20%)	0.71	1 (20%) 3 2	65, 68, 91, 97	0
54	1x	72/77 (93%)	-0.43	0 100 100	28, 58, 83, 92	0
54	2x	72/77 (93%)	0.06	1 (1%) 73 64	41, 79, 91, 102	0
55	1z	12/14 (85%)	1.12	4 (33%) 1 1	23, 39, 59, 84	0
55	2z	12/14 (85%)	0.79	2 (16%) 4 3	26, 42, 64, 85	0
All	All	20520/21472 (95%)	0.14	747 (3%) 46 37	16, 62, 92, 112	0

The worst 5 of 747 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	2z	12	PRO	7.2
32	1a	980	G	6.1
7	1H	2	SER	5.8
55	1z	12	PRO	5.8
32	1a	981	G	5.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	PSU	2x	55	20/21	0.77	0.13	67,79,90,98	0
54	5MU	2x	54	21/22	0.87	0.11	66,79,92,102	0
54	5MC	2x	32	21/22	0.89	0.14	72,77,87,99	0
54	4SU	2x	8	20/21	0.91	0.09	68,80,91,95	0
54	5MU	1x	54	21/22	0.92	0.09	48,57,75,82	0
54	PSU	1x	55	20/21	0.93	0.08	49,60,75,77	0
54	5MC	1x	32	21/22	0.94	0.10	50,57,66,75	0
54	4SU	1x	8	20/21	0.96	0.07	51,58,69,71	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
56	MG	1a	1791	1/1	0.21	0.29	89,89,89,89	0
56	MG	2a	3137	1/1	0.24	0.22	97,97,97,97	0
56	MG	1A	3409	1/1	0.35	0.37	81,81,81,81	0
56	MG	1a	1780	1/1	0.49	0.23	93,93,93,93	0
56	MG	1B	214	1/1	0.52	0.24	80,80,80,80	0
56	MG	2A	3469	1/1	0.60	0.29	67,67,67,67	0
56	MG	1A	3893	1/1	0.60	0.19	69,69,69,69	0
56	MG	2a	3244	1/1	0.60	0.20	76,76,76,76	0
56	MG	1a	1787	1/1	0.61	0.30	70,70,70,70	0
56	MG	2a	3152	1/1	0.61	0.26	89,89,89,89	0
56	MG	2a	3077	1/1	0.61	0.24	95,95,95,95	0
56	MG	1a	1788	1/1	0.62	0.31	81,81,81,81	0
56	MG	2a	3027	1/1	0.63	0.13	88,88,88,88	0
56	MG	2A	3495	1/1	0.64	0.36	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1812	1/1	0.64	0.30	78,78,78,78	0
56	MG	1a	1789	1/1	0.64	0.26	78,78,78,78	0
56	MG	1A	3451	1/1	0.65	0.17	81,81,81,81	0
56	MG	2a	3168	1/1	0.65	0.17	83,83,83,83	0
56	MG	2a	3220	1/1	0.65	0.44	87,87,87,87	0
56	MG	1A	3339	1/1	0.65	0.25	78,78,78,78	0
56	MG	2a	3213	1/1	0.66	0.18	87,87,87,87	0
56	MG	1A	3954	1/1	0.66	0.23	83,83,83,83	0
56	MG	1a	1804	1/1	0.66	0.23	88,88,88,88	0
56	MG	1A	3940	1/1	0.67	0.20	78,78,78,78	0
56	MG	1a	1786	1/1	0.67	0.25	83,83,83,83	0
56	MG	1a	1881	1/1	0.67	0.27	84,84,84,84	0
56	MG	2a	3040	1/1	0.67	0.27	83,83,83,83	0
56	MG	2A	3459	1/1	0.67	0.26	70,70,70,70	0
56	MG	2a	3108	1/1	0.67	0.23	79,79,79,79	0
56	MG	1A	4020	1/1	0.68	0.21	67,67,67,67	0
56	MG	1A	3481	1/1	0.68	0.18	76,76,76,76	0
56	MG	1a	1760	1/1	0.69	0.33	78,78,78,78	0
56	MG	1a	1813	1/1	0.69	0.15	99,99,99,99	0
56	MG	2a	3149	1/1	0.69	0.30	100,100,100,100	0
56	MG	2A	3502	1/1	0.69	0.27	75,75,75,75	0
56	MG	1a	1762	1/1	0.70	0.16	80,80,80,80	0
56	MG	2a	3178	1/1	0.70	0.31	75,75,75,75	0
56	MG	2a	3023	1/1	0.70	0.35	74,74,74,74	0
56	MG	1A	3340	1/1	0.70	0.16	56,56,56,56	0
56	MG	2a	3155	1/1	0.70	0.22	91,91,91,91	0
56	MG	2A	3578	1/1	0.71	0.14	58,58,58,58	0
56	MG	1A	3262	1/1	0.71	0.16	58,58,58,58	0
56	MG	2a	3186	1/1	0.71	0.22	80,80,80,80	0
56	MG	2a	3191	1/1	0.71	0.28	66,66,66,66	0
56	MG	1a	1667	1/1	0.71	0.45	68,68,68,68	0
56	MG	1a	1753	1/1	0.71	0.15	83,83,83,83	0
56	MG	2A	3437	1/1	0.71	0.26	83,83,83,83	0
56	MG	1a	1613	1/1	0.72	0.27	76,76,76,76	0
56	MG	1A	3476	1/1	0.72	0.16	66,66,66,66	0
56	MG	1a	1688	1/1	0.72	0.25	76,76,76,76	0
56	MG	1A	3990	1/1	0.72	0.28	64,64,64,64	0
56	MG	2A	3525	1/1	0.72	0.16	53,53,53,53	0
56	MG	1a	1826	1/1	0.72	0.26	80,80,80,80	0
56	MG	2B	3008	1/1	0.72	0.23	73,73,73,73	0
56	MG	1a	1756	1/1	0.72	0.26	93,93,93,93	0
56	MG	1r	3002	1/1	0.72	0.20	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3256	1/1	0.72	0.16	79,79,79,79	0
56	MG	2a	3041	1/1	0.72	0.24	79,79,79,79	0
56	MG	2a	3243	1/1	0.72	0.16	58,58,58,58	0
56	MG	1B	225	1/1	0.72	0.14	77,77,77,77	0
56	MG	2a	3056	1/1	0.73	0.48	79,79,79,79	0
56	MG	1a	1889	1/1	0.73	0.22	64,64,64,64	0
56	MG	1A	3994	1/1	0.73	0.15	51,51,51,51	0
56	MG	2A	3180	1/1	0.73	0.23	52,52,52,52	0
56	MG	1A	3068	1/1	0.73	0.25	67,67,67,67	0
56	MG	1a	1768	1/1	0.74	0.20	90,90,90,90	0
56	MG	1l	101	1/1	0.74	0.15	83,83,83,83	0
56	MG	2a	3197	1/1	0.74	0.22	74,74,74,74	0
56	MG	1A	3984	1/1	0.74	0.21	77,77,77,77	0
56	MG	1A	3069	1/1	0.74	0.10	65,65,65,65	0
56	MG	2G	3001	1/1	0.74	0.15	60,60,60,60	0
56	MG	1E	307	1/1	0.74	0.19	74,74,74,74	0
56	MG	1A	3508	1/1	0.75	0.15	64,64,64,64	0
56	MG	2a	3084	1/1	0.75	0.22	75,75,75,75	0
56	MG	1A	3964	1/1	0.75	0.25	76,76,76,76	0
56	MG	1A	3322	1/1	0.75	0.20	63,63,63,63	0
56	MG	1A	3901	1/1	0.75	0.21	68,68,68,68	0
56	MG	1G	3002	1/1	0.75	0.24	69,69,69,69	0
56	MG	1x	110	1/1	0.75	0.26	78,78,78,78	0
56	MG	2B	3002	1/1	0.75	0.21	70,70,70,70	0
56	MG	2a	3176	1/1	0.75	0.34	87,87,87,87	0
56	MG	2A	3023	1/1	0.75	0.07	55,55,55,55	0
56	MG	1N	204	1/1	0.75	0.15	59,59,59,59	0
56	MG	1A	3364	1/1	0.75	0.26	57,57,57,57	0
56	MG	2A	3288	1/1	0.75	0.20	70,70,70,70	0
56	MG	2A	3394	1/1	0.75	0.27	61,61,61,61	0
56	MG	2A	3395	1/1	0.75	0.19	78,78,78,78	0
56	MG	2a	3047	1/1	0.75	0.11	89,89,89,89	0
56	MG	14	502	1/1	0.75	0.23	79,79,79,79	0
56	MG	1B	221	1/1	0.76	0.17	63,63,63,63	0
56	MG	2a	3048	1/1	0.76	0.15	91,91,91,91	0
56	MG	1A	3514	1/1	0.76	0.19	72,72,72,72	0
56	MG	1a	1891	1/1	0.76	0.32	82,82,82,82	0
56	MG	1A	3817	1/1	0.76	0.26	61,61,61,61	0
56	MG	18	101	1/1	0.76	0.21	66,66,66,66	0
56	MG	1a	1759	1/1	0.76	0.23	82,82,82,82	0
56	MG	2a	3215	1/1	0.76	0.32	80,80,80,80	0
56	MG	1a	1820	1/1	0.76	0.31	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3439	1/1	0.76	0.17	50,50,50,50	0
56	MG	2A	3503	1/1	0.76	0.13	61,61,61,61	0
56	MG	2a	3014	1/1	0.77	0.28	74,74,74,74	0
56	MG	1A	3665	1/1	0.77	0.23	64,64,64,64	0
56	MG	2a	3153	1/1	0.77	0.16	99,99,99,99	0
56	MG	1A	3745	1/1	0.77	0.26	54,54,54,54	0
56	MG	2a	3158	1/1	0.77	0.32	72,72,72,72	0
56	MG	2A	3498	1/1	0.77	0.13	69,69,69,69	0
56	MG	1a	1766	1/1	0.77	0.21	79,79,79,79	0
56	MG	1a	1752	1/1	0.77	0.21	72,72,72,72	0
56	MG	2a	3124	1/1	0.78	0.33	76,76,76,76	0
56	MG	2a	3133	1/1	0.78	0.17	93,93,93,93	0
56	MG	2A	3278	1/1	0.78	0.17	65,65,65,65	0
56	MG	1A	3921	1/1	0.78	0.18	80,80,80,80	0
56	MG	1N	201	1/1	0.78	0.23	70,70,70,70	0
56	MG	2a	3010	1/1	0.78	0.26	83,83,83,83	0
56	MG	1A	3501	1/1	0.78	0.14	83,83,83,83	0
56	MG	2A	3404	1/1	0.78	0.24	69,69,69,69	0
56	MG	1P	201	1/1	0.78	0.21	55,55,55,55	0
56	MG	2a	3034	1/1	0.78	0.42	72,72,72,72	0
56	MG	1A	3941	1/1	0.78	0.22	73,73,73,73	0
56	MG	1A	3472	1/1	0.78	0.17	66,66,66,66	0
56	MG	1a	1795	1/1	0.78	0.16	64,64,64,64	0
56	MG	1A	3303	1/1	0.78	0.24	48,48,48,48	0
56	MG	2A	3137	1/1	0.78	0.15	55,55,55,55	0
56	MG	1A	3980	1/1	0.78	0.39	63,63,63,63	0
56	MG	2a	3081	1/1	0.78	0.25	69,69,69,69	0
56	MG	2a	3233	1/1	0.78	0.25	66,66,66,66	0
56	MG	2A	3206	1/1	0.78	0.19	64,64,64,64	0
56	MG	1A	3098	1/1	0.78	0.30	71,71,71,71	0
56	MG	2d	503	1/1	0.78	0.21	72,72,72,72	0
56	MG	2A	3202	1/1	0.79	0.10	50,50,50,50	0
56	MG	2a	3088	1/1	0.79	0.26	73,73,73,73	0
56	MG	1A	3368	1/1	0.79	0.22	50,50,50,50	0
56	MG	2A	3529	1/1	0.79	0.16	62,62,62,62	0
56	MG	1A	3815	1/1	0.79	0.14	52,52,52,52	0
56	MG	2A	3267	1/1	0.79	0.24	63,63,63,63	0
56	MG	1A	3415	1/1	0.79	0.19	73,73,73,73	0
56	MG	2B	3010	1/1	0.79	0.26	66,66,66,66	0
56	MG	1A	3842	1/1	0.79	0.29	55,55,55,55	0
56	MG	2a	3004	1/1	0.79	0.12	87,87,87,87	0
56	MG	2A	3320	1/1	0.79	0.19	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3159	1/1	0.79	0.24	76,76,76,76	0
56	MG	1T	203	1/1	0.79	0.17	69,69,69,69	0
56	MG	2a	3020	1/1	0.79	0.15	72,72,72,72	0
56	MG	1a	1906	1/1	0.79	0.12	83,83,83,83	0
56	MG	1A	3852	1/1	0.79	0.21	72,72,72,72	0
56	MG	1B	223	1/1	0.79	0.17	74,74,74,74	0
56	MG	2A	3438	1/1	0.79	0.33	70,70,70,70	0
56	MG	2a	3201	1/1	0.79	0.15	83,83,83,83	0
56	MG	2a	3210	1/1	0.79	0.25	69,69,69,69	0
56	MG	2A	3457	1/1	0.79	0.20	55,55,55,55	0
56	MG	1A	3438	1/1	0.79	0.15	62,62,62,62	0
56	MG	2A	3083	1/1	0.79	0.23	66,66,66,66	0
56	MG	2A	3093	1/1	0.79	0.27	64,64,64,64	0
56	MG	2a	3058	1/1	0.79	0.13	66,66,66,66	0
56	MG	1A	3376	1/1	0.79	0.17	60,60,60,60	0
56	MG	1a	1617	1/1	0.79	0.39	74,74,74,74	0
56	MG	2A	3360	1/1	0.80	0.20	73,73,73,73	0
56	MG	1A	3011	1/1	0.80	0.39	65,65,65,65	0
56	MG	2a	3144	1/1	0.80	0.25	75,75,75,75	0
56	MG	2a	3002	1/1	0.80	0.25	68,68,68,68	0
56	MG	1A	3949	1/1	0.80	0.17	59,59,59,59	0
56	MG	1A	3330	1/1	0.80	0.23	62,62,62,62	0
56	MG	2a	3154	1/1	0.80	0.25	84,84,84,84	0
56	MG	2A	3431	1/1	0.80	0.19	68,68,68,68	0
56	MG	1a	1663	1/1	0.80	0.18	67,67,67,67	0
56	MG	1A	3850	1/1	0.80	0.23	80,80,80,80	0
56	MG	1A	3073	1/1	0.80	0.12	74,74,74,74	0
56	MG	2a	3169	1/1	0.80	0.13	75,75,75,75	0
56	MG	1a	1712	1/1	0.80	0.27	65,65,65,65	0
56	MG	2A	3462	1/1	0.80	0.27	74,74,74,74	0
56	MG	1A	3867	1/1	0.80	0.33	40,40,40,40	0
56	MG	1a	1800	1/1	0.80	0.21	84,84,84,84	0
56	MG	1A	3989	1/1	0.80	0.27	70,70,70,70	0
56	MG	1a	1810	1/1	0.80	0.18	86,86,86,86	0
56	MG	1A	3402	1/1	0.80	0.17	73,73,73,73	0
56	MG	1A	3462	1/1	0.80	0.20	45,45,45,45	0
56	MG	1T	205	1/1	0.80	0.23	66,66,66,66	0
56	MG	1A	3091	1/1	0.80	0.21	61,61,61,61	0
56	MG	2a	3226	1/1	0.80	0.36	75,75,75,75	0
56	MG	2A	3580	1/1	0.80	0.17	51,51,51,51	0
56	MG	2a	3099	1/1	0.80	0.27	63,63,63,63	0
56	MG	1a	1866	1/1	0.80	0.39	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3412	1/1	0.80	0.29	77,77,77,77	0
56	MG	2n	502	1/1	0.80	0.43	73,73,73,73	0
56	MG	2A	3364	1/1	0.81	0.15	55,55,55,55	0
56	MG	2A	3390	1/1	0.81	0.21	63,63,63,63	0
56	MG	1A	3816	1/1	0.81	0.11	67,67,67,67	0
56	MG	1x	107	1/1	0.81	0.16	64,64,64,64	0
56	MG	2a	3007	1/1	0.81	0.20	91,91,91,91	0
56	MG	1A	3307	1/1	0.81	0.20	75,75,75,75	0
56	MG	1A	3702	1/1	0.81	0.20	73,73,73,73	0
56	MG	2a	3017	1/1	0.81	0.31	68,68,68,68	0
56	MG	2A	3025	1/1	0.81	0.20	61,61,61,61	0
56	MG	2A	3074	1/1	0.81	0.12	47,47,47,47	0
56	MG	2a	3164	1/1	0.81	0.30	65,65,65,65	0
56	MG	2A	3451	1/1	0.81	0.18	63,63,63,63	0
56	MG	1A	3963	1/1	0.81	0.20	54,54,54,54	0
56	MG	1B	208	1/1	0.81	0.20	61,61,61,61	0
56	MG	2A	3135	1/1	0.81	0.10	48,48,48,48	0
56	MG	2a	3045	1/1	0.81	0.10	81,81,81,81	0
56	MG	1a	1680	1/1	0.81	0.20	57,57,57,57	0
56	MG	1a	1770	1/1	0.81	0.16	87,87,87,87	0
56	MG	1A	3296	1/1	0.81	0.20	47,47,47,47	0
56	MG	2a	3205	1/1	0.81	0.32	78,78,78,78	0
56	MG	1a	1827	1/1	0.81	0.22	63,63,63,63	0
56	MG	1a	1843	1/1	0.81	0.21	71,71,71,71	0
56	MG	1a	1695	1/1	0.81	0.20	77,77,77,77	0
56	MG	1A	3922	1/1	0.81	0.19	75,75,75,75	0
56	MG	1A	3640	1/1	0.81	0.16	70,70,70,70	0
56	MG	1A	3986	1/1	0.81	0.16	44,44,44,44	0
56	MG	2a	3102	1/1	0.81	0.32	72,72,72,72	0
56	MG	2A	3333	1/1	0.81	0.25	61,61,61,61	0
56	MG	1a	1754	1/1	0.81	0.13	53,53,53,53	0
56	MG	2a	3125	1/1	0.81	0.31	66,66,66,66	0
56	MG	1A	3297	1/1	0.82	0.29	59,59,59,59	0
56	MG	2A	3359	1/1	0.82	0.20	75,75,75,75	0
56	MG	2a	3140	1/1	0.82	0.23	83,83,83,83	0
56	MG	1b	3001	1/1	0.82	0.25	83,83,83,83	0
56	MG	1q	202	1/1	0.82	0.26	62,62,62,62	0
56	MG	1A	3022	1/1	0.82	0.14	66,66,66,66	0
56	MG	1A	3444	1/1	0.82	0.17	65,65,65,65	0
56	MG	1A	3450	1/1	0.82	0.19	64,64,64,64	0
56	MG	1a	1748	1/1	0.82	0.25	61,61,61,61	0
56	MG	1A	3575	1/1	0.82	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3068	1/1	0.82	0.29	68,68,68,68	0
56	MG	1A	3585	1/1	0.82	0.09	68,68,68,68	0
56	MG	2A	3441	1/1	0.82	0.15	51,51,51,51	0
56	MG	1A	3866	1/1	0.82	0.17	65,65,65,65	0
56	MG	2a	3175	1/1	0.82	0.17	53,53,53,53	0
56	MG	2a	3038	1/1	0.82	0.18	85,85,85,85	0
56	MG	2A	3453	1/1	0.82	0.29	83,83,83,83	0
56	MG	1A	3277	1/1	0.82	0.23	68,68,68,68	0
56	MG	2a	3188	1/1	0.82	0.27	74,74,74,74	0
56	MG	2A	3132	1/1	0.82	0.12	62,62,62,62	0
56	MG	1A	3341	1/1	0.82	0.14	58,58,58,58	0
56	MG	1A	3686	1/1	0.82	0.16	58,58,58,58	0
56	MG	1A	3345	1/1	0.82	0.22	64,64,64,64	0
56	MG	1A	3001	1/1	0.82	0.15	45,45,45,45	0
56	MG	1a	1836	1/1	0.82	0.25	59,59,59,59	0
56	MG	2A	3246	1/1	0.82	0.18	67,67,67,67	0
56	MG	2A	3509	1/1	0.82	0.17	80,80,80,80	0
56	MG	1A	3808	1/1	0.82	0.32	57,57,57,57	0
56	MG	1a	1624	1/1	0.82	0.16	65,65,65,65	0
56	MG	2A	3565	1/1	0.82	0.17	62,62,62,62	0
56	MG	1a	1774	1/1	0.82	0.26	63,63,63,63	0
56	MG	1A	3811	1/1	0.82	0.12	50,50,50,50	0
56	MG	1A	3943	1/1	0.82	0.22	35,35,35,35	0
56	MG	1a	1775	1/1	0.83	0.28	65,65,65,65	0
56	MG	1A	3480	1/1	0.83	0.20	75,75,75,75	0
56	MG	2a	3089	1/1	0.83	0.21	75,75,75,75	0
56	MG	2A	3032	1/1	0.83	0.24	50,50,50,50	0
56	MG	1a	1782	1/1	0.83	0.12	67,67,67,67	0
56	MG	1A	4006	1/1	0.83	0.11	77,77,77,77	0
56	MG	1a	1601	1/1	0.83	0.15	66,66,66,66	0
56	MG	2A	3500	1/1	0.83	0.13	57,57,57,57	0
56	MG	1A	3716	1/1	0.83	0.14	53,53,53,53	0
56	MG	1A	3244	1/1	0.83	0.24	55,55,55,55	0
56	MG	2a	3138	1/1	0.83	0.20	73,73,73,73	0
56	MG	1A	3491	1/1	0.83	0.13	83,83,83,83	0
56	MG	1a	1654	1/1	0.83	0.15	67,67,67,67	0
56	MG	1B	215	1/1	0.83	0.13	68,68,68,68	0
56	MG	1A	3020	1/1	0.83	0.16	56,56,56,56	0
56	MG	2A	3205	1/1	0.83	0.17	62,62,62,62	0
56	MG	1A	3442	1/1	0.83	0.40	57,57,57,57	0
56	MG	2A	3240	1/1	0.83	0.29	57,57,57,57	0
56	MG	1A	3401	1/1	0.83	0.15	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3516	1/1	0.83	0.13	75,75,75,75	0
56	MG	1A	3839	1/1	0.83	0.12	54,54,54,54	0
56	MG	2a	3001	1/1	0.83	0.23	54,54,54,54	0
56	MG	1a	1735	1/1	0.83	0.19	72,72,72,72	0
56	MG	1H	204	1/1	0.83	0.12	62,62,62,62	0
56	MG	2A	3297	1/1	0.83	0.13	49,49,49,49	0
56	MG	1A	3556	1/1	0.83	0.17	70,70,70,70	0
56	MG	2a	3182	1/1	0.83	0.10	64,64,64,64	0
56	MG	1N	202	1/1	0.83	0.30	49,49,49,49	0
56	MG	2A	3335	1/1	0.83	0.18	52,52,52,52	0
56	MG	1A	3304	1/1	0.83	0.18	74,74,74,74	0
56	MG	2a	3194	1/1	0.83	0.39	75,75,75,75	0
56	MG	1a	1867	1/1	0.83	0.14	51,51,51,51	0
56	MG	1O	201	1/1	0.83	0.13	54,54,54,54	0
56	MG	1A	3161	1/1	0.83	0.18	61,61,61,61	0
56	MG	2A	3393	1/1	0.83	0.19	71,71,71,71	0
56	MG	1A	3308	1/1	0.83	0.30	64,64,64,64	0
56	MG	1A	3167	1/1	0.83	0.19	59,59,59,59	0
56	MG	1Y	502	1/1	0.83	0.23	59,59,59,59	0
56	MG	1Z	303	1/1	0.83	0.11	64,64,64,64	0
56	MG	2a	3227	1/1	0.83	0.24	81,81,81,81	0
56	MG	10	105	1/1	0.83	0.24	57,57,57,57	0
56	MG	1x	101	1/1	0.83	0.24	69,69,69,69	0
56	MG	1a	1771	1/1	0.83	0.15	75,75,75,75	0
56	MG	1A	3422	1/1	0.83	0.10	72,72,72,72	0
56	MG	1x	111	1/1	0.83	0.26	80,80,80,80	0
56	MG	2q	201	1/1	0.83	0.25	71,71,71,71	0
56	MG	2x	3004	1/1	0.83	0.15	74,74,74,74	0
56	MG	1a	1604	1/1	0.84	0.32	70,70,70,70	0
56	MG	1A	3315	1/1	0.84	0.08	51,51,51,51	0
56	MG	1A	3798	1/1	0.84	0.16	59,59,59,59	0
56	MG	1A	3054	1/1	0.84	0.30	56,56,56,56	0
56	MG	1a	1625	1/1	0.84	0.22	78,78,78,78	0
56	MG	1a	1650	1/1	0.84	0.30	72,72,72,72	0
56	MG	1a	1652	1/1	0.84	0.33	65,65,65,65	0
56	MG	1A	3219	1/1	0.84	0.23	63,63,63,63	0
56	MG	2A	3076	1/1	0.84	0.27	61,61,61,61	0
56	MG	2A	3482	1/1	0.84	0.23	63,63,63,63	0
56	MG	2a	3134	1/1	0.84	0.33	79,79,79,79	0
56	MG	2A	3082	1/1	0.84	0.19	56,56,56,56	0
56	MG	1E	303	1/1	0.84	0.30	51,51,51,51	0
56	MG	1A	3331	1/1	0.84	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3142	1/1	0.84	0.18	83,83,83,83	0
56	MG	2A	3098	1/1	0.84	0.16	53,53,53,53	0
56	MG	2A	3129	1/1	0.84	0.13	55,55,55,55	0
56	MG	2a	3150	1/1	0.84	0.18	63,63,63,63	0
56	MG	1a	1677	1/1	0.84	0.25	61,61,61,61	0
56	MG	2A	3521	1/1	0.84	0.12	59,59,59,59	0
56	MG	1A	3067	1/1	0.84	0.11	64,64,64,64	0
56	MG	1A	3517	1/1	0.84	0.25	56,56,56,56	0
56	MG	2a	3157	1/1	0.84	0.33	66,66,66,66	0
56	MG	2A	3174	1/1	0.84	0.17	48,48,48,48	0
56	MG	1a	1807	1/1	0.84	0.13	71,71,71,71	0
56	MG	1a	1690	1/1	0.84	0.25	82,82,82,82	0
56	MG	1A	3837	1/1	0.84	0.23	74,74,74,74	0
56	MG	1A	3039	1/1	0.84	0.13	54,54,54,54	0
56	MG	1A	3459	1/1	0.84	0.20	57,57,57,57	0
56	MG	1A	3053	1/1	0.84	0.18	38,38,38,38	0
56	MG	1A	3413	1/1	0.84	0.14	60,60,60,60	0
56	MG	1A	3859	1/1	0.84	0.16	59,59,59,59	0
56	MG	1A	3991	1/1	0.84	0.20	53,53,53,53	0
56	MG	1a	1864	1/1	0.84	0.20	68,68,68,68	0
56	MG	2a	3008	1/1	0.84	0.27	60,60,60,60	0
56	MG	2A	3292	1/1	0.84	0.13	60,60,60,60	0
56	MG	1a	1865	1/1	0.84	0.13	65,65,65,65	0
56	MG	1a	1755	1/1	0.84	0.17	60,60,60,60	0
56	MG	1A	3414	1/1	0.84	0.17	79,79,79,79	0
56	MG	1a	1758	1/1	0.84	0.10	64,64,64,64	0
56	MG	1A	3678	1/1	0.84	0.12	67,67,67,67	0
56	MG	1A	4010	1/1	0.84	0.31	58,58,58,58	0
56	MG	2a	3036	1/1	0.84	0.16	73,73,73,73	0
56	MG	1a	1892	1/1	0.84	0.32	67,67,67,67	0
56	MG	2A	3369	1/1	0.84	0.17	65,65,65,65	0
56	MG	1A	3285	1/1	0.84	0.50	79,79,79,79	0
56	MG	2a	3234	1/1	0.84	0.32	79,79,79,79	0
56	MG	1A	4035	1/1	0.84	0.20	81,81,81,81	0
56	MG	1f	3001	1/1	0.84	0.19	66,66,66,66	0
56	MG	1A	3350	1/1	0.84	0.14	65,65,65,65	0
56	MG	2A	3396	1/1	0.84	0.15	44,44,44,44	0
56	MG	1a	1769	1/1	0.84	0.19	74,74,74,74	0
56	MG	1A	3487	1/1	0.84	0.21	64,64,64,64	0
56	MG	1A	3975	1/1	0.85	0.11	63,63,63,63	0
56	MG	1H	203	1/1	0.85	0.17	60,60,60,60	0
56	MG	1A	3642	1/1	0.85	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3239	1/1	0.85	0.19	41,41,41,41	0
56	MG	2a	3093	1/1	0.85	0.20	62,62,62,62	0
56	MG	1A	3269	1/1	0.85	0.16	56,56,56,56	0
56	MG	2A	3097	1/1	0.85	0.18	54,54,54,54	0
56	MG	1A	3513	1/1	0.85	0.12	72,72,72,72	0
56	MG	2a	3109	1/1	0.85	0.37	73,73,73,73	0
56	MG	1a	1732	1/1	0.85	0.24	53,53,53,53	0
56	MG	1A	3090	1/1	0.85	0.19	53,53,53,53	0
56	MG	1A	3479	1/1	0.85	0.17	78,78,78,78	0
56	MG	2A	3497	1/1	0.85	0.14	49,49,49,49	0
56	MG	1a	1750	1/1	0.85	0.18	72,72,72,72	0
56	MG	2A	3138	1/1	0.85	0.14	62,62,62,62	0
56	MG	1a	1829	1/1	0.85	0.21	73,73,73,73	0
56	MG	1A	3720	1/1	0.85	0.26	64,64,64,64	0
56	MG	2A	3189	1/1	0.85	0.26	61,61,61,61	0
56	MG	2a	3148	1/1	0.85	0.15	77,77,77,77	0
56	MG	2A	3511	1/1	0.85	0.10	50,50,50,50	0
56	MG	1A	3253	1/1	0.85	0.21	81,81,81,81	0
56	MG	1A	3899	1/1	0.85	0.20	53,53,53,53	0
56	MG	1A	4012	1/1	0.85	0.30	81,81,81,81	0
56	MG	2A	3535	1/1	0.85	0.12	69,69,69,69	0
56	MG	2A	3213	1/1	0.85	0.14	67,67,67,67	0
56	MG	1A	4018	1/1	0.85	0.18	62,62,62,62	0
56	MG	2A	3244	1/1	0.85	0.15	73,73,73,73	0
56	MG	1A	3765	1/1	0.85	0.16	56,56,56,56	0
56	MG	1A	3550	1/1	0.85	0.18	58,58,58,58	0
56	MG	1a	1885	1/1	0.85	0.18	66,66,66,66	0
56	MG	2E	305	1/1	0.85	0.14	68,68,68,68	0
56	MG	1B	207	1/1	0.85	0.34	70,70,70,70	0
56	MG	1A	3385	1/1	0.85	0.17	51,51,51,51	0
56	MG	2A	3290	1/1	0.85	0.17	57,57,57,57	0
56	MG	1B	213	1/1	0.85	0.33	65,65,65,65	0
56	MG	1A	3386	1/1	0.85	0.11	51,51,51,51	0
56	MG	1A	3580	1/1	0.85	0.12	68,68,68,68	0
56	MG	1a	1618	1/1	0.85	0.09	65,65,65,65	0
56	MG	1h	3001	1/1	0.85	0.19	74,74,74,74	0
56	MG	1o	3001	1/1	0.85	0.14	77,77,77,77	0
56	MG	1A	3305	1/1	0.85	0.13	83,83,83,83	0
56	MG	1A	3599	1/1	0.85	0.17	51,51,51,51	0
56	MG	1a	1641	1/1	0.85	0.17	70,70,70,70	0
56	MG	2a	3030	1/1	0.85	0.15	59,59,59,59	0
56	MG	1a	1645	1/1	0.85	0.19	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3823	1/1	0.85	0.14	39,39,39,39	0
56	MG	1D	305	1/1	0.85	0.17	58,58,58,58	0
56	MG	2a	3039	1/1	0.85	0.23	75,75,75,75	0
56	MG	2A	3006	1/1	0.85	0.08	71,71,71,71	0
56	MG	1A	3828	1/1	0.85	0.17	55,55,55,55	0
56	MG	2a	3241	1/1	0.85	0.31	67,67,67,67	0
56	MG	2A	3397	1/1	0.85	0.20	64,64,64,64	0
56	MG	1a	1658	1/1	0.85	0.13	68,68,68,68	0
56	MG	2A	3417	1/1	0.85	0.17	62,62,62,62	0
56	MG	2A	3425	1/1	0.85	0.40	72,72,72,72	0
56	MG	2p	101	1/1	0.85	0.29	68,68,68,68	0
56	MG	1A	3492	1/1	0.85	0.08	81,81,81,81	0
56	MG	1F	306	1/1	0.85	0.14	64,64,64,64	0
56	MG	2x	3006	1/1	0.85	0.16	78,78,78,78	0
56	MG	1a	1642	1/1	0.86	0.30	68,68,68,68	0
56	MG	2A	3007	1/1	0.86	0.15	50,50,50,50	0
56	MG	2A	3013	1/1	0.86	0.25	67,67,67,67	0
56	MG	2A	3022	1/1	0.86	0.08	63,63,63,63	0
56	MG	1A	3230	1/1	0.86	0.16	61,61,61,61	0
56	MG	1A	3433	1/1	0.86	0.17	50,50,50,50	0
56	MG	1A	3436	1/1	0.86	0.12	68,68,68,68	0
56	MG	2A	3038	1/1	0.86	0.21	50,50,50,50	0
56	MG	2A	3063	1/1	0.86	0.17	56,56,56,56	0
56	MG	1A	3961	1/1	0.86	0.19	47,47,47,47	0
56	MG	1E	304	1/1	0.86	0.10	64,64,64,64	0
56	MG	1A	3306	1/1	0.86	0.19	62,62,62,62	0
56	MG	1F	302	1/1	0.86	0.30	56,56,56,56	0
56	MG	1A	3594	1/1	0.86	0.23	62,62,62,62	0
56	MG	1A	3295	1/1	0.86	0.20	63,63,63,63	0
56	MG	2A	3467	1/1	0.86	0.20	58,58,58,58	0
56	MG	1A	3490	1/1	0.86	0.15	66,66,66,66	0
56	MG	1A	3982	1/1	0.86	0.24	74,74,74,74	0
56	MG	2A	3483	1/1	0.86	0.13	47,47,47,47	0
56	MG	1a	1816	1/1	0.86	0.14	88,88,88,88	0
56	MG	2a	3143	1/1	0.86	0.11	90,90,90,90	0
56	MG	1A	3146	1/1	0.86	0.09	43,43,43,43	0
56	MG	1a	1821	1/1	0.86	0.11	77,77,77,77	0
56	MG	1a	1824	1/1	0.86	0.19	52,52,52,52	0
56	MG	1a	1700	1/1	0.86	0.28	80,80,80,80	0
56	MG	2A	3154	1/1	0.86	0.28	55,55,55,55	0
56	MG	1A	3342	1/1	0.86	0.11	40,40,40,40	0
56	MG	2A	3178	1/1	0.86	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1718	1/1	0.86	0.25	64,64,64,64	0
56	MG	1A	3988	1/1	0.86	0.32	38,38,38,38	0
56	MG	2A	3198	1/1	0.86	0.28	53,53,53,53	0
56	MG	1A	3848	1/1	0.86	0.22	57,57,57,57	0
56	MG	2A	3537	1/1	0.86	0.21	59,59,59,59	0
56	MG	1A	3264	1/1	0.86	0.23	66,66,66,66	0
56	MG	1A	3505	1/1	0.86	0.10	66,66,66,66	0
56	MG	1A	3317	1/1	0.86	0.15	67,67,67,67	0
56	MG	2A	3225	1/1	0.86	0.21	42,42,42,42	0
56	MG	1A	3709	1/1	0.86	0.20	54,54,54,54	0
56	MG	1a	1878	1/1	0.86	0.17	78,78,78,78	0
56	MG	2E	304	1/1	0.86	0.57	74,74,74,74	0
56	MG	1A	3454	1/1	0.86	0.21	50,50,50,50	0
56	MG	1A	3021	1/1	0.86	0.17	48,48,48,48	0
56	MG	1a	1888	1/1	0.86	0.24	75,75,75,75	0
56	MG	2A	3268	1/1	0.86	0.15	63,63,63,63	0
56	MG	10	106	1/1	0.86	0.15	62,62,62,62	0
56	MG	1A	3247	1/1	0.86	0.35	72,72,72,72	0
56	MG	1A	3374	1/1	0.86	0.08	59,59,59,59	0
56	MG	2A	3291	1/1	0.86	0.20	56,56,56,56	0
56	MG	1A	4031	1/1	0.86	0.37	54,54,54,54	0
56	MG	2a	3217	1/1	0.86	0.22	59,59,59,59	0
56	MG	18	102	1/1	0.86	0.15	66,66,66,66	0
56	MG	2a	3225	1/1	0.86	0.31	67,67,67,67	0
56	MG	1A	3916	1/1	0.86	0.17	60,60,60,60	0
56	MG	2A	3324	1/1	0.86	0.11	64,64,64,64	0
56	MG	1B	203	1/1	0.86	0.27	66,66,66,66	0
56	MG	1a	1609	1/1	0.86	0.26	60,60,60,60	0
56	MG	2A	3357	1/1	0.86	0.15	75,75,75,75	0
56	MG	1A	3770	1/1	0.86	0.16	68,68,68,68	0
56	MG	1A	3793	1/1	0.86	0.16	72,72,72,72	0
56	MG	2d	502	1/1	0.86	0.37	61,61,61,61	0
56	MG	1t	3001	1/1	0.86	0.21	64,64,64,64	0
56	MG	1A	3927	1/1	0.86	0.30	59,59,59,59	0
56	MG	2A	3386	1/1	0.86	0.15	57,57,57,57	0
56	MG	1A	3938	1/1	0.86	0.17	47,47,47,47	0
56	MG	1A	3528	1/1	0.86	0.21	54,54,54,54	0
56	MG	1A	3474	1/1	0.86	0.12	59,59,59,59	0
56	MG	1a	1697	1/1	0.87	0.26	70,70,70,70	0
56	MG	2A	3027	1/1	0.87	0.18	64,64,64,64	0
56	MG	2A	3030	1/1	0.87	0.17	57,57,57,57	0
56	MG	2A	3391	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
56	MG	1A	3485	1/1	0.87	0.18	67,67,67,67	0
56	MG	1A	3378	1/1	0.87	0.15	53,53,53,53	0
56	MG	2a	3054	1/1	0.87	0.10	83,83,83,83	0
56	MG	2A	3048	1/1	0.87	0.25	57,57,57,57	0
56	MG	1A	3597	1/1	0.87	0.13	49,49,49,49	0
56	MG	1a	1722	1/1	0.87	0.22	60,60,60,60	0
56	MG	1a	1815	1/1	0.87	0.18	70,70,70,70	0
56	MG	1A	3337	1/1	0.87	0.18	48,48,48,48	0
56	MG	1A	3088	1/1	0.87	0.21	52,52,52,52	0
56	MG	1a	1737	1/1	0.87	0.34	66,66,66,66	0
56	MG	1a	1743	1/1	0.87	0.39	71,71,71,71	0
56	MG	1A	3393	1/1	0.87	0.21	46,46,46,46	0
56	MG	1a	1749	1/1	0.87	0.15	66,66,66,66	0
56	MG	2A	3099	1/1	0.87	0.23	45,45,45,45	0
56	MG	2A	3115	1/1	0.87	0.27	54,54,54,54	0
56	MG	2a	3118	1/1	0.87	0.24	68,68,68,68	0
56	MG	1A	3834	1/1	0.87	0.23	58,58,58,58	0
56	MG	1A	3240	1/1	0.87	0.14	48,48,48,48	0
56	MG	1A	3309	1/1	0.87	0.19	65,65,65,65	0
56	MG	1a	1848	1/1	0.87	0.12	85,85,85,85	0
56	MG	1a	1855	1/1	0.87	0.32	75,75,75,75	0
56	MG	2A	3475	1/1	0.87	0.23	67,67,67,67	0
56	MG	2A	3140	1/1	0.87	0.21	62,62,62,62	0
56	MG	1A	3680	1/1	0.87	0.21	71,71,71,71	0
56	MG	2A	3486	1/1	0.87	0.12	51,51,51,51	0
56	MG	2A	3167	1/1	0.87	0.22	58,58,58,58	0
56	MG	1A	3507	1/1	0.87	0.15	93,93,93,93	0
56	MG	1a	1619	1/1	0.87	0.17	71,71,71,71	0
56	MG	1a	1621	1/1	0.87	0.17	83,83,83,83	0
56	MG	1A	3983	1/1	0.87	0.18	62,62,62,62	0
56	MG	2A	3192	1/1	0.87	0.08	45,45,45,45	0
56	MG	2A	3196	1/1	0.87	0.09	37,37,37,37	0
56	MG	1A	3698	1/1	0.87	0.20	46,46,46,46	0
56	MG	2A	3520	1/1	0.87	0.29	75,75,75,75	0
56	MG	1a	1627	1/1	0.87	0.20	68,68,68,68	0
56	MG	2A	3523	1/1	0.87	0.15	57,57,57,57	0
56	MG	1a	1639	1/1	0.87	0.07	70,70,70,70	0
56	MG	1A	3199	1/1	0.87	0.26	48,48,48,48	0
56	MG	2A	3212	1/1	0.87	0.25	58,58,58,58	0
56	MG	1A	3858	1/1	0.87	0.14	52,52,52,52	0
56	MG	2A	3220	1/1	0.87	0.30	50,50,50,50	0
56	MG	2A	3572	1/1	0.87	0.25	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1644	1/1	0.87	0.17	68,68,68,68	0
56	MG	1a	1895	1/1	0.87	0.14	56,56,56,56	0
56	MG	1A	3316	1/1	0.87	0.10	81,81,81,81	0
56	MG	2B	3003	1/1	0.87	0.22	64,64,64,64	0
56	MG	2a	3193	1/1	0.87	0.20	76,76,76,76	0
56	MG	1A	3151	1/1	0.87	0.10	49,49,49,49	0
56	MG	2a	3195	1/1	0.87	0.15	53,53,53,53	0
56	MG	2B	3009	1/1	0.87	0.34	57,57,57,57	0
56	MG	1A	3009	1/1	0.87	0.19	50,50,50,50	0
56	MG	1a	1779	1/1	0.87	0.13	73,73,73,73	0
56	MG	1A	3738	1/1	0.87	0.10	18,18,18,18	0
56	MG	2A	3276	1/1	0.87	0.16	58,58,58,58	0
56	MG	26	101	1/1	0.87	0.08	46,46,46,46	0
56	MG	1A	3288	1/1	0.87	0.12	70,70,70,70	0
56	MG	1a	1783	1/1	0.87	0.19	75,75,75,75	0
56	MG	1a	1785	1/1	0.87	0.14	66,66,66,66	0
56	MG	1A	3421	1/1	0.87	0.10	65,65,65,65	0
56	MG	1A	3292	1/1	0.87	0.10	44,44,44,44	0
56	MG	1A	3779	1/1	0.87	0.11	45,45,45,45	0
56	MG	1A	3426	1/1	0.87	0.32	67,67,67,67	0
56	MG	2A	3005	1/1	0.87	0.22	70,70,70,70	0
56	MG	2a	3018	1/1	0.87	0.18	66,66,66,66	0
56	MG	1A	3336	1/1	0.87	0.16	61,61,61,61	0
56	MG	1A	3936	1/1	0.87	0.12	39,39,39,39	0
56	MG	2A	3345	1/1	0.87	0.19	68,68,68,68	0
56	MG	2k	3001	1/1	0.87	0.20	70,70,70,70	0
56	MG	2A	3008	1/1	0.87	0.21	59,59,59,59	0
56	MG	1A	3435	1/1	0.87	0.10	62,62,62,62	0
56	MG	2a	3035	1/1	0.87	0.20	76,76,76,76	0
56	MG	1a	1802	1/1	0.87	0.10	77,77,77,77	0
56	MG	1a	1803	1/1	0.87	0.14	80,80,80,80	0
56	MG	1A	3283	1/1	0.88	0.13	60,60,60,60	0
56	MG	1A	3903	1/1	0.88	0.15	66,66,66,66	0
56	MG	2A	3423	1/1	0.88	0.32	71,71,71,71	0
56	MG	1a	1860	1/1	0.88	0.24	61,61,61,61	0
56	MG	2A	3426	1/1	0.88	0.30	67,67,67,67	0
56	MG	2A	3429	1/1	0.88	0.27	64,64,64,64	0
56	MG	1A	3723	1/1	0.88	0.13	49,49,49,49	0
56	MG	2a	3057	1/1	0.88	0.20	75,75,75,75	0
56	MG	2A	3433	1/1	0.88	0.16	62,62,62,62	0
56	MG	2a	3076	1/1	0.88	0.29	68,68,68,68	0
56	MG	1A	3917	1/1	0.88	0.20	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3249	1/1	0.88	0.20	53,53,53,53	0
56	MG	1B	209	1/1	0.88	0.19	61,61,61,61	0
56	MG	1A	3744	1/1	0.88	0.15	63,63,63,63	0
56	MG	1A	3012	1/1	0.88	0.10	45,45,45,45	0
56	MG	2A	3455	1/1	0.88	0.18	67,67,67,67	0
56	MG	2A	3162	1/1	0.88	0.15	47,47,47,47	0
56	MG	1A	3259	1/1	0.88	0.15	66,66,66,66	0
56	MG	1A	3075	1/1	0.88	0.20	60,60,60,60	0
56	MG	2A	3463	1/1	0.88	0.11	58,58,58,58	0
56	MG	2a	3117	1/1	0.88	0.26	68,68,68,68	0
56	MG	2A	3466	1/1	0.88	0.07	56,56,56,56	0
56	MG	2a	3120	1/1	0.88	0.19	66,66,66,66	0
56	MG	1a	1626	1/1	0.88	0.25	69,69,69,69	0
56	MG	1A	3515	1/1	0.88	0.24	75,75,75,75	0
56	MG	1a	1636	1/1	0.88	0.26	68,68,68,68	0
56	MG	1B	224	1/1	0.88	0.20	69,69,69,69	0
56	MG	2a	3135	1/1	0.88	0.16	61,61,61,61	0
56	MG	1a	1772	1/1	0.88	0.14	66,66,66,66	0
56	MG	1A	3786	1/1	0.88	0.17	67,67,67,67	0
56	MG	2A	3492	1/1	0.88	0.15	45,45,45,45	0
56	MG	2A	3200	1/1	0.88	0.13	41,41,41,41	0
56	MG	1D	302	1/1	0.88	0.16	33,33,33,33	0
56	MG	2A	3203	1/1	0.88	0.17	58,58,58,58	0
56	MG	1a	1776	1/1	0.88	0.19	76,76,76,76	0
56	MG	1h	3003	1/1	0.88	0.27	79,79,79,79	0
56	MG	1A	3400	1/1	0.88	0.11	48,48,48,48	0
56	MG	1A	3311	1/1	0.88	0.09	57,57,57,57	0
56	MG	2A	3215	1/1	0.88	0.15	63,63,63,63	0
56	MG	1r	3001	1/1	0.88	0.17	68,68,68,68	0
56	MG	1A	3182	1/1	0.88	0.12	59,59,59,59	0
56	MG	1a	1651	1/1	0.88	0.17	61,61,61,61	0
56	MG	1A	3406	1/1	0.88	0.12	56,56,56,56	0
56	MG	1x	106	1/1	0.88	0.34	54,54,54,54	0
56	MG	1A	3408	1/1	0.88	0.19	66,66,66,66	0
56	MG	1A	3468	1/1	0.88	0.09	59,59,59,59	0
56	MG	2A	3541	1/1	0.88	0.11	67,67,67,67	0
56	MG	2a	3172	1/1	0.88	0.20	78,78,78,78	0
56	MG	1A	3344	1/1	0.88	0.14	54,54,54,54	0
56	MG	2A	3270	1/1	0.88	0.18	61,61,61,61	0
56	MG	1A	3979	1/1	0.88	0.19	59,59,59,59	0
56	MG	2a	3181	1/1	0.88	0.26	71,71,71,71	0
56	MG	1A	3268	1/1	0.88	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2B	3001	1/1	0.88	0.23	65,65,65,65	0
56	MG	2a	3187	1/1	0.88	0.12	56,56,56,56	0
56	MG	2A	3279	1/1	0.88	0.18	71,71,71,71	0
56	MG	2A	3286	1/1	0.88	0.11	47,47,47,47	0
56	MG	1a	1794	1/1	0.88	0.22	63,63,63,63	0
56	MG	1A	3981	1/1	0.88	0.24	63,63,63,63	0
56	MG	1A	3349	1/1	0.88	0.20	51,51,51,51	0
56	MG	1A	3300	1/1	0.88	0.22	51,51,51,51	0
56	MG	2a	3198	1/1	0.88	0.21	76,76,76,76	0
56	MG	2A	3294	1/1	0.88	0.20	58,58,58,58	0
56	MG	1A	3360	1/1	0.88	0.16	61,61,61,61	0
56	MG	1A	3362	1/1	0.88	0.18	42,42,42,42	0
56	MG	1A	3029	1/1	0.88	0.19	57,57,57,57	0
56	MG	1A	3424	1/1	0.88	0.15	62,62,62,62	0
56	MG	1a	1715	1/1	0.88	0.14	76,76,76,76	0
56	MG	2A	3339	1/1	0.88	0.12	55,55,55,55	0
56	MG	1A	3489	1/1	0.88	0.19	55,55,55,55	0
56	MG	1Z	301	1/1	0.88	0.12	74,74,74,74	0
56	MG	2A	3052	1/1	0.88	0.33	66,66,66,66	0
56	MG	2a	3231	1/1	0.88	0.26	79,79,79,79	0
56	MG	1a	1728	1/1	0.88	0.27	55,55,55,55	0
56	MG	1A	3365	1/1	0.88	0.35	44,44,44,44	0
56	MG	1a	1734	1/1	0.88	0.32	66,66,66,66	0
56	MG	2a	3022	1/1	0.88	0.31	70,70,70,70	0
56	MG	2A	3075	1/1	0.88	0.32	75,75,75,75	0
56	MG	1A	3429	1/1	0.88	0.17	53,53,53,53	0
56	MG	1A	3325	1/1	0.88	0.10	75,75,75,75	0
56	MG	1A	3495	1/1	0.88	0.23	51,51,51,51	0
56	MG	2A	3084	1/1	0.88	0.11	51,51,51,51	0
56	MG	1A	3704	1/1	0.88	0.14	34,34,34,34	0
56	MG	2a	3037	1/1	0.88	0.20	72,72,72,72	0
56	MG	1A	3070	1/1	0.88	0.08	65,65,65,65	0
56	MG	1A	3503	1/1	0.88	0.16	82,82,82,82	0
56	MG	1A	4027	1/1	0.89	0.17	72,72,72,72	0
56	MG	1A	3327	1/1	0.89	0.12	64,64,64,64	0
56	MG	2A	3184	1/1	0.89	0.21	59,59,59,59	0
56	MG	2a	3060	1/1	0.89	0.31	63,63,63,63	0
56	MG	2a	3070	1/1	0.89	0.14	57,57,57,57	0
56	MG	1A	3208	1/1	0.89	0.17	57,57,57,57	0
56	MG	1Z	302	1/1	0.89	0.36	73,73,73,73	0
56	MG	1A	4036	1/1	0.89	0.30	44,44,44,44	0
56	MG	2a	3083	1/1	0.89	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3946	1/1	0.89	0.10	51,51,51,51	0
56	MG	2A	3460	1/1	0.89	0.10	53,53,53,53	0
56	MG	1A	3662	1/1	0.89	0.12	55,55,55,55	0
56	MG	1A	3425	1/1	0.89	0.09	57,57,57,57	0
56	MG	1A	3147	1/1	0.89	0.15	49,49,49,49	0
56	MG	1x	102	1/1	0.89	0.18	69,69,69,69	0
56	MG	2a	3107	1/1	0.89	0.18	63,63,63,63	0
56	MG	1x	105	1/1	0.89	0.23	57,57,57,57	0
56	MG	1A	3679	1/1	0.89	0.15	51,51,51,51	0
56	MG	2a	3112	1/1	0.89	0.18	67,67,67,67	0
56	MG	1A	3371	1/1	0.89	0.15	39,39,39,39	0
56	MG	1x	109	1/1	0.89	0.20	73,73,73,73	0
56	MG	1a	1717	1/1	0.89	0.14	69,69,69,69	0
56	MG	2a	3121	1/1	0.89	0.21	57,57,57,57	0
56	MG	2a	3122	1/1	0.89	0.27	69,69,69,69	0
56	MG	1A	3800	1/1	0.89	0.08	55,55,55,55	0
56	MG	2A	3239	1/1	0.89	0.13	49,49,49,49	0
56	MG	2a	3129	1/1	0.89	0.24	73,73,73,73	0
56	MG	2A	3002	1/1	0.89	0.16	59,59,59,59	0
56	MG	2A	3243	1/1	0.89	0.14	62,62,62,62	0
56	MG	1A	3977	1/1	0.89	0.20	50,50,50,50	0
56	MG	1a	1723	1/1	0.89	0.16	60,60,60,60	0
56	MG	1a	1606	1/1	0.89	0.20	73,73,73,73	0
56	MG	2A	3505	1/1	0.89	0.08	48,48,48,48	0
56	MG	1A	3868	1/1	0.89	0.17	65,65,65,65	0
56	MG	1A	3874	1/1	0.89	0.09	45,45,45,45	0
56	MG	1A	3883	1/1	0.89	0.11	66,66,66,66	0
56	MG	2a	3147	1/1	0.89	0.13	74,74,74,74	0
56	MG	1a	1736	1/1	0.89	0.14	63,63,63,63	0
56	MG	1D	301	1/1	0.89	0.24	58,58,58,58	0
56	MG	1A	3805	1/1	0.89	0.13	47,47,47,47	0
56	MG	2A	3029	1/1	0.89	0.23	59,59,59,59	0
56	MG	1a	1620	1/1	0.89	0.10	79,79,79,79	0
56	MG	1A	3332	1/1	0.89	0.18	61,61,61,61	0
56	MG	1A	3183	1/1	0.89	0.10	59,59,59,59	0
56	MG	2A	3544	1/1	0.89	0.18	61,61,61,61	0
56	MG	2A	3039	1/1	0.89	0.21	65,65,65,65	0
56	MG	2A	3566	1/1	0.89	0.20	58,58,58,58	0
56	MG	2A	3293	1/1	0.89	0.11	57,57,57,57	0
56	MG	2A	3044	1/1	0.89	0.10	46,46,46,46	0
56	MG	1a	1751	1/1	0.89	0.29	63,63,63,63	0
56	MG	1A	3902	1/1	0.89	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3323	1/1	0.89	0.08	54,54,54,54	0
56	MG	1E	306	1/1	0.89	0.39	74,74,74,74	0
56	MG	1A	3195	1/1	0.89	0.16	45,45,45,45	0
56	MG	1a	1837	1/1	0.89	0.25	50,50,50,50	0
56	MG	1a	1635	1/1	0.89	0.12	64,64,64,64	0
56	MG	1a	1845	1/1	0.89	0.18	52,52,52,52	0
56	MG	2A	3346	1/1	0.89	0.33	65,65,65,65	0
56	MG	2A	3352	1/1	0.89	0.21	66,66,66,66	0
56	MG	1A	3576	1/1	0.89	0.17	48,48,48,48	0
56	MG	2A	3358	1/1	0.89	0.21	53,53,53,53	0
56	MG	1a	1638	1/1	0.89	0.28	57,57,57,57	0
56	MG	1A	3357	1/1	0.89	0.14	50,50,50,50	0
56	MG	1A	3819	1/1	0.89	0.12	89,89,89,89	0
56	MG	1a	1761	1/1	0.89	0.17	66,66,66,66	0
56	MG	2A	3384	1/1	0.89	0.20	47,47,47,47	0
56	MG	1A	3477	1/1	0.89	0.22	67,67,67,67	0
56	MG	2a	3206	1/1	0.89	0.25	62,62,62,62	0
56	MG	2a	3015	1/1	0.89	0.08	79,79,79,79	0
56	MG	2A	3388	1/1	0.89	0.14	46,46,46,46	0
56	MG	1a	1763	1/1	0.89	0.09	76,76,76,76	0
56	MG	1A	3999	1/1	0.89	0.16	71,71,71,71	0
56	MG	2A	3392	1/1	0.89	0.23	43,43,43,43	0
56	MG	2A	3126	1/1	0.89	0.18	54,54,54,54	0
56	MG	1A	3926	1/1	0.89	0.26	66,66,66,66	0
56	MG	1a	1646	1/1	0.89	0.17	68,68,68,68	0
56	MG	1A	3051	1/1	0.89	0.18	57,57,57,57	0
56	MG	1A	3391	1/1	0.89	0.16	56,56,56,56	0
56	MG	1A	4015	1/1	0.89	0.25	61,61,61,61	0
56	MG	2a	3239	1/1	0.89	0.32	60,60,60,60	0
56	MG	1a	1653	1/1	0.89	0.10	70,70,70,70	0
56	MG	1A	3206	1/1	0.89	0.13	51,51,51,51	0
56	MG	1a	1900	1/1	0.89	0.22	62,62,62,62	0
56	MG	2A	3163	1/1	0.89	0.26	64,64,64,64	0
56	MG	2A	3166	1/1	0.89	0.15	51,51,51,51	0
56	MG	2a	3043	1/1	0.89	0.10	85,85,85,85	0
56	MG	1A	3631	1/1	0.89	0.10	55,55,55,55	0
56	MG	2a	3046	1/1	0.89	0.12	77,77,77,77	0
56	MG	2A	3432	1/1	0.89	0.23	64,64,64,64	0
56	MG	2A	3171	1/1	0.89	0.12	52,52,52,52	0
56	MG	2x	3005	1/1	0.89	0.14	70,70,70,70	0
56	MG	1a	1778	1/1	0.89	0.24	78,78,78,78	0
56	MG	1A	4034	1/1	0.90	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2F	301	1/1	0.90	0.16	63,63,63,63	0
56	MG	2A	3249	1/1	0.90	0.17	57,57,57,57	0
56	MG	2Q	201	1/1	0.90	0.27	55,55,55,55	0
56	MG	2A	3251	1/1	0.90	0.22	55,55,55,55	0
56	MG	1a	1608	1/1	0.90	0.17	68,68,68,68	0
56	MG	2A	3257	1/1	0.90	0.18	62,62,62,62	0
56	MG	2a	3003	1/1	0.90	0.25	60,60,60,60	0
56	MG	1h	3002	1/1	0.90	0.12	64,64,64,64	0
56	MG	1A	3419	1/1	0.90	0.22	52,52,52,52	0
56	MG	1A	3266	1/1	0.90	0.15	78,78,78,78	0
56	MG	1A	4039	1/1	0.90	0.18	56,56,56,56	0
56	MG	1A	3141	1/1	0.90	0.15	56,56,56,56	0
56	MG	1A	3423	1/1	0.90	0.21	62,62,62,62	0
56	MG	2A	3280	1/1	0.90	0.13	46,46,46,46	0
56	MG	1A	3184	1/1	0.90	0.06	61,61,61,61	0
56	MG	1A	3270	1/1	0.90	0.25	63,63,63,63	0
56	MG	1A	3271	1/1	0.90	0.25	66,66,66,66	0
56	MG	1A	3612	1/1	0.90	0.10	24,24,24,24	0
56	MG	1a	1765	1/1	0.90	0.14	65,65,65,65	0
56	MG	1A	3428	1/1	0.90	0.09	55,55,55,55	0
56	MG	2a	3033	1/1	0.90	0.21	76,76,76,76	0
56	MG	1A	3488	1/1	0.90	0.20	53,53,53,53	0
56	MG	1a	1629	1/1	0.90	0.22	54,54,54,54	0
56	MG	2A	3301	1/1	0.90	0.09	48,48,48,48	0
56	MG	2A	3318	1/1	0.90	0.23	64,64,64,64	0
56	MG	1a	1633	1/1	0.90	0.19	52,52,52,52	0
56	MG	2A	3001	1/1	0.90	0.14	55,55,55,55	0
56	MG	1A	3381	1/1	0.90	0.10	61,61,61,61	0
56	MG	2A	3331	1/1	0.90	0.12	36,36,36,36	0
56	MG	2A	3004	1/1	0.90	0.12	55,55,55,55	0
56	MG	1A	3430	1/1	0.90	0.27	41,41,41,41	0
56	MG	1A	3827	1/1	0.90	0.09	27,27,27,27	0
56	MG	1A	3028	1/1	0.90	0.15	58,58,58,58	0
56	MG	1A	3956	1/1	0.90	0.14	69,69,69,69	0
56	MG	2a	3051	1/1	0.90	0.22	76,76,76,76	0
56	MG	2a	3053	1/1	0.90	0.07	83,83,83,83	0
56	MG	1A	3830	1/1	0.90	0.15	54,54,54,54	0
56	MG	2a	3055	1/1	0.90	0.11	70,70,70,70	0
56	MG	1D	316	1/1	0.90	0.15	76,76,76,76	0
56	MG	1A	3278	1/1	0.90	0.16	72,72,72,72	0
56	MG	1A	3246	1/1	0.90	0.32	65,65,65,65	0
56	MG	1a	1647	1/1	0.90	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3028	1/1	0.90	0.10	48,48,48,48	0
56	MG	2A	3366	1/1	0.90	0.20	58,58,58,58	0
56	MG	2A	3367	1/1	0.90	0.10	52,52,52,52	0
56	MG	1E	305	1/1	0.90	0.08	58,58,58,58	0
56	MG	2A	3381	1/1	0.90	0.19	45,45,45,45	0
56	MG	2A	3382	1/1	0.90	0.11	71,71,71,71	0
56	MG	1A	3313	1/1	0.90	0.15	71,71,71,71	0
56	MG	1A	3840	1/1	0.90	0.22	67,67,67,67	0
56	MG	2a	3092	1/1	0.90	0.36	65,65,65,65	0
56	MG	2A	3034	1/1	0.90	0.14	61,61,61,61	0
56	MG	1A	3978	1/1	0.90	0.11	59,59,59,59	0
56	MG	1A	3050	1/1	0.90	0.24	63,63,63,63	0
56	MG	1A	3845	1/1	0.90	0.17	57,57,57,57	0
56	MG	1a	1662	1/1	0.90	0.15	73,73,73,73	0
56	MG	1A	3693	1/1	0.90	0.14	58,58,58,58	0
56	MG	1a	1664	1/1	0.90	0.15	57,57,57,57	0
56	MG	1a	1801	1/1	0.90	0.12	70,70,70,70	0
56	MG	1A	3348	1/1	0.90	0.16	63,63,63,63	0
56	MG	2a	3119	1/1	0.90	0.35	62,62,62,62	0
56	MG	2A	3398	1/1	0.90	0.08	57,57,57,57	0
56	MG	1a	1671	1/1	0.90	0.23	61,61,61,61	0
56	MG	1a	1672	1/1	0.90	0.12	61,61,61,61	0
56	MG	2A	3077	1/1	0.90	0.39	63,63,63,63	0
56	MG	1a	1676	1/1	0.90	0.29	51,51,51,51	0
56	MG	2a	3126	1/1	0.90	0.09	66,66,66,66	0
56	MG	2a	3128	1/1	0.90	0.37	63,63,63,63	0
56	MG	1A	3014	1/1	0.90	0.11	58,58,58,58	0
56	MG	2a	3130	1/1	0.90	0.21	58,58,58,58	0
56	MG	2a	3131	1/1	0.90	0.15	63,63,63,63	0
56	MG	1a	1678	1/1	0.90	0.16	60,60,60,60	0
56	MG	2A	3430	1/1	0.90	0.17	57,57,57,57	0
56	MG	1a	1679	1/1	0.90	0.15	52,52,52,52	0
56	MG	2A	3095	1/1	0.90	0.14	48,48,48,48	0
56	MG	1A	3854	1/1	0.90	0.26	76,76,76,76	0
56	MG	2a	3139	1/1	0.90	0.14	94,94,94,94	0
56	MG	1A	3448	1/1	0.90	0.13	58,58,58,58	0
56	MG	1a	1818	1/1	0.90	0.08	78,78,78,78	0
56	MG	2A	3105	1/1	0.90	0.10	55,55,55,55	0
56	MG	2A	3448	1/1	0.90	0.12	65,65,65,65	0
56	MG	1A	3512	1/1	0.90	0.08	53,53,53,53	0
56	MG	2A	3116	1/1	0.90	0.15	55,55,55,55	0
56	MG	2A	3117	1/1	0.90	0.26	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1693	1/1	0.90	0.17	65,65,65,65	0
56	MG	2A	3128	1/1	0.90	0.28	61,61,61,61	0
56	MG	1A	3861	1/1	0.90	0.14	68,68,68,68	0
56	MG	1a	1825	1/1	0.90	0.25	61,61,61,61	0
56	MG	1A	3052	1/1	0.90	0.10	48,48,48,48	0
56	MG	2A	3465	1/1	0.90	0.14	46,46,46,46	0
56	MG	1a	1698	1/1	0.90	0.18	75,75,75,75	0
56	MG	1a	1828	1/1	0.90	0.14	67,67,67,67	0
56	MG	1T	204	1/1	0.90	0.14	72,72,72,72	0
56	MG	2A	3151	1/1	0.90	0.17	45,45,45,45	0
56	MG	1a	1834	1/1	0.90	0.18	72,72,72,72	0
56	MG	1a	1702	1/1	0.90	0.17	67,67,67,67	0
56	MG	1A	3351	1/1	0.90	0.14	59,59,59,59	0
56	MG	1U	204	1/1	0.90	0.34	44,44,44,44	0
56	MG	1A	3993	1/1	0.90	0.15	73,73,73,73	0
56	MG	1A	3257	1/1	0.90	0.31	68,68,68,68	0
56	MG	1A	3728	1/1	0.90	0.10	23,23,23,23	0
56	MG	1A	4001	1/1	0.90	0.22	52,52,52,52	0
56	MG	1a	1725	1/1	0.90	0.30	59,59,59,59	0
56	MG	2A	3183	1/1	0.90	0.20	58,58,58,58	0
56	MG	2a	3189	1/1	0.90	0.16	57,57,57,57	0
56	MG	1A	3217	1/1	0.90	0.11	48,48,48,48	0
56	MG	2A	3508	1/1	0.90	0.13	61,61,61,61	0
56	MG	1A	3127	1/1	0.90	0.19	50,50,50,50	0
56	MG	1A	3463	1/1	0.90	0.22	53,53,53,53	0
56	MG	2A	3513	1/1	0.90	0.16	38,38,38,38	0
56	MG	2A	3514	1/1	0.90	0.10	58,58,58,58	0
56	MG	2a	3200	1/1	0.90	0.18	56,56,56,56	0
56	MG	2A	3518	1/1	0.90	0.18	67,67,67,67	0
56	MG	1a	1869	1/1	0.90	0.13	63,63,63,63	0
56	MG	1a	1876	1/1	0.90	0.14	61,61,61,61	0
56	MG	13	101	1/1	0.90	0.22	52,52,52,52	0
56	MG	2a	3212	1/1	0.90	0.20	56,56,56,56	0
56	MG	1A	3329	1/1	0.90	0.14	50,50,50,50	0
56	MG	15	105	1/1	0.90	0.10	57,57,57,57	0
56	MG	2A	3534	1/1	0.90	0.09	52,52,52,52	0
56	MG	1a	1887	1/1	0.90	0.27	66,66,66,66	0
56	MG	1a	1742	1/1	0.90	0.18	61,61,61,61	0
56	MG	1A	3128	1/1	0.90	0.24	49,49,49,49	0
56	MG	2A	3542	1/1	0.90	0.18	50,50,50,50	0
56	MG	2A	3543	1/1	0.90	0.07	66,66,66,66	0
56	MG	1a	1745	1/1	0.90	0.20	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3552	1/1	0.90	0.20	50,50,50,50	0
56	MG	1a	1747	1/1	0.90	0.27	59,59,59,59	0
56	MG	2A	3216	1/1	0.90	0.24	44,44,44,44	0
56	MG	2A	3567	1/1	0.90	0.13	54,54,54,54	0
56	MG	1A	3574	1/1	0.90	0.13	57,57,57,57	0
56	MG	18	104	1/1	0.90	0.16	59,59,59,59	0
56	MG	2A	3227	1/1	0.90	0.25	49,49,49,49	0
56	MG	2e	3001	1/1	0.90	0.13	68,68,68,68	0
56	MG	2A	3231	1/1	0.90	0.18	53,53,53,53	0
56	MG	2k	3002	1/1	0.90	0.09	66,66,66,66	0
56	MG	2l	202	1/1	0.90	0.11	57,57,57,57	0
56	MG	2A	3233	1/1	0.90	0.29	62,62,62,62	0
56	MG	2A	3234	1/1	0.90	0.32	52,52,52,52	0
56	MG	1A	3906	1/1	0.90	0.10	42,42,42,42	0
56	MG	2x	3001	1/1	0.90	0.15	79,79,79,79	0
56	MG	2x	3002	1/1	0.90	0.18	58,58,58,58	0
56	MG	1A	3915	1/1	0.90	0.11	38,38,38,38	0
56	MG	1b	3002	1/1	0.90	0.07	87,87,87,87	0
56	MG	1e	202	1/1	0.90	0.15	66,66,66,66	0
56	MG	1A	3159	1/1	0.91	0.16	42,42,42,42	0
56	MG	2a	3019	1/1	0.91	0.17	67,67,67,67	0
56	MG	2A	3337	1/1	0.91	0.10	41,41,41,41	0
56	MG	1a	1808	1/1	0.91	0.14	85,85,85,85	0
56	MG	1A	3673	1/1	0.91	0.18	52,52,52,52	0
56	MG	2a	3026	1/1	0.91	0.52	72,72,72,72	0
56	MG	2A	3053	1/1	0.91	0.20	49,49,49,49	0
56	MG	2A	3055	1/1	0.91	0.25	46,46,46,46	0
56	MG	2A	3056	1/1	0.91	0.23	57,57,57,57	0
56	MG	1a	1811	1/1	0.91	0.13	71,71,71,71	0
56	MG	2A	3066	1/1	0.91	0.17	54,54,54,54	0
56	MG	1A	3496	1/1	0.91	0.14	68,68,68,68	0
56	MG	2A	3362	1/1	0.91	0.20	54,54,54,54	0
56	MG	2A	3363	1/1	0.91	0.18	53,53,53,53	0
56	MG	2A	3073	1/1	0.91	0.11	37,37,37,37	0
56	MG	1A	3499	1/1	0.91	0.12	81,81,81,81	0
56	MG	1N	205	1/1	0.91	0.12	53,53,53,53	0
56	MG	2a	3042	1/1	0.91	0.18	78,78,78,78	0
56	MG	1A	3359	1/1	0.91	0.21	51,51,51,51	0
56	MG	1A	3841	1/1	0.91	0.18	41,41,41,41	0
56	MG	1Q	3003	1/1	0.91	0.10	54,54,54,54	0
56	MG	1Q	3004	1/1	0.91	0.17	46,46,46,46	0
56	MG	1R	205	1/1	0.91	0.19	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3088	1/1	0.91	0.09	46,46,46,46	0
56	MG	2A	3092	1/1	0.91	0.20	55,55,55,55	0
56	MG	1A	3445	1/1	0.91	0.10	58,58,58,58	0
56	MG	1A	3263	1/1	0.91	0.17	56,56,56,56	0
56	MG	1A	3846	1/1	0.91	0.09	43,43,43,43	0
56	MG	1A	3449	1/1	0.91	0.32	77,77,77,77	0
56	MG	1W	3004	1/1	0.91	0.17	43,43,43,43	0
56	MG	1a	1714	1/1	0.91	0.10	58,58,58,58	0
56	MG	2a	3065	1/1	0.91	0.08	84,84,84,84	0
56	MG	2A	3109	1/1	0.91	0.27	66,66,66,66	0
56	MG	1A	3110	1/1	0.91	0.11	39,39,39,39	0
56	MG	1A	3166	1/1	0.91	0.18	47,47,47,47	0
56	MG	1A	3992	1/1	0.91	0.10	50,50,50,50	0
56	MG	2a	3082	1/1	0.91	0.32	61,61,61,61	0
56	MG	2A	3124	1/1	0.91	0.10	62,62,62,62	0
56	MG	1A	3114	1/1	0.91	0.21	48,48,48,48	0
56	MG	10	101	1/1	0.91	0.19	68,68,68,68	0
56	MG	2A	3428	1/1	0.91	0.15	64,64,64,64	0
56	MG	1a	1849	1/1	0.91	0.13	54,54,54,54	0
56	MG	1a	1853	1/1	0.91	0.06	56,56,56,56	0
56	MG	2a	3094	1/1	0.91	0.20	51,51,51,51	0
56	MG	1A	3171	1/1	0.91	0.20	47,47,47,47	0
56	MG	2a	3100	1/1	0.91	0.25	57,57,57,57	0
56	MG	1a	1858	1/1	0.91	0.18	69,69,69,69	0
56	MG	1A	3461	1/1	0.91	0.24	46,46,46,46	0
56	MG	1a	1861	1/1	0.91	0.20	68,68,68,68	0
56	MG	2A	3149	1/1	0.91	0.25	59,59,59,59	0
56	MG	2A	3439	1/1	0.91	0.12	54,54,54,54	0
56	MG	2A	3440	1/1	0.91	0.13	62,62,62,62	0
56	MG	1A	3417	1/1	0.91	0.11	60,60,60,60	0
56	MG	1a	1733	1/1	0.91	0.27	53,53,53,53	0
56	MG	2A	3157	1/1	0.91	0.18	47,47,47,47	0
56	MG	1A	3025	1/1	0.91	0.14	60,60,60,60	0
56	MG	13	102	1/1	0.91	0.16	63,63,63,63	0
56	MG	1A	3521	1/1	0.91	0.17	46,46,46,46	0
56	MG	1A	3522	1/1	0.91	0.20	62,62,62,62	0
56	MG	17	104	1/1	0.91	0.22	57,57,57,57	0
56	MG	2A	3461	1/1	0.91	0.08	78,78,78,78	0
56	MG	2A	3172	1/1	0.91	0.14	47,47,47,47	0
56	MG	1a	1879	1/1	0.91	0.14	51,51,51,51	0
56	MG	1A	3873	1/1	0.91	0.11	25,25,25,25	0
56	MG	1a	1884	1/1	0.91	0.21	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3245	1/1	0.91	0.24	64,64,64,64	0
56	MG	1A	3758	1/1	0.91	0.13	66,66,66,66	0
56	MG	2A	3187	1/1	0.91	0.09	53,53,53,53	0
56	MG	2A	3480	1/1	0.91	0.14	74,74,74,74	0
56	MG	19	502	1/1	0.91	0.16	46,46,46,46	0
56	MG	2A	3190	1/1	0.91	0.24	61,61,61,61	0
56	MG	2a	3141	1/1	0.91	0.08	57,57,57,57	0
56	MG	1A	4023	1/1	0.91	0.22	40,40,40,40	0
56	MG	2A	3487	1/1	0.91	0.17	60,60,60,60	0
56	MG	2A	3195	1/1	0.91	0.23	58,58,58,58	0
56	MG	1A	4025	1/1	0.91	0.14	51,51,51,51	0
56	MG	1A	3272	1/1	0.91	0.15	70,70,70,70	0
56	MG	1A	3055	1/1	0.91	0.20	55,55,55,55	0
56	MG	1a	1898	1/1	0.91	0.26	65,65,65,65	0
56	MG	1A	3778	1/1	0.91	0.09	20,20,20,20	0
56	MG	1a	1905	1/1	0.91	0.12	83,83,83,83	0
56	MG	1A	3567	1/1	0.91	0.17	51,51,51,51	0
56	MG	2A	3507	1/1	0.91	0.10	48,48,48,48	0
56	MG	2a	3156	1/1	0.91	0.19	70,70,70,70	0
56	MG	1a	1615	1/1	0.91	0.07	83,83,83,83	0
56	MG	1A	3062	1/1	0.91	0.24	57,57,57,57	0
56	MG	1A	4037	1/1	0.91	0.11	62,62,62,62	0
56	MG	2a	3160	1/1	0.91	0.21	59,59,59,59	0
56	MG	2a	3162	1/1	0.91	0.10	47,47,47,47	0
56	MG	1A	3787	1/1	0.91	0.08	45,45,45,45	0
56	MG	1A	4049	1/1	0.91	0.15	57,57,57,57	0
56	MG	1A	4050	1/1	0.91	0.09	53,53,53,53	0
56	MG	2A	3519	1/1	0.91	0.14	53,53,53,53	0
56	MG	1B	201	1/1	0.91	0.07	44,44,44,44	0
56	MG	1A	3788	1/1	0.91	0.06	25,25,25,25	0
56	MG	1A	3384	1/1	0.91	0.11	66,66,66,66	0
56	MG	1A	3794	1/1	0.91	0.19	62,62,62,62	0
56	MG	2A	3526	1/1	0.91	0.11	54,54,54,54	0
56	MG	2a	3184	1/1	0.91	0.17	56,56,56,56	0
56	MG	2A	3237	1/1	0.91	0.19	48,48,48,48	0
56	MG	1A	3071	1/1	0.91	0.10	52,52,52,52	0
56	MG	1r	3003	1/1	0.91	0.08	58,58,58,58	0
56	MG	2A	3536	1/1	0.91	0.15	67,67,67,67	0
56	MG	1A	3799	1/1	0.91	0.28	54,54,54,54	0
56	MG	1a	1634	1/1	0.91	0.18	66,66,66,66	0
56	MG	1A	3044	1/1	0.91	0.15	50,50,50,50	0
56	MG	2A	3247	1/1	0.91	0.18	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3389	1/1	0.91	0.12	50,50,50,50	0
56	MG	2A	3550	1/1	0.91	0.25	37,37,37,37	0
56	MG	1A	3806	1/1	0.91	0.23	56,56,56,56	0
56	MG	2A	3563	1/1	0.91	0.17	58,58,58,58	0
56	MG	2a	3204	1/1	0.91	0.21	62,62,62,62	0
56	MG	1A	3482	1/1	0.91	0.19	61,61,61,61	0
56	MG	1A	3346	1/1	0.91	0.21	33,33,33,33	0
56	MG	2a	3208	1/1	0.91	0.15	68,68,68,68	0
56	MG	2a	3209	1/1	0.91	0.21	76,76,76,76	0
56	MG	2A	3259	1/1	0.91	0.14	40,40,40,40	0
56	MG	1A	3813	1/1	0.91	0.17	55,55,55,55	0
56	MG	1A	3256	1/1	0.91	0.14	51,51,51,51	0
56	MG	1A	3148	1/1	0.91	0.23	42,42,42,42	0
56	MG	2a	3216	1/1	0.91	0.15	57,57,57,57	0
56	MG	1A	3629	1/1	0.91	0.22	58,58,58,58	0
56	MG	2A	3277	1/1	0.91	0.11	36,36,36,36	0
56	MG	1A	3952	1/1	0.91	0.14	57,57,57,57	0
56	MG	1a	1784	1/1	0.91	0.12	73,73,73,73	0
56	MG	1A	3294	1/1	0.91	0.16	60,60,60,60	0
56	MG	2a	3228	1/1	0.91	0.09	67,67,67,67	0
56	MG	1A	3820	1/1	0.91	0.10	50,50,50,50	0
56	MG	2a	3232	1/1	0.91	0.20	62,62,62,62	0
56	MG	1A	3437	1/1	0.91	0.25	56,56,56,56	0
56	MG	2A	3010	1/1	0.91	0.16	51,51,51,51	0
56	MG	2a	3238	1/1	0.91	0.23	61,61,61,61	0
56	MG	2E	306	1/1	0.91	0.28	43,43,43,43	0
56	MG	1A	3826	1/1	0.91	0.11	35,35,35,35	0
56	MG	1A	3100	1/1	0.91	0.12	31,31,31,31	0
56	MG	2O	203	1/1	0.91	0.17	57,57,57,57	0
56	MG	1E	308	1/1	0.91	0.18	70,70,70,70	0
56	MG	25	502	1/1	0.91	0.30	56,56,56,56	0
56	MG	1a	1660	1/1	0.91	0.18	54,54,54,54	0
56	MG	1A	3967	1/1	0.91	0.13	53,53,53,53	0
56	MG	1A	3970	1/1	0.91	0.27	53,53,53,53	0
56	MG	2A	3311	1/1	0.91	0.15	44,44,44,44	0
56	MG	2A	3316	1/1	0.91	0.19	43,43,43,43	0
56	MG	1A	3405	1/1	0.91	0.09	59,59,59,59	0
56	MG	1H	201	1/1	0.91	0.30	54,54,54,54	0
56	MG	2a	3009	1/1	0.91	0.23	81,81,81,81	0
56	MG	1a	1669	1/1	0.91	0.33	62,62,62,62	0
56	MG	1A	3829	1/1	0.91	0.11	56,56,56,56	0
56	MG	1a	1805	1/1	0.91	0.16	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1806	1/1	0.91	0.20	67,67,67,67	0
57	ZN	24	501	1/1	0.91	0.08	126,126,126,126	0
56	MG	1A	3911	1/1	0.92	0.10	66,66,66,66	0
56	MG	1A	3706	1/1	0.92	0.08	38,38,38,38	0
56	MG	2A	3229	1/1	0.92	0.10	46,46,46,46	0
56	MG	1A	3131	1/1	0.92	0.07	32,32,32,32	0
56	MG	2B	3004	1/1	0.92	0.25	59,59,59,59	0
56	MG	1A	3710	1/1	0.92	0.08	48,48,48,48	0
56	MG	1A	3498	1/1	0.92	0.29	50,50,50,50	0
56	MG	1A	3434	1/1	0.92	0.31	41,41,41,41	0
56	MG	2D	302	1/1	0.92	0.13	57,57,57,57	0
56	MG	2D	303	1/1	0.92	0.14	60,60,60,60	0
56	MG	2E	302	1/1	0.92	0.34	63,63,63,63	0
56	MG	1a	1729	1/1	0.92	0.28	57,57,57,57	0
56	MG	1a	1730	1/1	0.92	0.24	49,49,49,49	0
56	MG	1A	3379	1/1	0.92	0.08	47,47,47,47	0
56	MG	1A	3334	1/1	0.92	0.09	55,55,55,55	0
56	MG	2A	3245	1/1	0.92	0.15	78,78,78,78	0
56	MG	2O	201	1/1	0.92	0.12	54,54,54,54	0
56	MG	1e	204	1/1	0.92	0.10	64,64,64,64	0
56	MG	1A	3730	1/1	0.92	0.08	33,33,33,33	0
56	MG	2Q	203	1/1	0.92	0.11	52,52,52,52	0
56	MG	20	8001	1/1	0.92	0.13	72,72,72,72	0
56	MG	1A	3250	1/1	0.92	0.15	42,42,42,42	0
56	MG	2A	3250	1/1	0.92	0.16	61,61,61,61	0
56	MG	1Q	3006	1/1	0.92	0.16	48,48,48,48	0
56	MG	1A	3139	1/1	0.92	0.12	28,28,28,28	0
56	MG	1k	3001	1/1	0.92	0.22	65,65,65,65	0
56	MG	1A	3190	1/1	0.92	0.11	59,59,59,59	0
56	MG	2a	3005	1/1	0.92	0.28	51,51,51,51	0
56	MG	2a	3006	1/1	0.92	0.14	66,66,66,66	0
56	MG	2A	3265	1/1	0.92	0.15	59,59,59,59	0
56	MG	1A	3751	1/1	0.92	0.10	40,40,40,40	0
56	MG	1A	3511	1/1	0.92	0.20	51,51,51,51	0
56	MG	1A	3140	1/1	0.92	0.14	50,50,50,50	0
56	MG	2a	3013	1/1	0.92	0.08	73,73,73,73	0
56	MG	2A	3271	1/1	0.92	0.19	36,36,36,36	0
56	MG	1A	3768	1/1	0.92	0.12	82,82,82,82	0
56	MG	1W	3006	1/1	0.92	0.17	42,42,42,42	0
56	MG	1A	3197	1/1	0.92	0.13	30,30,30,30	0
56	MG	1A	3771	1/1	0.92	0.07	54,54,54,54	0
56	MG	1A	3959	1/1	0.92	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3038	1/1	0.92	0.10	52,52,52,52	0
56	MG	1A	3446	1/1	0.92	0.09	52,52,52,52	0
56	MG	2a	3024	1/1	0.92	0.20	58,58,58,58	0
56	MG	1A	3782	1/1	0.92	0.07	43,43,43,43	0
56	MG	1A	3966	1/1	0.92	0.08	52,52,52,52	0
56	MG	2a	3029	1/1	0.92	0.26	59,59,59,59	0
56	MG	1A	3783	1/1	0.92	0.08	22,22,22,22	0
56	MG	2a	3032	1/1	0.92	0.25	65,65,65,65	0
56	MG	1A	3447	1/1	0.92	0.14	75,75,75,75	0
56	MG	1A	3399	1/1	0.92	0.16	68,68,68,68	0
56	MG	1A	3006	1/1	0.92	0.26	61,61,61,61	0
56	MG	15	103	1/1	0.92	0.17	45,45,45,45	0
56	MG	1A	3789	1/1	0.92	0.13	31,31,31,31	0
56	MG	1A	3016	1/1	0.92	0.23	49,49,49,49	0
56	MG	2A	3317	1/1	0.92	0.14	40,40,40,40	0
56	MG	1A	3265	1/1	0.92	0.11	55,55,55,55	0
56	MG	2A	3319	1/1	0.92	0.21	57,57,57,57	0
56	MG	1A	3796	1/1	0.92	0.47	42,42,42,42	0
56	MG	1A	3532	1/1	0.92	0.14	43,43,43,43	0
56	MG	2a	3044	1/1	0.92	0.10	95,95,95,95	0
56	MG	2A	3018	1/1	0.92	0.21	57,57,57,57	0
56	MG	2A	3327	1/1	0.92	0.14	68,68,68,68	0
56	MG	2A	3020	1/1	0.92	0.22	60,60,60,60	0
56	MG	1A	3536	1/1	0.92	0.21	62,62,62,62	0
56	MG	2a	3050	1/1	0.92	0.18	71,71,71,71	0
56	MG	1A	3347	1/1	0.92	0.20	41,41,41,41	0
56	MG	2a	3052	1/1	0.92	0.06	73,73,73,73	0
56	MG	1A	3985	1/1	0.92	0.23	73,73,73,73	0
56	MG	2A	3026	1/1	0.92	0.16	56,56,56,56	0
56	MG	2A	3340	1/1	0.92	0.18	51,51,51,51	0
56	MG	1a	1605	1/1	0.92	0.10	84,84,84,84	0
56	MG	1A	3552	1/1	0.92	0.15	58,58,58,58	0
56	MG	1a	1607	1/1	0.92	0.13	66,66,66,66	0
56	MG	2A	3354	1/1	0.92	0.25	75,75,75,75	0
56	MG	1a	1777	1/1	0.92	0.17	73,73,73,73	0
56	MG	1A	3456	1/1	0.92	0.11	58,58,58,58	0
56	MG	2a	3072	1/1	0.92	0.14	64,64,64,64	0
56	MG	2A	3033	1/1	0.92	0.23	55,55,55,55	0
56	MG	1A	3214	1/1	0.92	0.18	34,34,34,34	0
56	MG	1A	3460	1/1	0.92	0.10	51,51,51,51	0
56	MG	1a	1614	1/1	0.92	0.26	57,57,57,57	0
56	MG	1A	3407	1/1	0.92	0.10	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3046	1/1	0.92	0.25	62,62,62,62	0
56	MG	2a	3086	1/1	0.92	0.35	65,65,65,65	0
56	MG	1A	3103	1/1	0.92	0.26	41,41,41,41	0
56	MG	1A	3057	1/1	0.92	0.11	56,56,56,56	0
56	MG	2a	3090	1/1	0.92	0.12	60,60,60,60	0
56	MG	2a	3091	1/1	0.92	0.29	63,63,63,63	0
56	MG	2A	3375	1/1	0.92	0.15	50,50,50,50	0
56	MG	2A	3378	1/1	0.92	0.14	53,53,53,53	0
56	MG	2A	3380	1/1	0.92	0.12	45,45,45,45	0
56	MG	1A	3227	1/1	0.92	0.21	65,65,65,65	0
56	MG	1A	3818	1/1	0.92	0.16	62,62,62,62	0
56	MG	1A	4000	1/1	0.92	0.17	54,54,54,54	0
56	MG	2A	3057	1/1	0.92	0.26	50,50,50,50	0
56	MG	2A	3062	1/1	0.92	0.21	33,33,33,33	0
56	MG	1a	1622	1/1	0.92	0.28	74,74,74,74	0
56	MG	2a	3110	1/1	0.92	0.18	53,53,53,53	0
56	MG	2A	3064	1/1	0.92	0.24	56,56,56,56	0
56	MG	2a	3115	1/1	0.92	0.19	52,52,52,52	0
56	MG	2a	3116	1/1	0.92	0.31	51,51,51,51	0
56	MG	2A	3065	1/1	0.92	0.29	58,58,58,58	0
56	MG	1A	3588	1/1	0.92	0.20	69,69,69,69	0
56	MG	1A	3591	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	4007	1/1	0.92	0.14	58,58,58,58	0
56	MG	1a	1799	1/1	0.92	0.14	76,76,76,76	0
56	MG	1A	3822	1/1	0.92	0.07	34,34,34,34	0
56	MG	1A	3155	1/1	0.92	0.15	51,51,51,51	0
56	MG	2A	3402	1/1	0.92	0.18	55,55,55,55	0
56	MG	1A	3595	1/1	0.92	0.17	47,47,47,47	0
56	MG	2A	3411	1/1	0.92	0.17	39,39,39,39	0
56	MG	2A	3415	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3416	1/1	0.92	0.10	56,56,56,56	0
56	MG	2A	3080	1/1	0.92	0.06	37,37,37,37	0
56	MG	1A	3473	1/1	0.92	0.12	63,63,63,63	0
56	MG	2A	3424	1/1	0.92	0.12	50,50,50,50	0
56	MG	1A	3005	1/1	0.92	0.31	60,60,60,60	0
56	MG	2a	3136	1/1	0.92	0.21	72,72,72,72	0
56	MG	1A	3276	1/1	0.92	0.25	74,74,74,74	0
56	MG	1A	3623	1/1	0.92	0.15	40,40,40,40	0
56	MG	2A	3089	1/1	0.92	0.06	45,45,45,45	0
56	MG	1A	3627	1/1	0.92	0.10	20,20,20,20	0
56	MG	1a	1640	1/1	0.92	0.19	77,77,77,77	0
56	MG	1A	3835	1/1	0.92	0.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3416	1/1	0.92	0.21	70,70,70,70	0
56	MG	2A	3435	1/1	0.92	0.09	53,53,53,53	0
56	MG	2a	3145	1/1	0.92	0.09	91,91,91,91	0
56	MG	1A	3122	1/1	0.92	0.37	60,60,60,60	0
56	MG	1A	3635	1/1	0.92	0.09	56,56,56,56	0
56	MG	2A	3102	1/1	0.92	0.09	41,41,41,41	0
56	MG	1a	1814	1/1	0.92	0.20	63,63,63,63	0
56	MG	2A	3107	1/1	0.92	0.17	50,50,50,50	0
56	MG	2A	3447	1/1	0.92	0.19	77,77,77,77	0
56	MG	2A	3108	1/1	0.92	0.15	47,47,47,47	0
56	MG	1A	3126	1/1	0.92	0.18	55,55,55,55	0
56	MG	2A	3452	1/1	0.92	0.12	59,59,59,59	0
56	MG	2A	3113	1/1	0.92	0.10	54,54,54,54	0
56	MG	1A	3420	1/1	0.92	0.06	50,50,50,50	0
56	MG	1a	1817	1/1	0.92	0.14	49,49,49,49	0
56	MG	1A	4046	1/1	0.92	0.08	56,56,56,56	0
56	MG	1a	1819	1/1	0.92	0.12	58,58,58,58	0
56	MG	1A	3650	1/1	0.92	0.17	46,46,46,46	0
56	MG	2a	3166	1/1	0.92	0.26	63,63,63,63	0
56	MG	2A	3127	1/1	0.92	0.11	54,54,54,54	0
56	MG	1A	3658	1/1	0.92	0.08	21,21,21,21	0
56	MG	1a	1823	1/1	0.92	0.16	69,69,69,69	0
56	MG	2a	3174	1/1	0.92	0.14	56,56,56,56	0
56	MG	2A	3130	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3659	1/1	0.92	0.16	73,73,73,73	0
56	MG	1A	3013	1/1	0.92	0.20	64,64,64,64	0
56	MG	2A	3473	1/1	0.92	0.08	40,40,40,40	0
56	MG	2A	3474	1/1	0.92	0.08	58,58,58,58	0
56	MG	1A	3366	1/1	0.92	0.24	46,46,46,46	0
56	MG	1A	3853	1/1	0.92	0.20	49,49,49,49	0
56	MG	2A	3139	1/1	0.92	0.21	47,47,47,47	0
56	MG	1A	3668	1/1	0.92	0.26	84,84,84,84	0
56	MG	1A	3670	1/1	0.92	0.10	56,56,56,56	0
56	MG	2A	3150	1/1	0.92	0.15	56,56,56,56	0
56	MG	2A	3489	1/1	0.92	0.18	43,43,43,43	0
56	MG	1A	3486	1/1	0.92	0.12	65,65,65,65	0
56	MG	2A	3494	1/1	0.92	0.15	69,69,69,69	0
56	MG	1a	1666	1/1	0.92	0.07	55,55,55,55	0
56	MG	1A	3860	1/1	0.92	0.15	72,72,72,72	0
56	MG	1a	1838	1/1	0.92	0.14	62,62,62,62	0
56	MG	1A	3284	1/1	0.92	0.16	52,52,52,52	0
56	MG	1A	3370	1/1	0.92	0.26	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3037	1/1	0.92	0.15	65,65,65,65	0
56	MG	2A	3169	1/1	0.92	0.31	54,54,54,54	0
56	MG	2A	3170	1/1	0.92	0.11	35,35,35,35	0
56	MG	1A	3681	1/1	0.92	0.07	39,39,39,39	0
56	MG	1a	1852	1/1	0.92	0.12	77,77,77,77	0
56	MG	2a	3211	1/1	0.92	0.20	60,60,60,60	0
56	MG	2A	3173	1/1	0.92	0.17	49,49,49,49	0
56	MG	1A	3869	1/1	0.92	0.18	85,85,85,85	0
56	MG	1A	3372	1/1	0.92	0.08	56,56,56,56	0
56	MG	2A	3516	1/1	0.92	0.08	38,38,38,38	0
56	MG	2A	3517	1/1	0.92	0.10	47,47,47,47	0
56	MG	2a	3218	1/1	0.92	0.27	55,55,55,55	0
56	MG	1A	3690	1/1	0.92	0.20	41,41,41,41	0
56	MG	1A	3876	1/1	0.92	0.20	68,68,68,68	0
56	MG	1A	3691	1/1	0.92	0.14	59,59,59,59	0
56	MG	2A	3185	1/1	0.92	0.33	43,43,43,43	0
56	MG	2A	3522	1/1	0.92	0.14	39,39,39,39	0
56	MG	2a	3229	1/1	0.92	0.21	66,66,66,66	0
56	MG	2A	3186	1/1	0.92	0.19	43,43,43,43	0
56	MG	1a	1863	1/1	0.92	0.15	47,47,47,47	0
56	MG	1A	3885	1/1	0.92	0.09	56,56,56,56	0
56	MG	1A	3887	1/1	0.92	0.07	29,29,29,29	0
56	MG	2A	3533	1/1	0.92	0.11	47,47,47,47	0
56	MG	1A	3692	1/1	0.92	0.16	57,57,57,57	0
56	MG	2A	3193	1/1	0.92	0.28	63,63,63,63	0
56	MG	1A	3894	1/1	0.92	0.20	58,58,58,58	0
56	MG	1A	3286	1/1	0.92	0.06	45,45,45,45	0
56	MG	1a	1873	1/1	0.92	0.10	56,56,56,56	0
56	MG	1a	1699	1/1	0.92	0.22	71,71,71,71	0
56	MG	1A	3130	1/1	0.92	0.29	48,48,48,48	0
56	MG	1a	1701	1/1	0.92	0.22	50,50,50,50	0
56	MG	2A	3547	1/1	0.92	0.18	37,37,37,37	0
56	MG	1A	3700	1/1	0.92	0.23	37,37,37,37	0
56	MG	2l	203	1/1	0.92	0.20	67,67,67,67	0
56	MG	2A	3551	1/1	0.92	0.33	55,55,55,55	0
56	MG	1a	1883	1/1	0.92	0.19	58,58,58,58	0
56	MG	2A	3559	1/1	0.92	0.16	61,61,61,61	0
56	MG	2A	3209	1/1	0.92	0.37	49,49,49,49	0
56	MG	1a	1711	1/1	0.92	0.13	54,54,54,54	0
56	MG	1F	307	1/1	0.92	0.21	49,49,49,49	0
56	MG	1a	1713	1/1	0.92	0.35	65,65,65,65	0
56	MG	1A	3493	1/1	0.92	0.06	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3377	1/1	0.92	0.29	67,67,67,67	0
56	MG	2a	3012	1/1	0.93	0.31	69,69,69,69	0
56	MG	1a	1842	1/1	0.93	0.11	61,61,61,61	0
56	MG	1A	3441	1/1	0.93	0.12	50,50,50,50	0
56	MG	1T	201	1/1	0.93	0.10	59,59,59,59	0
56	MG	1A	3671	1/1	0.93	0.13	47,47,47,47	0
56	MG	1A	3387	1/1	0.93	0.10	64,64,64,64	0
56	MG	2A	3100	1/1	0.93	0.29	62,62,62,62	0
56	MG	1A	3338	1/1	0.93	0.08	55,55,55,55	0
56	MG	2A	3104	1/1	0.93	0.09	42,42,42,42	0
56	MG	2A	3372	1/1	0.93	0.20	62,62,62,62	0
56	MG	2A	3373	1/1	0.93	0.06	47,47,47,47	0
56	MG	1A	3251	1/1	0.93	0.12	60,60,60,60	0
56	MG	2A	3377	1/1	0.93	0.07	21,21,21,21	0
56	MG	1A	3392	1/1	0.93	0.09	55,55,55,55	0
56	MG	1a	1716	1/1	0.93	0.12	68,68,68,68	0
56	MG	1A	3832	1/1	0.93	0.20	68,68,68,68	0
56	MG	2A	3111	1/1	0.93	0.40	62,62,62,62	0
56	MG	2A	3383	1/1	0.93	0.19	64,64,64,64	0
56	MG	1A	3252	1/1	0.93	0.16	53,53,53,53	0
56	MG	2A	3385	1/1	0.93	0.12	43,43,43,43	0
56	MG	1A	3152	1/1	0.93	0.22	50,50,50,50	0
56	MG	1A	3255	1/1	0.93	0.12	44,44,44,44	0
56	MG	1a	1724	1/1	0.93	0.23	70,70,70,70	0
56	MG	2A	3119	1/1	0.93	0.21	46,46,46,46	0
56	MG	1A	3298	1/1	0.93	0.20	52,52,52,52	0
56	MG	1a	1726	1/1	0.93	0.19	66,66,66,66	0
56	MG	1A	3023	1/1	0.93	0.25	57,57,57,57	0
56	MG	1A	3518	1/1	0.93	0.18	52,52,52,52	0
56	MG	1a	1874	1/1	0.93	0.17	64,64,64,64	0
56	MG	1a	1875	1/1	0.93	0.27	65,65,65,65	0
56	MG	2A	3131	1/1	0.93	0.13	48,48,48,48	0
56	MG	2A	3399	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3453	1/1	0.93	0.11	49,49,49,49	0
56	MG	1a	1877	1/1	0.93	0.22	56,56,56,56	0
56	MG	2A	3405	1/1	0.93	0.20	45,45,45,45	0
56	MG	2A	3409	1/1	0.93	0.15	59,59,59,59	0
56	MG	1A	3844	1/1	0.93	0.17	63,63,63,63	0
56	MG	2A	3412	1/1	0.93	0.10	45,45,45,45	0
56	MG	1A	3404	1/1	0.93	0.07	82,82,82,82	0
56	MG	1A	3523	1/1	0.93	0.18	59,59,59,59	0
56	MG	1a	1882	1/1	0.93	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3418	1/1	0.93	0.22	62,62,62,62	0
56	MG	2A	3143	1/1	0.93	0.20	51,51,51,51	0
56	MG	1A	3302	1/1	0.93	0.10	33,33,33,33	0
56	MG	1A	3204	1/1	0.93	0.07	38,38,38,38	0
56	MG	1A	3205	1/1	0.93	0.15	55,55,55,55	0
56	MG	2A	3152	1/1	0.93	0.13	48,48,48,48	0
56	MG	2a	3080	1/1	0.93	0.26	61,61,61,61	0
56	MG	1a	1739	1/1	0.93	0.22	72,72,72,72	0
56	MG	16	103	1/1	0.93	0.08	57,57,57,57	0
56	MG	2A	3158	1/1	0.93	0.23	52,52,52,52	0
56	MG	1A	3540	1/1	0.93	0.18	41,41,41,41	0
56	MG	2a	3085	1/1	0.93	0.24	61,61,61,61	0
56	MG	1a	1890	1/1	0.93	0.25	58,58,58,58	0
56	MG	1A	4003	1/1	0.93	0.17	24,24,24,24	0
56	MG	1A	4005	1/1	0.93	0.20	31,31,31,31	0
56	MG	1A	3712	1/1	0.93	0.10	58,58,58,58	0
56	MG	1A	3856	1/1	0.93	0.16	52,52,52,52	0
56	MG	19	503	1/1	0.93	0.14	61,61,61,61	0
56	MG	1a	1903	1/1	0.93	0.18	56,56,56,56	0
56	MG	2A	3442	1/1	0.93	0.27	66,66,66,66	0
56	MG	2A	3446	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	3548	1/1	0.93	0.12	65,65,65,65	0
56	MG	2a	3101	1/1	0.93	0.36	64,64,64,64	0
56	MG	1a	1603	1/1	0.93	0.08	59,59,59,59	0
56	MG	2A	3175	1/1	0.93	0.06	40,40,40,40	0
56	MG	1A	3040	1/1	0.93	0.21	58,58,58,58	0
56	MG	1A	3722	1/1	0.93	0.20	56,56,56,56	0
56	MG	2A	3181	1/1	0.93	0.21	43,43,43,43	0
56	MG	2a	3111	1/1	0.93	0.18	46,46,46,46	0
56	MG	1d	302	1/1	0.93	0.17	70,70,70,70	0
56	MG	1A	3017	1/1	0.93	0.11	47,47,47,47	0
56	MG	1e	203	1/1	0.93	0.13	76,76,76,76	0
56	MG	1A	3725	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	3209	1/1	0.93	0.19	41,41,41,41	0
56	MG	2A	3188	1/1	0.93	0.18	49,49,49,49	0
56	MG	1A	3353	1/1	0.93	0.17	57,57,57,57	0
56	MG	1a	1611	1/1	0.93	0.09	85,85,85,85	0
56	MG	1A	3573	1/1	0.93	0.09	74,74,74,74	0
56	MG	2a	3123	1/1	0.93	0.24	57,57,57,57	0
56	MG	1A	3165	1/1	0.93	0.15	48,48,48,48	0
56	MG	2A	3194	1/1	0.93	0.26	45,45,45,45	0
56	MG	1A	3358	1/1	0.93	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1o	3002	1/1	0.93	0.14	55,55,55,55	0
56	MG	1a	1764	1/1	0.93	0.11	67,67,67,67	0
56	MG	1a	1616	1/1	0.93	0.13	76,76,76,76	0
56	MG	1A	3875	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3045	1/1	0.93	0.07	53,53,53,53	0
56	MG	2A	3204	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	3877	1/1	0.93	0.17	61,61,61,61	0
56	MG	1A	4038	1/1	0.93	0.14	66,66,66,66	0
56	MG	2A	3493	1/1	0.93	0.09	41,41,41,41	0
56	MG	1A	3880	1/1	0.93	0.09	42,42,42,42	0
56	MG	1x	103	1/1	0.93	0.14	70,70,70,70	0
56	MG	1A	4041	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	3757	1/1	0.93	0.09	41,41,41,41	0
56	MG	1A	3099	1/1	0.93	0.17	42,42,42,42	0
56	MG	2A	3218	1/1	0.93	0.15	64,64,64,64	0
56	MG	2A	3219	1/1	0.93	0.23	38,38,38,38	0
56	MG	1A	3418	1/1	0.93	0.22	43,43,43,43	0
56	MG	2a	3146	1/1	0.93	0.10	66,66,66,66	0
56	MG	1A	3766	1/1	0.93	0.11	49,49,49,49	0
56	MG	1a	1628	1/1	0.93	0.09	57,57,57,57	0
56	MG	1A	3170	1/1	0.93	0.18	32,32,32,32	0
56	MG	2A	3510	1/1	0.93	0.16	62,62,62,62	0
56	MG	1a	1631	1/1	0.93	0.17	44,44,44,44	0
56	MG	1A	3897	1/1	0.93	0.23	33,33,33,33	0
56	MG	1A	3589	1/1	0.93	0.25	65,65,65,65	0
56	MG	2A	3515	1/1	0.93	0.10	63,63,63,63	0
56	MG	1A	3900	1/1	0.93	0.32	42,42,42,42	0
56	MG	1A	3314	1/1	0.93	0.14	57,57,57,57	0
56	MG	1A	3228	1/1	0.93	0.20	51,51,51,51	0
56	MG	1A	3048	1/1	0.93	0.11	41,41,41,41	0
56	MG	1A	3596	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3907	1/1	0.93	0.07	13,13,13,13	0
56	MG	1a	1790	1/1	0.93	0.11	33,33,33,33	0
56	MG	2A	3021	1/1	0.93	0.20	60,60,60,60	0
56	MG	2A	3524	1/1	0.93	0.08	33,33,33,33	0
56	MG	1A	3484	1/1	0.93	0.06	70,70,70,70	0
56	MG	2a	3171	1/1	0.93	0.08	77,77,77,77	0
56	MG	1a	1792	1/1	0.93	0.11	59,59,59,59	0
56	MG	2A	3527	1/1	0.93	0.15	68,68,68,68	0
56	MG	1a	1793	1/1	0.93	0.17	68,68,68,68	0
56	MG	2A	3254	1/1	0.93	0.20	60,60,60,60	0
56	MG	1A	3237	1/1	0.93	0.16	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3180	1/1	0.93	0.08	79,79,79,79	0
56	MG	1B	226	1/1	0.93	0.11	47,47,47,47	0
56	MG	1a	1798	1/1	0.93	0.08	64,64,64,64	0
56	MG	2A	3264	1/1	0.93	0.21	65,65,65,65	0
56	MG	2a	3185	1/1	0.93	0.13	79,79,79,79	0
56	MG	2A	3538	1/1	0.93	0.18	52,52,52,52	0
56	MG	2A	3539	1/1	0.93	0.21	48,48,48,48	0
56	MG	1A	3602	1/1	0.93	0.13	41,41,41,41	0
56	MG	1A	3605	1/1	0.93	0.12	35,35,35,35	0
56	MG	1A	3607	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3321	1/1	0.93	0.33	52,52,52,52	0
56	MG	1A	3177	1/1	0.93	0.18	56,56,56,56	0
56	MG	2A	3275	1/1	0.93	0.09	34,34,34,34	0
56	MG	1A	3179	1/1	0.93	0.09	47,47,47,47	0
56	MG	1A	3243	1/1	0.93	0.15	43,43,43,43	0
56	MG	2A	3043	1/1	0.93	0.21	58,58,58,58	0
56	MG	1A	3937	1/1	0.93	0.29	51,51,51,51	0
56	MG	1A	3328	1/1	0.93	0.19	56,56,56,56	0
56	MG	2A	3282	1/1	0.93	0.08	31,31,31,31	0
56	MG	1A	3280	1/1	0.93	0.17	70,70,70,70	0
56	MG	2A	3570	1/1	0.93	0.07	50,50,50,50	0
56	MG	1E	310	1/1	0.93	0.17	45,45,45,45	0
56	MG	2A	3574	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3575	1/1	0.93	0.31	47,47,47,47	0
56	MG	2A	3576	1/1	0.93	0.19	50,50,50,50	0
56	MG	1A	3801	1/1	0.93	0.12	52,52,52,52	0
56	MG	1F	305	1/1	0.93	0.23	28,28,28,28	0
56	MG	1A	3804	1/1	0.93	0.14	50,50,50,50	0
56	MG	1A	3004	1/1	0.93	0.29	44,44,44,44	0
56	MG	2A	3059	1/1	0.93	0.13	50,50,50,50	0
56	MG	2A	3061	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3300	1/1	0.93	0.09	42,42,42,42	0
56	MG	1A	3058	1/1	0.93	0.06	49,49,49,49	0
56	MG	2A	3302	1/1	0.93	0.12	64,64,64,64	0
56	MG	1A	3950	1/1	0.93	0.13	55,55,55,55	0
56	MG	1A	3647	1/1	0.93	0.12	55,55,55,55	0
56	MG	2a	3230	1/1	0.93	0.09	70,70,70,70	0
56	MG	1A	3061	1/1	0.93	0.29	51,51,51,51	0
56	MG	1A	3655	1/1	0.93	0.19	56,56,56,56	0
56	MG	1A	3958	1/1	0.93	0.14	46,46,46,46	0
56	MG	2A	3069	1/1	0.93	0.19	55,55,55,55	0
56	MG	2E	307	1/1	0.93	0.10	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3070	1/1	0.93	0.32	58,58,58,58	0
56	MG	1A	3383	1/1	0.93	0.12	51,51,51,51	0
56	MG	2a	3242	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3326	1/1	0.93	0.13	34,34,34,34	0
56	MG	1a	1682	1/1	0.93	0.15	70,70,70,70	0
56	MG	2A	3328	1/1	0.93	0.09	45,45,45,45	0
56	MG	1a	1684	1/1	0.93	0.19	58,58,58,58	0
56	MG	2V	201	1/1	0.93	0.33	51,51,51,51	0
56	MG	1A	3076	1/1	0.93	0.14	42,42,42,42	0
56	MG	1N	208	1/1	0.93	0.07	60,60,60,60	0
56	MG	2A	3336	1/1	0.93	0.16	49,49,49,49	0
56	MG	2A	3078	1/1	0.93	0.08	53,53,53,53	0
56	MG	1a	1691	1/1	0.93	0.11	50,50,50,50	0
56	MG	1A	3080	1/1	0.93	0.14	52,52,52,52	0
56	MG	1A	3664	1/1	0.93	0.09	57,57,57,57	0
56	MG	2t	201	1/1	0.93	0.20	62,62,62,62	0
56	MG	1P	202	1/1	0.93	0.13	46,46,46,46	0
56	MG	2A	3348	1/1	0.93	0.21	72,72,72,72	0
56	MG	2A	3086	1/1	0.93	0.06	30,30,30,30	0
56	MG	1A	3196	1/1	0.93	0.17	45,45,45,45	0
56	MG	1A	3667	1/1	0.93	0.14	42,42,42,42	0
56	MG	1A	3440	1/1	0.93	0.09	51,51,51,51	0
56	MG	2A	3094	1/1	0.94	0.12	48,48,48,48	0
56	MG	1a	1686	1/1	0.94	0.19	53,53,53,53	0
56	MG	2A	3096	1/1	0.94	0.13	40,40,40,40	0
56	MG	1a	1846	1/1	0.94	0.08	71,71,71,71	0
56	MG	1a	1847	1/1	0.94	0.18	54,54,54,54	0
56	MG	1A	3395	1/1	0.94	0.14	59,59,59,59	0
56	MG	1A	3396	1/1	0.94	0.11	58,58,58,58	0
56	MG	2A	3101	1/1	0.94	0.12	60,60,60,60	0
56	MG	1a	1851	1/1	0.94	0.16	49,49,49,49	0
56	MG	1A	3944	1/1	0.94	0.21	19,19,19,19	0
56	MG	2A	3368	1/1	0.94	0.22	63,63,63,63	0
56	MG	1A	3398	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3106	1/1	0.94	0.14	33,33,33,33	0
56	MG	1A	3669	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3374	1/1	0.94	0.13	57,57,57,57	0
56	MG	2a	3021	1/1	0.94	0.07	78,78,78,78	0
56	MG	1A	3242	1/1	0.94	0.23	48,48,48,48	0
56	MG	1a	1859	1/1	0.94	0.14	72,72,72,72	0
56	MG	1N	203	1/1	0.94	0.22	46,46,46,46	0
56	MG	1A	3951	1/1	0.94	0.07	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3114	1/1	0.94	0.13	34,34,34,34	0
56	MG	1A	3008	1/1	0.94	0.19	51,51,51,51	0
56	MG	1A	3115	1/1	0.94	0.19	40,40,40,40	0
56	MG	1A	3675	1/1	0.94	0.14	39,39,39,39	0
56	MG	2A	3118	1/1	0.94	0.22	56,56,56,56	0
56	MG	1a	1709	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3121	1/1	0.94	0.15	42,42,42,42	0
56	MG	1a	1710	1/1	0.94	0.18	54,54,54,54	0
56	MG	1a	1868	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3677	1/1	0.94	0.12	50,50,50,50	0
56	MG	1a	1870	1/1	0.94	0.07	56,56,56,56	0
56	MG	1a	1872	1/1	0.94	0.10	67,67,67,67	0
56	MG	1A	3143	1/1	0.94	0.22	55,55,55,55	0
56	MG	1Q	3001	1/1	0.94	0.26	47,47,47,47	0
56	MG	1A	3274	1/1	0.94	0.06	69,69,69,69	0
56	MG	1A	3310	1/1	0.94	0.09	65,65,65,65	0
56	MG	1Q	3005	1/1	0.94	0.17	53,53,53,53	0
56	MG	1A	3458	1/1	0.94	0.12	72,72,72,72	0
56	MG	1R	203	1/1	0.94	0.12	56,56,56,56	0
56	MG	1a	1720	1/1	0.94	0.23	43,43,43,43	0
56	MG	1R	204	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3144	1/1	0.94	0.21	53,53,53,53	0
56	MG	1A	3684	1/1	0.94	0.11	41,41,41,41	0
56	MG	1A	3275	1/1	0.94	0.08	53,53,53,53	0
56	MG	1A	3968	1/1	0.94	0.15	65,65,65,65	0
56	MG	1A	3352	1/1	0.94	0.28	49,49,49,49	0
56	MG	2A	3153	1/1	0.94	0.19	42,42,42,42	0
56	MG	2A	3419	1/1	0.94	0.23	51,51,51,51	0
56	MG	1A	3312	1/1	0.94	0.09	60,60,60,60	0
56	MG	1A	3976	1/1	0.94	0.20	49,49,49,49	0
56	MG	2a	3061	1/1	0.94	0.07	72,72,72,72	0
56	MG	2a	3063	1/1	0.94	0.11	66,66,66,66	0
56	MG	1W	3001	1/1	0.94	0.29	52,52,52,52	0
56	MG	2A	3161	1/1	0.94	0.16	46,46,46,46	0
56	MG	2a	3071	1/1	0.94	0.23	58,58,58,58	0
56	MG	2A	3427	1/1	0.94	0.14	68,68,68,68	0
56	MG	1A	3354	1/1	0.94	0.16	54,54,54,54	0
56	MG	1W	3005	1/1	0.94	0.07	41,41,41,41	0
56	MG	1a	1893	1/1	0.94	0.19	59,59,59,59	0
56	MG	1a	1894	1/1	0.94	0.21	56,56,56,56	0
56	MG	1A	3410	1/1	0.94	0.08	51,51,51,51	0
56	MG	1A	3838	1/1	0.94	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3696	1/1	0.94	0.08	62,62,62,62	0
56	MG	1A	3464	1/1	0.94	0.13	43,43,43,43	0
56	MG	1a	1738	1/1	0.94	0.08	59,59,59,59	0
56	MG	1A	3466	1/1	0.94	0.11	48,48,48,48	0
56	MG	1A	3701	1/1	0.94	0.06	22,22,22,22	0
56	MG	1A	3356	1/1	0.94	0.09	49,49,49,49	0
56	MG	1c	3001	1/1	0.94	0.23	68,68,68,68	0
56	MG	2A	3443	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	3559	1/1	0.94	0.07	36,36,36,36	0
56	MG	1d	303	1/1	0.94	0.15	62,62,62,62	0
56	MG	10	107	1/1	0.94	0.10	58,58,58,58	0
56	MG	2A	3450	1/1	0.94	0.19	52,52,52,52	0
56	MG	1A	3470	1/1	0.94	0.08	57,57,57,57	0
56	MG	1A	3987	1/1	0.94	0.11	35,35,35,35	0
56	MG	1A	3847	1/1	0.94	0.06	81,81,81,81	0
56	MG	2A	3454	1/1	0.94	0.22	58,58,58,58	0
56	MG	1A	3116	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	3065	1/1	0.94	0.09	60,60,60,60	0
56	MG	15	104	1/1	0.94	0.25	49,49,49,49	0
56	MG	2A	3191	1/1	0.94	0.15	45,45,45,45	0
56	MG	1A	3002	1/1	0.94	0.17	43,43,43,43	0
56	MG	1A	3279	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3212	1/1	0.94	0.15	49,49,49,49	0
56	MG	1q	201	1/1	0.94	0.19	68,68,68,68	0
56	MG	1A	3581	1/1	0.94	0.15	51,51,51,51	0
56	MG	1A	3857	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3199	1/1	0.94	0.19	47,47,47,47	0
56	MG	2A	3472	1/1	0.94	0.11	54,54,54,54	0
56	MG	18	103	1/1	0.94	0.10	49,49,49,49	0
56	MG	1A	3583	1/1	0.94	0.11	33,33,33,33	0
56	MG	1A	3724	1/1	0.94	0.19	55,55,55,55	0
56	MG	1A	3319	1/1	0.94	0.07	55,55,55,55	0
56	MG	1A	4004	1/1	0.94	0.29	31,31,31,31	0
56	MG	1A	3282	1/1	0.94	0.23	47,47,47,47	0
56	MG	2A	3208	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3862	1/1	0.94	0.09	25,25,25,25	0
56	MG	2a	3132	1/1	0.94	0.14	71,71,71,71	0
56	MG	1A	3863	1/1	0.94	0.16	49,49,49,49	0
56	MG	2A	3491	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3865	1/1	0.94	0.15	32,32,32,32	0
56	MG	2A	3214	1/1	0.94	0.22	49,49,49,49	0
56	MG	1A	3018	1/1	0.94	0.32	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3323	1/1	0.94	0.06	46,46,46,46	0
56	MG	2A	3217	1/1	0.94	0.26	45,45,45,45	0
56	MG	1A	4016	1/1	0.94	0.13	58,58,58,58	0
56	MG	1A	4017	1/1	0.94	0.17	41,41,41,41	0
56	MG	2A	3501	1/1	0.94	0.10	43,43,43,43	0
56	MG	1a	1612	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3221	1/1	0.94	0.15	35,35,35,35	0
56	MG	2A	3003	1/1	0.94	0.07	58,58,58,58	0
56	MG	1A	3741	1/1	0.94	0.12	32,32,32,32	0
56	MG	1A	4019	1/1	0.94	0.15	93,93,93,93	0
56	MG	1A	3592	1/1	0.94	0.12	42,42,42,42	0
56	MG	1A	4022	1/1	0.94	0.17	66,66,66,66	0
56	MG	1A	3871	1/1	0.94	0.19	67,67,67,67	0
56	MG	2a	3151	1/1	0.94	0.06	64,64,64,64	0
56	MG	2A	3009	1/1	0.94	0.18	56,56,56,56	0
56	MG	1A	3483	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3077	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3016	1/1	0.94	0.08	59,59,59,59	0
56	MG	2A	3017	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3326	1/1	0.94	0.08	63,63,63,63	0
56	MG	1A	4032	1/1	0.94	0.25	47,47,47,47	0
56	MG	1A	3031	1/1	0.94	0.10	51,51,51,51	0
56	MG	1A	3223	1/1	0.94	0.18	55,55,55,55	0
56	MG	1A	3601	1/1	0.94	0.11	28,28,28,28	0
56	MG	1A	3881	1/1	0.94	0.12	63,63,63,63	0
56	MG	2a	3165	1/1	0.94	0.25	50,50,50,50	0
56	MG	2A	3252	1/1	0.94	0.27	56,56,56,56	0
56	MG	2A	3253	1/1	0.94	0.15	68,68,68,68	0
56	MG	1A	3882	1/1	0.94	0.07	36,36,36,36	0
56	MG	1A	3375	1/1	0.94	0.11	59,59,59,59	0
56	MG	2A	3528	1/1	0.94	0.07	56,56,56,56	0
56	MG	1A	3287	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	4042	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3262	1/1	0.94	0.14	55,55,55,55	0
56	MG	2a	3177	1/1	0.94	0.16	52,52,52,52	0
56	MG	1A	3224	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3888	1/1	0.94	0.22	37,37,37,37	0
56	MG	1a	1796	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3889	1/1	0.94	0.09	53,53,53,53	0
56	MG	2A	3035	1/1	0.94	0.17	59,59,59,59	0
56	MG	2A	3540	1/1	0.94	0.16	39,39,39,39	0
56	MG	2A	3036	1/1	0.94	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3891	1/1	0.94	0.12	51,51,51,51	0
56	MG	1a	1637	1/1	0.94	0.23	64,64,64,64	0
56	MG	2A	3040	1/1	0.94	0.12	43,43,43,43	0
56	MG	1B	202	1/1	0.94	0.20	59,59,59,59	0
56	MG	2a	3192	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3772	1/1	0.94	0.09	61,61,61,61	0
56	MG	1B	206	1/1	0.94	0.10	38,38,38,38	0
56	MG	1A	3777	1/1	0.94	0.14	43,43,43,43	0
56	MG	2A	3555	1/1	0.94	0.06	43,43,43,43	0
56	MG	2A	3283	1/1	0.94	0.06	51,51,51,51	0
56	MG	1A	3609	1/1	0.94	0.14	28,28,28,28	0
56	MG	2A	3287	1/1	0.94	0.07	46,46,46,46	0
56	MG	2a	3202	1/1	0.94	0.19	70,70,70,70	0
56	MG	2a	3203	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3898	1/1	0.94	0.20	36,36,36,36	0
56	MG	1A	3291	1/1	0.94	0.07	55,55,55,55	0
56	MG	2A	3569	1/1	0.94	0.10	41,41,41,41	0
56	MG	1A	3226	1/1	0.94	0.17	53,53,53,53	0
56	MG	1A	3258	1/1	0.94	0.07	45,45,45,45	0
56	MG	1A	3628	1/1	0.94	0.15	63,63,63,63	0
56	MG	2A	3060	1/1	0.94	0.14	42,42,42,42	0
56	MG	1A	3188	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3577	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3105	1/1	0.94	0.09	39,39,39,39	0
56	MG	2A	3579	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3160	1/1	0.94	0.08	42,42,42,42	0
56	MG	2A	3582	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	3232	1/1	0.94	0.11	57,57,57,57	0
56	MG	1A	3136	1/1	0.94	0.18	47,47,47,47	0
56	MG	1A	3019	1/1	0.94	0.13	61,61,61,61	0
56	MG	1a	1661	1/1	0.94	0.13	57,57,57,57	0
56	MG	2B	3005	1/1	0.94	0.23	51,51,51,51	0
56	MG	1A	3797	1/1	0.94	0.13	73,73,73,73	0
56	MG	1D	310	1/1	0.94	0.17	33,33,33,33	0
56	MG	2A	3071	1/1	0.94	0.21	56,56,56,56	0
56	MG	2D	301	1/1	0.94	0.10	54,54,54,54	0
56	MG	2A	3321	1/1	0.94	0.11	53,53,53,53	0
56	MG	1D	315	1/1	0.94	0.08	56,56,56,56	0
56	MG	2a	3237	1/1	0.94	0.10	69,69,69,69	0
56	MG	1A	3920	1/1	0.94	0.11	23,23,23,23	0
56	MG	1A	3649	1/1	0.94	0.10	28,28,28,28	0
56	MG	1a	1668	1/1	0.94	0.08	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3390	1/1	0.94	0.10	54,54,54,54	0
56	MG	1A	3925	1/1	0.94	0.10	54,54,54,54	0
56	MG	1A	3506	1/1	0.94	0.16	57,57,57,57	0
56	MG	1A	3267	1/1	0.94	0.19	57,57,57,57	0
56	MG	2N	8001	1/1	0.94	0.07	59,59,59,59	0
56	MG	1a	1832	1/1	0.94	0.10	54,54,54,54	0
56	MG	2f	3001	1/1	0.94	0.07	58,58,58,58	0
56	MG	1A	3932	1/1	0.94	0.13	46,46,46,46	0
56	MG	2A	3338	1/1	0.94	0.11	54,54,54,54	0
56	MG	2Q	202	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3934	1/1	0.94	0.14	62,62,62,62	0
56	MG	2R	8001	1/1	0.94	0.14	50,50,50,50	0
56	MG	2U	201	1/1	0.94	0.08	40,40,40,40	0
56	MG	1A	3343	1/1	0.94	0.16	31,31,31,31	0
56	MG	2A	3343	1/1	0.94	0.17	60,60,60,60	0
56	MG	1A	3509	1/1	0.94	0.15	60,60,60,60	0
56	MG	2A	3091	1/1	0.94	0.21	37,37,37,37	0
56	MG	28	8001	1/1	0.94	0.24	56,56,56,56	0
56	MG	2A	3347	1/1	0.94	0.08	55,55,55,55	0
56	MG	1A	3663	1/1	0.94	0.18	55,55,55,55	0
56	MG	1A	3198	1/1	0.94	0.13	41,41,41,41	0
56	MG	1A	3809	1/1	0.95	0.17	40,40,40,40	0
56	MG	1A	4021	1/1	0.95	0.09	33,33,33,33	0
56	MG	1a	1850	1/1	0.95	0.18	46,46,46,46	0
56	MG	1A	3810	1/1	0.95	0.11	63,63,63,63	0
56	MG	1A	3361	1/1	0.95	0.12	59,59,59,59	0
56	MG	2A	3242	1/1	0.95	0.11	55,55,55,55	0
56	MG	1A	3225	1/1	0.95	0.21	40,40,40,40	0
56	MG	15	101	1/1	0.95	0.16	43,43,43,43	0
56	MG	1A	3904	1/1	0.95	0.13	44,44,44,44	0
56	MG	1A	4029	1/1	0.95	0.32	40,40,40,40	0
56	MG	1A	3905	1/1	0.95	0.13	39,39,39,39	0
56	MG	1a	1727	1/1	0.95	0.21	39,39,39,39	0
56	MG	1a	1862	1/1	0.95	0.13	53,53,53,53	0
56	MG	2A	3468	1/1	0.95	0.09	64,64,64,64	0
56	MG	2A	3072	1/1	0.95	0.20	55,55,55,55	0
56	MG	2A	3470	1/1	0.95	0.06	42,42,42,42	0
56	MG	1A	3814	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	4033	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3154	1/1	0.95	0.32	44,44,44,44	0
56	MG	1A	3261	1/1	0.95	0.32	68,68,68,68	0
56	MG	2a	3067	1/1	0.95	0.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3069	1/1	0.95	0.24	65,65,65,65	0
56	MG	2A	3478	1/1	0.95	0.07	47,47,47,47	0
56	MG	1A	3587	1/1	0.95	0.15	42,42,42,42	0
56	MG	2A	3258	1/1	0.95	0.08	32,32,32,32	0
56	MG	2a	3074	1/1	0.95	0.14	63,63,63,63	0
56	MG	1A	3135	1/1	0.95	0.19	44,44,44,44	0
56	MG	1A	3497	1/1	0.95	0.22	56,56,56,56	0
56	MG	1A	3157	1/1	0.95	0.29	30,30,30,30	0
56	MG	2A	3488	1/1	0.95	0.10	31,31,31,31	0
56	MG	1a	1871	1/1	0.95	0.18	58,58,58,58	0
56	MG	19	504	1/1	0.95	0.09	56,56,56,56	0
56	MG	2A	3085	1/1	0.95	0.07	34,34,34,34	0
56	MG	1A	3699	1/1	0.95	0.07	17,17,17,17	0
56	MG	2A	3087	1/1	0.95	0.07	36,36,36,36	0
56	MG	2a	3087	1/1	0.95	0.29	60,60,60,60	0
56	MG	2A	3272	1/1	0.95	0.21	61,61,61,61	0
56	MG	1A	3229	1/1	0.95	0.12	55,55,55,55	0
56	MG	1a	1741	1/1	0.95	0.44	68,68,68,68	0
56	MG	1A	3924	1/1	0.95	0.14	67,67,67,67	0
56	MG	1A	3452	1/1	0.95	0.20	42,42,42,42	0
56	MG	1A	3158	1/1	0.95	0.09	37,37,37,37	0
56	MG	1a	1746	1/1	0.95	0.25	60,60,60,60	0
56	MG	2a	3096	1/1	0.95	0.12	72,72,72,72	0
56	MG	2A	3504	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	4051	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	3074	1/1	0.95	0.20	61,61,61,61	0
56	MG	2A	3285	1/1	0.95	0.12	58,58,58,58	0
56	MG	2a	3103	1/1	0.95	0.25	59,59,59,59	0
56	MG	1A	3931	1/1	0.95	0.12	49,49,49,49	0
56	MG	1A	3455	1/1	0.95	0.14	52,52,52,52	0
56	MG	1B	204	1/1	0.95	0.14	53,53,53,53	0
56	MG	2A	3289	1/1	0.95	0.19	44,44,44,44	0
56	MG	1A	3301	1/1	0.95	0.20	33,33,33,33	0
56	MG	1A	3831	1/1	0.95	0.10	54,54,54,54	0
56	MG	2a	3114	1/1	0.95	0.18	70,70,70,70	0
56	MG	1A	3236	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3833	1/1	0.95	0.16	56,56,56,56	0
56	MG	1B	212	1/1	0.95	0.19	47,47,47,47	0
56	MG	2A	3296	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3095	1/1	0.95	0.08	41,41,41,41	0
56	MG	1A	3046	1/1	0.95	0.08	60,60,60,60	0
56	MG	1A	3836	1/1	0.95	0.06	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3718	1/1	0.95	0.10	18,18,18,18	0
56	MG	2A	3304	1/1	0.95	0.08	40,40,40,40	0
56	MG	2A	3305	1/1	0.95	0.13	38,38,38,38	0
56	MG	2A	3308	1/1	0.95	0.19	41,41,41,41	0
56	MG	1a	1896	1/1	0.95	0.09	45,45,45,45	0
56	MG	1A	3945	1/1	0.95	0.20	30,30,30,30	0
56	MG	1A	3118	1/1	0.95	0.17	20,20,20,20	0
56	MG	2A	3531	1/1	0.95	0.17	58,58,58,58	0
56	MG	2A	3532	1/1	0.95	0.09	56,56,56,56	0
56	MG	1a	1902	1/1	0.95	0.18	59,59,59,59	0
56	MG	1A	3241	1/1	0.95	0.20	49,49,49,49	0
56	MG	1A	3380	1/1	0.95	0.15	39,39,39,39	0
56	MG	1A	3618	1/1	0.95	0.12	40,40,40,40	0
56	MG	1A	3203	1/1	0.95	0.50	47,47,47,47	0
56	MG	1A	3624	1/1	0.95	0.11	35,35,35,35	0
56	MG	2A	3123	1/1	0.95	0.13	51,51,51,51	0
56	MG	1A	3142	1/1	0.95	0.15	43,43,43,43	0
56	MG	1A	3957	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3007	1/1	0.95	0.11	53,53,53,53	0
56	MG	2A	3332	1/1	0.95	0.11	50,50,50,50	0
56	MG	1e	201	1/1	0.95	0.10	59,59,59,59	0
56	MG	2A	3334	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3549	1/1	0.95	0.13	43,43,43,43	0
56	MG	1A	3739	1/1	0.95	0.10	22,22,22,22	0
56	MG	1A	3010	1/1	0.95	0.28	53,53,53,53	0
56	MG	1A	3630	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3851	1/1	0.95	0.10	42,42,42,42	0
56	MG	2A	3556	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3558	1/1	0.95	0.08	37,37,37,37	0
56	MG	2A	3134	1/1	0.95	0.07	35,35,35,35	0
56	MG	2A	3561	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3519	1/1	0.95	0.12	33,33,33,33	0
56	MG	2A	3136	1/1	0.95	0.21	45,45,45,45	0
56	MG	2A	3344	1/1	0.95	0.15	32,32,32,32	0
56	MG	1A	3632	1/1	0.95	0.16	45,45,45,45	0
56	MG	1E	309	1/1	0.95	0.13	32,32,32,32	0
56	MG	1A	3035	1/1	0.95	0.14	58,58,58,58	0
56	MG	1A	3638	1/1	0.95	0.14	22,22,22,22	0
56	MG	2A	3573	1/1	0.95	0.10	42,42,42,42	0
56	MG	2a	3163	1/1	0.95	0.14	55,55,55,55	0
56	MG	2A	3351	1/1	0.95	0.17	62,62,62,62	0
56	MG	1A	3972	1/1	0.95	0.06	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3973	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3145	1/1	0.95	0.13	50,50,50,50	0
56	MG	2A	3146	1/1	0.95	0.19	41,41,41,41	0
56	MG	2a	3170	1/1	0.95	0.17	53,53,53,53	0
56	MG	1A	3759	1/1	0.95	0.05	54,54,54,54	0
56	MG	1q	204	1/1	0.95	0.18	58,58,58,58	0
56	MG	1a	1648	1/1	0.95	0.40	64,64,64,64	0
56	MG	1A	3762	1/1	0.95	0.10	51,51,51,51	0
56	MG	1G	3003	1/1	0.95	0.06	59,59,59,59	0
56	MG	1A	3173	1/1	0.95	0.14	24,24,24,24	0
56	MG	2A	3156	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3427	1/1	0.95	0.18	41,41,41,41	0
56	MG	2B	3007	1/1	0.95	0.11	55,55,55,55	0
56	MG	1A	3525	1/1	0.95	0.06	60,60,60,60	0
56	MG	2a	3183	1/1	0.95	0.23	54,54,54,54	0
56	MG	1a	1657	1/1	0.95	0.08	72,72,72,72	0
56	MG	1A	3769	1/1	0.95	0.11	37,37,37,37	0
56	MG	1a	1659	1/1	0.95	0.18	60,60,60,60	0
56	MG	1A	3648	1/1	0.95	0.15	51,51,51,51	0
56	MG	1a	1797	1/1	0.95	0.12	42,42,42,42	0
56	MG	2E	301	1/1	0.95	0.08	24,24,24,24	0
56	MG	1A	3248	1/1	0.95	0.21	60,60,60,60	0
56	MG	2E	303	1/1	0.95	0.25	53,53,53,53	0
56	MG	1A	3530	1/1	0.95	0.11	29,29,29,29	0
56	MG	1A	3654	1/1	0.95	0.16	60,60,60,60	0
56	MG	1A	3175	1/1	0.95	0.20	36,36,36,36	0
56	MG	2a	3196	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	3534	1/1	0.95	0.27	65,65,65,65	0
56	MG	1A	3281	1/1	0.95	0.22	59,59,59,59	0
56	MG	2a	3199	1/1	0.95	0.24	59,59,59,59	0
56	MG	1A	3660	1/1	0.95	0.13	38,38,38,38	0
56	MG	2A	3176	1/1	0.95	0.15	44,44,44,44	0
56	MG	1P	203	1/1	0.95	0.10	67,67,67,67	0
56	MG	1A	3538	1/1	0.95	0.10	14,14,14,14	0
56	MG	1Q	3002	1/1	0.95	0.21	38,38,38,38	0
56	MG	1a	1673	1/1	0.95	0.08	46,46,46,46	0
56	MG	1a	1809	1/1	0.95	0.09	67,67,67,67	0
56	MG	2a	3207	1/1	0.95	0.10	58,58,58,58	0
56	MG	2Q	204	1/1	0.95	0.15	46,46,46,46	0
56	MG	2Q	205	1/1	0.95	0.06	57,57,57,57	0
56	MG	1A	3056	1/1	0.95	0.13	49,49,49,49	0
56	MG	2A	3015	1/1	0.95	0.14	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3541	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3149	1/1	0.95	0.12	34,34,34,34	0
56	MG	2a	3214	1/1	0.95	0.15	75,75,75,75	0
56	MG	1A	3878	1/1	0.95	0.21	60,60,60,60	0
56	MG	1A	3791	1/1	0.95	0.10	60,60,60,60	0
56	MG	1A	3394	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3218	1/1	0.95	0.20	52,52,52,52	0
56	MG	1A	3355	1/1	0.95	0.11	51,51,51,51	0
56	MG	2a	3222	1/1	0.95	0.13	67,67,67,67	0
56	MG	2A	3408	1/1	0.95	0.07	47,47,47,47	0
56	MG	1A	4002	1/1	0.95	0.09	71,71,71,71	0
56	MG	1A	3884	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3558	1/1	0.95	0.10	27,27,27,27	0
56	MG	2A	3197	1/1	0.95	0.10	47,47,47,47	0
56	MG	1U	201	1/1	0.95	0.09	38,38,38,38	0
56	MG	1a	1694	1/1	0.95	0.08	41,41,41,41	0
56	MG	1U	203	1/1	0.95	0.40	40,40,40,40	0
56	MG	2a	3011	1/1	0.95	0.36	68,68,68,68	0
56	MG	2A	3201	1/1	0.95	0.13	52,52,52,52	0
56	MG	2a	3235	1/1	0.95	0.17	64,64,64,64	0
56	MG	2a	3236	1/1	0.95	0.14	67,67,67,67	0
56	MG	2A	3422	1/1	0.95	0.16	52,52,52,52	0
56	MG	1a	1696	1/1	0.95	0.08	67,67,67,67	0
56	MG	1A	3181	1/1	0.95	0.23	46,46,46,46	0
56	MG	2a	3240	1/1	0.95	0.19	65,65,65,65	0
56	MG	1U	205	1/1	0.95	0.25	43,43,43,43	0
56	MG	1A	3220	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3570	1/1	0.95	0.12	18,18,18,18	0
56	MG	2A	3037	1/1	0.95	0.28	62,62,62,62	0
56	MG	1A	3572	1/1	0.95	0.11	51,51,51,51	0
56	MG	2A	3210	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	4011	1/1	0.95	0.15	48,48,48,48	0
56	MG	1a	1707	1/1	0.95	0.21	46,46,46,46	0
56	MG	2A	3041	1/1	0.95	0.15	49,49,49,49	0
56	MG	1A	3802	1/1	0.95	0.12	64,64,64,64	0
56	MG	2l	201	1/1	0.95	0.13	64,64,64,64	0
56	MG	1A	4013	1/1	0.95	0.12	47,47,47,47	0
56	MG	1a	1839	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3047	1/1	0.95	0.11	46,46,46,46	0
56	MG	1a	1840	1/1	0.95	0.13	67,67,67,67	0
56	MG	1A	3109	1/1	0.95	0.12	69,69,69,69	0
56	MG	1A	3895	1/1	0.95	0.21	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3223	1/1	0.95	0.18	39,39,39,39	0
56	MG	1A	3066	1/1	0.95	0.27	63,63,63,63	0
56	MG	2A	3226	1/1	0.95	0.38	52,52,52,52	0
56	MG	1A	3289	1/1	0.95	0.19	49,49,49,49	0
56	MG	1A	3403	1/1	0.95	0.17	49,49,49,49	0
56	MG	2A	3058	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3965	1/1	0.96	0.09	35,35,35,35	0
56	MG	2A	3434	1/1	0.96	0.09	55,55,55,55	0
56	MG	1A	3210	1/1	0.96	0.16	46,46,46,46	0
56	MG	2A	3436	1/1	0.96	0.16	68,68,68,68	0
56	MG	2A	3031	1/1	0.96	0.23	55,55,55,55	0
56	MG	2A	3211	1/1	0.96	0.12	52,52,52,52	0
56	MG	1A	3726	1/1	0.96	0.07	29,29,29,29	0
56	MG	1G	3001	1/1	0.96	0.09	47,47,47,47	0
56	MG	1A	3606	1/1	0.96	0.12	43,43,43,43	0
56	MG	1A	3211	1/1	0.96	0.21	46,46,46,46	0
56	MG	1A	3849	1/1	0.96	0.09	55,55,55,55	0
56	MG	1A	3363	1/1	0.96	0.12	42,42,42,42	0
56	MG	1a	1665	1/1	0.96	0.10	47,47,47,47	0
56	MG	2a	3049	1/1	0.96	0.05	91,91,91,91	0
56	MG	1A	3974	1/1	0.96	0.18	48,48,48,48	0
56	MG	2A	3449	1/1	0.96	0.12	62,62,62,62	0
56	MG	1A	3457	1/1	0.96	0.11	48,48,48,48	0
56	MG	1A	3613	1/1	0.96	0.10	30,30,30,30	0
56	MG	1A	3742	1/1	0.96	0.15	60,60,60,60	0
56	MG	1a	1670	1/1	0.96	0.15	60,60,60,60	0
56	MG	1A	3743	1/1	0.96	0.06	60,60,60,60	0
56	MG	1a	1822	1/1	0.96	0.07	74,74,74,74	0
56	MG	2A	3456	1/1	0.96	0.07	41,41,41,41	0
56	MG	2a	3059	1/1	0.96	0.18	58,58,58,58	0
56	MG	2A	3228	1/1	0.96	0.19	44,44,44,44	0
56	MG	1A	3324	1/1	0.96	0.07	66,66,66,66	0
56	MG	2a	3062	1/1	0.96	0.06	66,66,66,66	0
56	MG	2A	3050	1/1	0.96	0.05	44,44,44,44	0
56	MG	2A	3051	1/1	0.96	0.16	49,49,49,49	0
56	MG	1A	3620	1/1	0.96	0.10	19,19,19,19	0
56	MG	2a	3068	1/1	0.96	0.07	43,43,43,43	0
56	MG	2A	3235	1/1	0.96	0.42	55,55,55,55	0
56	MG	2A	3464	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3747	1/1	0.96	0.11	28,28,28,28	0
56	MG	2A	3054	1/1	0.96	0.06	41,41,41,41	0
56	MG	1O	202	1/1	0.96	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3241	1/1	0.96	0.17	56,56,56,56	0
56	MG	1A	3072	1/1	0.96	0.09	53,53,53,53	0
56	MG	2a	3078	1/1	0.96	0.08	49,49,49,49	0
56	MG	2a	3079	1/1	0.96	0.32	55,55,55,55	0
56	MG	1A	3753	1/1	0.96	0.08	67,67,67,67	0
56	MG	1A	3027	1/1	0.96	0.09	60,60,60,60	0
56	MG	1a	1830	1/1	0.96	0.08	55,55,55,55	0
56	MG	1a	1681	1/1	0.96	0.09	44,44,44,44	0
56	MG	1a	1833	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3367	1/1	0.96	0.13	51,51,51,51	0
56	MG	1a	1683	1/1	0.96	0.23	56,56,56,56	0
56	MG	1A	3520	1/1	0.96	0.09	41,41,41,41	0
56	MG	1A	3761	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3484	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	3036	1/1	0.96	0.25	52,52,52,52	0
56	MG	2A	3067	1/1	0.96	0.24	57,57,57,57	0
56	MG	1a	1689	1/1	0.96	0.04	60,60,60,60	0
56	MG	1A	3764	1/1	0.96	0.06	54,54,54,54	0
56	MG	1A	3369	1/1	0.96	0.14	49,49,49,49	0
56	MG	1a	1692	1/1	0.96	0.16	50,50,50,50	0
56	MG	2a	3097	1/1	0.96	0.20	47,47,47,47	0
56	MG	2A	3261	1/1	0.96	0.08	34,34,34,34	0
56	MG	1A	3093	1/1	0.96	0.17	46,46,46,46	0
56	MG	2A	3263	1/1	0.96	0.12	24,24,24,24	0
56	MG	1A	3465	1/1	0.96	0.34	36,36,36,36	0
56	MG	1A	3872	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3526	1/1	0.96	0.14	50,50,50,50	0
56	MG	1T	202	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3527	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3290	1/1	0.96	0.12	47,47,47,47	0
56	MG	2A	3079	1/1	0.96	0.20	51,51,51,51	0
56	MG	2A	3273	1/1	0.96	0.07	36,36,36,36	0
56	MG	2a	3113	1/1	0.96	0.30	51,51,51,51	0
56	MG	1A	3176	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3775	1/1	0.96	0.10	22,22,22,22	0
56	MG	1A	3776	1/1	0.96	0.09	44,44,44,44	0
56	MG	1a	1703	1/1	0.96	0.10	48,48,48,48	0
56	MG	1a	1706	1/1	0.96	0.14	52,52,52,52	0
56	MG	2A	3512	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3531	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	3373	1/1	0.96	0.06	49,49,49,49	0
56	MG	1V	201	1/1	0.96	0.24	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3284	1/1	0.96	0.22	65,65,65,65	0
56	MG	1A	3533	1/1	0.96	0.09	37,37,37,37	0
56	MG	1W	3003	1/1	0.96	0.19	37,37,37,37	0
56	MG	1A	3781	1/1	0.96	0.06	28,28,28,28	0
56	MG	2a	3127	1/1	0.96	0.23	51,51,51,51	0
56	MG	1A	4008	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	3145	1/1	0.96	0.08	37,37,37,37	0
56	MG	1X	3001	1/1	0.96	0.11	44,44,44,44	0
56	MG	1X	3002	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3221	1/1	0.96	0.19	56,56,56,56	0
56	MG	1a	1719	1/1	0.96	0.17	47,47,47,47	0
56	MG	1A	3886	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3333	1/1	0.96	0.13	51,51,51,51	0
56	MG	1A	3178	1/1	0.96	0.21	50,50,50,50	0
56	MG	1A	3117	1/1	0.96	0.06	41,41,41,41	0
56	MG	10	102	1/1	0.96	0.07	56,56,56,56	0
56	MG	10	104	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3303	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3546	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3547	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3478	1/1	0.96	0.30	51,51,51,51	0
56	MG	2A	3309	1/1	0.96	0.17	44,44,44,44	0
56	MG	2A	3310	1/1	0.96	0.06	46,46,46,46	0
56	MG	1A	3024	1/1	0.96	0.06	52,52,52,52	0
56	MG	2A	3312	1/1	0.96	0.17	39,39,39,39	0
56	MG	2A	3313	1/1	0.96	0.08	49,49,49,49	0
56	MG	2A	3315	1/1	0.96	0.12	40,40,40,40	0
56	MG	2A	3110	1/1	0.96	0.17	49,49,49,49	0
56	MG	1A	3896	1/1	0.96	0.23	32,32,32,32	0
56	MG	1A	3119	1/1	0.96	0.13	35,35,35,35	0
56	MG	1A	3299	1/1	0.96	0.26	30,30,30,30	0
56	MG	1A	3097	1/1	0.96	0.09	40,40,40,40	0
56	MG	1A	4026	1/1	0.96	0.18	41,41,41,41	0
56	MG	1A	3150	1/1	0.96	0.14	40,40,40,40	0
56	MG	2A	3554	1/1	0.96	0.16	44,44,44,44	0
56	MG	1A	4028	1/1	0.96	0.10	68,68,68,68	0
56	MG	1A	3564	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3557	1/1	0.96	0.13	45,45,45,45	0
56	MG	1a	1740	1/1	0.96	0.10	57,57,57,57	0
56	MG	17	101	1/1	0.96	0.27	34,34,34,34	0
56	MG	2A	3560	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3330	1/1	0.96	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3562	1/1	0.96	0.14	37,37,37,37	0
56	MG	17	102	1/1	0.96	0.09	33,33,33,33	0
56	MG	2A	3125	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3566	1/1	0.96	0.10	42,42,42,42	0
56	MG	1a	1897	1/1	0.96	0.10	50,50,50,50	0
56	MG	2A	3568	1/1	0.96	0.10	43,43,43,43	0
56	MG	1A	3186	1/1	0.96	0.09	47,47,47,47	0
56	MG	1A	3803	1/1	0.96	0.12	33,33,33,33	0
56	MG	1A	3568	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3569	1/1	0.96	0.12	25,25,25,25	0
56	MG	1A	3432	1/1	0.96	0.23	44,44,44,44	0
56	MG	1A	3571	1/1	0.96	0.14	66,66,66,66	0
56	MG	2A	3341	1/1	0.96	0.06	39,39,39,39	0
56	MG	1A	3124	1/1	0.96	0.29	54,54,54,54	0
56	MG	1A	3231	1/1	0.96	0.21	42,42,42,42	0
56	MG	1a	1602	1/1	0.96	0.20	51,51,51,51	0
56	MG	1A	3388	1/1	0.96	0.17	42,42,42,42	0
56	MG	2A	3581	1/1	0.96	0.05	51,51,51,51	0
56	MG	1A	3919	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	4045	1/1	0.96	0.28	50,50,50,50	0
56	MG	1a	1757	1/1	0.96	0.08	64,64,64,64	0
56	MG	2a	3190	1/1	0.96	0.08	67,67,67,67	0
56	MG	1A	3812	1/1	0.96	0.06	54,54,54,54	0
56	MG	1A	3685	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3125	1/1	0.96	0.10	49,49,49,49	0
56	MG	2B	3006	1/1	0.96	0.17	50,50,50,50	0
56	MG	1A	3234	1/1	0.96	0.17	54,54,54,54	0
56	MG	1A	3194	1/1	0.96	0.13	41,41,41,41	0
56	MG	1A	3153	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3582	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3928	1/1	0.96	0.17	51,51,51,51	0
56	MG	1B	205	1/1	0.96	0.11	49,49,49,49	0
56	MG	1a	1767	1/1	0.96	0.07	84,84,84,84	0
56	MG	1A	3694	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3695	1/1	0.96	0.12	63,63,63,63	0
56	MG	2A	3159	1/1	0.96	0.14	31,31,31,31	0
56	MG	2A	3160	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3273	1/1	0.96	0.26	45,45,45,45	0
56	MG	1A	3584	1/1	0.96	0.10	52,52,52,52	0
56	MG	1B	211	1/1	0.96	0.20	54,54,54,54	0
56	MG	2A	3164	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3165	1/1	0.96	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1773	1/1	0.96	0.13	57,57,57,57	0
56	MG	1A	3824	1/1	0.96	0.05	31,31,31,31	0
56	MG	2O	202	1/1	0.96	0.18	53,53,53,53	0
56	MG	2A	3168	1/1	0.96	0.19	51,51,51,51	0
56	MG	1A	3033	1/1	0.96	0.20	47,47,47,47	0
56	MG	1a	1623	1/1	0.96	0.09	79,79,79,79	0
56	MG	1x	104	1/1	0.96	0.15	47,47,47,47	0
56	MG	1A	3939	1/1	0.96	0.16	57,57,57,57	0
56	MG	2A	3387	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3586	1/1	0.96	0.10	32,32,32,32	0
56	MG	2a	3224	1/1	0.96	0.11	75,75,75,75	0
56	MG	1A	3034	1/1	0.96	0.14	42,42,42,42	0
56	MG	1x	108	1/1	0.96	0.08	57,57,57,57	0
56	MG	2Y	502	1/1	0.96	0.15	57,57,57,57	0
56	MG	1A	3942	1/1	0.96	0.32	34,34,34,34	0
56	MG	1A	3443	1/1	0.96	0.08	47,47,47,47	0
56	MG	2A	3179	1/1	0.96	0.15	43,43,43,43	0
56	MG	1A	3079	1/1	0.96	0.08	31,31,31,31	0
56	MG	1A	3705	1/1	0.96	0.20	35,35,35,35	0
56	MG	2A	3182	1/1	0.96	0.15	37,37,37,37	0
56	MG	1A	3397	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	3708	1/1	0.96	0.14	45,45,45,45	0
56	MG	1D	303	1/1	0.96	0.09	47,47,47,47	0
56	MG	1A	3049	1/1	0.96	0.09	49,49,49,49	0
56	MG	1A	3104	1/1	0.96	0.04	38,38,38,38	0
56	MG	2A	3406	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3134	1/1	0.96	0.14	31,31,31,31	0
56	MG	1A	3953	1/1	0.96	0.18	61,61,61,61	0
56	MG	2A	3410	1/1	0.96	0.08	40,40,40,40	0
56	MG	1D	317	1/1	0.96	0.07	69,69,69,69	0
56	MG	1E	301	1/1	0.96	0.07	58,58,58,58	0
56	MG	2A	3413	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	3715	1/1	0.96	0.10	49,49,49,49	0
56	MG	1a	1643	1/1	0.96	0.16	52,52,52,52	0
56	MG	1A	3083	1/1	0.96	0.06	29,29,29,29	0
56	MG	1A	3107	1/1	0.96	0.28	50,50,50,50	0
56	MG	1A	3318	1/1	0.96	0.06	46,46,46,46	0
56	MG	2A	3420	1/1	0.96	0.15	59,59,59,59	0
56	MG	2A	3019	1/1	0.96	0.09	47,47,47,47	0
56	MG	1A	3600	1/1	0.96	0.11	31,31,31,31	0
56	MG	1A	3960	1/1	0.96	0.08	41,41,41,41	0
56	MG	2a	3025	1/1	0.96	0.08	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1649	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	3137	1/1	0.96	0.20	49,49,49,49	0
56	MG	2A	3024	1/1	0.96	0.18	67,67,67,67	0
56	MG	1A	3843	1/1	0.96	0.06	37,37,37,37	0
56	MG	2x	3003	1/1	0.96	0.14	51,51,51,51	0
56	MG	1F	301	1/1	0.96	0.20	39,39,39,39	0
56	MG	1A	3085	1/1	0.96	0.10	41,41,41,41	0
56	MG	1F	304	1/1	0.96	0.18	40,40,40,40	0
56	MG	2A	3207	1/1	0.96	0.16	23,23,23,23	0
56	MG	1A	3590	1/1	0.97	0.09	56,56,56,56	0
56	MG	2A	3314	1/1	0.97	0.07	28,28,28,28	0
56	MG	1A	3682	1/1	0.97	0.10	59,59,59,59	0
56	MG	1A	3469	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3032	1/1	0.97	0.07	65,65,65,65	0
56	MG	1A	3593	1/1	0.97	0.10	30,30,30,30	0
56	MG	2a	3073	1/1	0.97	0.11	68,68,68,68	0
56	MG	1P	204	1/1	0.97	0.31	31,31,31,31	0
56	MG	1P	205	1/1	0.97	0.22	49,49,49,49	0
56	MG	1A	3892	1/1	0.97	0.11	46,46,46,46	0
56	MG	2A	3322	1/1	0.97	0.05	29,29,29,29	0
56	MG	2A	3155	1/1	0.97	0.11	33,33,33,33	0
56	MG	1A	3471	1/1	0.97	0.06	66,66,66,66	0
56	MG	1A	3041	1/1	0.97	0.17	56,56,56,56	0
56	MG	1A	3189	1/1	0.97	0.25	28,28,28,28	0
56	MG	1A	3060	1/1	0.97	0.12	51,51,51,51	0
56	MG	1A	4009	1/1	0.97	0.20	48,48,48,48	0
56	MG	1R	201	1/1	0.97	0.08	38,38,38,38	0
56	MG	1R	202	1/1	0.97	0.25	68,68,68,68	0
56	MG	1A	3475	1/1	0.97	0.07	61,61,61,61	0
56	MG	1A	3191	1/1	0.97	0.07	40,40,40,40	0
56	MG	2A	3011	1/1	0.97	0.20	42,42,42,42	0
56	MG	2A	3012	1/1	0.97	0.06	52,52,52,52	0
56	MG	1a	1675	1/1	0.97	0.10	62,62,62,62	0
56	MG	2A	3014	1/1	0.97	0.17	44,44,44,44	0
56	MG	1A	3431	1/1	0.97	0.05	14,14,14,14	0
56	MG	1R	206	1/1	0.97	0.09	34,34,34,34	0
56	MG	2A	3530	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	3192	1/1	0.97	0.06	50,50,50,50	0
56	MG	2a	3098	1/1	0.97	0.14	49,49,49,49	0
56	MG	1A	3604	1/1	0.97	0.07	26,26,26,26	0
56	MG	1A	3807	1/1	0.97	0.07	58,58,58,58	0
56	MG	1A	3047	1/1	0.97	0.28	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3233	1/1	0.97	0.32	54,54,54,54	0
56	MG	1A	3081	1/1	0.97	0.17	62,62,62,62	0
56	MG	2a	3104	1/1	0.97	0.06	40,40,40,40	0
56	MG	2a	3105	1/1	0.97	0.28	58,58,58,58	0
56	MG	2a	3106	1/1	0.97	0.24	59,59,59,59	0
56	MG	2A	3177	1/1	0.97	0.20	40,40,40,40	0
56	MG	1U	202	1/1	0.97	0.08	43,43,43,43	0
56	MG	1A	3703	1/1	0.97	0.07	58,58,58,58	0
56	MG	1A	3162	1/1	0.97	0.18	38,38,38,38	0
56	MG	1A	3910	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	3163	1/1	0.97	0.16	43,43,43,43	0
56	MG	1A	3537	1/1	0.97	0.07	37,37,37,37	0
56	MG	1W	3002	1/1	0.97	0.18	47,47,47,47	0
56	MG	2A	3545	1/1	0.97	0.09	50,50,50,50	0
56	MG	2A	3361	1/1	0.97	0.08	72,72,72,72	0
56	MG	2A	3548	1/1	0.97	0.11	42,42,42,42	0
56	MG	1A	3616	1/1	0.97	0.07	28,28,28,28	0
56	MG	1A	3238	1/1	0.97	0.20	53,53,53,53	0
56	MG	1A	3619	1/1	0.97	0.05	16,16,16,16	0
56	MG	1A	3164	1/1	0.97	0.22	51,51,51,51	0
56	MG	2A	3553	1/1	0.97	0.12	35,35,35,35	0
56	MG	1A	3714	1/1	0.97	0.10	32,32,32,32	0
56	MG	1A	3042	1/1	0.97	0.24	47,47,47,47	0
56	MG	1A	3923	1/1	0.97	0.05	37,37,37,37	0
56	MG	2A	3371	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3821	1/1	0.97	0.06	26,26,26,26	0
56	MG	1A	3543	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3717	1/1	0.97	0.10	44,44,44,44	0
56	MG	1A	3625	1/1	0.97	0.13	30,30,30,30	0
56	MG	1a	1704	1/1	0.97	0.16	40,40,40,40	0
56	MG	2A	3042	1/1	0.97	0.17	50,50,50,50	0
56	MG	2A	3379	1/1	0.97	0.11	42,42,42,42	0
56	MG	1a	1705	1/1	0.97	0.09	64,64,64,64	0
56	MG	1A	3200	1/1	0.97	0.09	54,54,54,54	0
56	MG	2A	3045	1/1	0.97	0.10	45,45,45,45	0
56	MG	10	103	1/1	0.97	0.07	69,69,69,69	0
56	MG	1A	3929	1/1	0.97	0.11	27,27,27,27	0
56	MG	2A	3571	1/1	0.97	0.18	43,43,43,43	0
56	MG	1A	4040	1/1	0.97	0.23	35,35,35,35	0
56	MG	2A	3049	1/1	0.97	0.10	33,33,33,33	0
56	MG	1A	3930	1/1	0.97	0.04	23,23,23,23	0
56	MG	1A	3201	1/1	0.97	0.21	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4043	1/1	0.97	0.06	45,45,45,45	0
56	MG	1A	4044	1/1	0.97	0.39	39,39,39,39	0
56	MG	1A	3320	1/1	0.97	0.14	49,49,49,49	0
56	MG	1A	3933	1/1	0.97	0.14	54,54,54,54	0
56	MG	1A	4047	1/1	0.97	0.09	36,36,36,36	0
56	MG	1A	3549	1/1	0.97	0.11	68,68,68,68	0
56	MG	1a	1854	1/1	0.97	0.15	51,51,51,51	0
56	MG	2A	3583	1/1	0.97	0.11	42,42,42,42	0
56	MG	1A	3120	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3121	1/1	0.97	0.24	42,42,42,42	0
56	MG	1a	1721	1/1	0.97	0.13	65,65,65,65	0
56	MG	2A	3400	1/1	0.97	0.08	31,31,31,31	0
56	MG	2A	3401	1/1	0.97	0.08	39,39,39,39	0
56	MG	16	101	1/1	0.97	0.14	51,51,51,51	0
56	MG	2A	3403	1/1	0.97	0.05	34,34,34,34	0
56	MG	1A	3727	1/1	0.97	0.07	25,25,25,25	0
56	MG	1A	3633	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3634	1/1	0.97	0.10	19,19,19,19	0
56	MG	2A	3407	1/1	0.97	0.08	31,31,31,31	0
56	MG	1A	3731	1/1	0.97	0.09	29,29,29,29	0
56	MG	1A	3733	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3737	1/1	0.97	0.14	29,29,29,29	0
56	MG	1A	3168	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3637	1/1	0.97	0.12	29,29,29,29	0
56	MG	1a	1731	1/1	0.97	0.07	55,55,55,55	0
56	MG	2A	3414	1/1	0.97	0.12	39,39,39,39	0
56	MG	18	105	1/1	0.97	0.12	43,43,43,43	0
56	MG	2a	3173	1/1	0.97	0.22	57,57,57,57	0
56	MG	1A	3169	1/1	0.97	0.21	41,41,41,41	0
56	MG	1B	210	1/1	0.97	0.04	45,45,45,45	0
56	MG	1A	3102	1/1	0.97	0.17	37,37,37,37	0
56	MG	1A	3641	1/1	0.97	0.06	22,22,22,22	0
56	MG	1A	3562	1/1	0.97	0.15	50,50,50,50	0
56	MG	2a	3179	1/1	0.97	0.04	47,47,47,47	0
56	MG	2A	3238	1/1	0.97	0.17	48,48,48,48	0
56	MG	1A	3563	1/1	0.97	0.11	50,50,50,50	0
56	MG	2P	201	1/1	0.97	0.15	33,33,33,33	0
56	MG	1A	3123	1/1	0.97	0.15	25,25,25,25	0
56	MG	1B	218	1/1	0.97	0.12	60,60,60,60	0
56	MG	2A	3081	1/1	0.97	0.06	37,37,37,37	0
56	MG	1A	3749	1/1	0.97	0.05	27,27,27,27	0
56	MG	1B	222	1/1	0.97	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
56	MG	1A	3955	1/1	0.97	0.16	47,47,47,47	0
56	MG	1A	3565	1/1	0.97	0.05	17,17,17,17	0
56	MG	2U	202	1/1	0.97	0.10	45,45,45,45	0
56	MG	1a	1610	1/1	0.97	0.05	52,52,52,52	0
56	MG	1A	3752	1/1	0.97	0.08	55,55,55,55	0
56	MG	1a	1886	1/1	0.97	0.16	53,53,53,53	0
56	MG	1A	3172	1/1	0.97	0.13	32,32,32,32	0
56	MG	2A	3090	1/1	0.97	0.04	51,51,51,51	0
56	MG	1A	3754	1/1	0.97	0.06	20,20,20,20	0
56	MG	1A	3755	1/1	0.97	0.05	65,65,65,65	0
56	MG	1A	3651	1/1	0.97	0.08	25,25,25,25	0
56	MG	1D	304	1/1	0.97	0.17	50,50,50,50	0
56	MG	1A	3652	1/1	0.97	0.03	24,24,24,24	0
56	MG	1D	306	1/1	0.97	0.14	43,43,43,43	0
56	MG	2A	3260	1/1	0.97	0.18	54,54,54,54	0
56	MG	1A	3063	1/1	0.97	0.17	52,52,52,52	0
56	MG	2A	3444	1/1	0.97	0.13	39,39,39,39	0
56	MG	1D	312	1/1	0.97	0.05	47,47,47,47	0
56	MG	1D	313	1/1	0.97	0.10	44,44,44,44	0
56	MG	1A	3086	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3657	1/1	0.97	0.06	19,19,19,19	0
56	MG	2A	3266	1/1	0.97	0.11	54,54,54,54	0
56	MG	1A	3411	1/1	0.97	0.09	51,51,51,51	0
56	MG	2A	3103	1/1	0.97	0.08	50,50,50,50	0
56	MG	2a	3016	1/1	0.97	0.07	58,58,58,58	0
56	MG	1a	1901	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3502	1/1	0.97	0.10	77,77,77,77	0
56	MG	1A	3064	1/1	0.97	0.08	41,41,41,41	0
56	MG	1a	1904	1/1	0.97	0.06	53,53,53,53	0
56	MG	2A	3274	1/1	0.97	0.09	47,47,47,47	0
56	MG	2A	3458	1/1	0.97	0.10	31,31,31,31	0
56	MG	2a	3219	1/1	0.97	0.09	58,58,58,58	0
56	MG	1A	3971	1/1	0.97	0.10	61,61,61,61	0
56	MG	2a	3221	1/1	0.97	0.14	57,57,57,57	0
56	MG	1A	3767	1/1	0.97	0.10	21,21,21,21	0
56	MG	2a	3223	1/1	0.97	0.13	57,57,57,57	0
56	MG	1A	3504	1/1	0.97	0.15	52,52,52,52	0
56	MG	1A	3216	1/1	0.97	0.11	66,66,66,66	0
56	MG	2A	3112	1/1	0.97	0.15	36,36,36,36	0
56	MG	2a	3028	1/1	0.97	0.27	61,61,61,61	0
56	MG	1a	1632	1/1	0.97	0.10	53,53,53,53	0
56	MG	2A	3281	1/1	0.97	0.20	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3031	1/1	0.97	0.23	48,48,48,48	0
56	MG	1A	3254	1/1	0.97	0.13	32,32,32,32	0
56	MG	1A	3089	1/1	0.97	0.22	44,44,44,44	0
56	MG	1A	3108	1/1	0.97	0.33	49,49,49,49	0
56	MG	1A	3335	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3510	1/1	0.97	0.17	39,39,39,39	0
56	MG	2A	3471	1/1	0.97	0.14	54,54,54,54	0
56	MG	1F	303	1/1	0.97	0.05	40,40,40,40	0
56	MG	1A	3043	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3003	1/1	0.97	0.08	58,58,58,58	0
56	MG	1A	3672	1/1	0.97	0.11	50,50,50,50	0
56	MG	2A	3476	1/1	0.97	0.05	45,45,45,45	0
56	MG	1A	3780	1/1	0.97	0.05	48,48,48,48	0
56	MG	2A	3479	1/1	0.97	0.06	31,31,31,31	0
56	MG	1A	3132	1/1	0.97	0.16	17,17,17,17	0
56	MG	2A	3481	1/1	0.97	0.07	41,41,41,41	0
56	MG	1l	201	1/1	0.97	0.12	62,62,62,62	0
56	MG	1A	3674	1/1	0.97	0.04	30,30,30,30	0
56	MG	2A	3295	1/1	0.97	0.05	50,50,50,50	0
56	MG	1A	3260	1/1	0.97	0.14	49,49,49,49	0
56	MG	1a	1781	1/1	0.97	0.09	87,87,87,87	0
56	MG	2A	3299	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3784	1/1	0.97	0.12	31,31,31,31	0
56	MG	1q	203	1/1	0.97	0.20	64,64,64,64	0
56	MG	1A	3879	1/1	0.97	0.06	24,24,24,24	0
56	MG	1A	3785	1/1	0.97	0.05	57,57,57,57	0
56	MG	1A	3222	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3112	1/1	0.97	0.17	35,35,35,35	0
56	MG	2A	3496	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3156	1/1	0.97	0.23	49,49,49,49	0
56	MG	1A	3185	1/1	0.97	0.07	44,44,44,44	0
56	MG	1A	3790	1/1	0.97	0.09	21,21,21,21	0
56	MG	1A	3998	1/1	0.97	0.11	51,51,51,51	0
56	MG	2a	3064	1/1	0.97	0.30	51,51,51,51	0
57	ZN	14	501	1/1	0.97	0.05	102,102,102,102	0
56	MG	1a	1655	1/1	0.97	0.05	60,60,60,60	0
57	ZN	2n	501	1/1	0.97	0.06	105,105,105,105	0
56	MG	1A	3092	1/1	0.98	0.08	40,40,40,40	0
56	MG	1A	4048	1/1	0.98	0.04	32,32,32,32	0
56	MG	1A	3707	1/1	0.98	0.07	40,40,40,40	0
56	MG	1A	3193	1/1	0.98	0.15	20,20,20,20	0
56	MG	1A	3653	1/1	0.98	0.04	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1630	1/1	0.98	0.08	38,38,38,38	0
56	MG	1A	3101	1/1	0.98	0.10	35,35,35,35	0
56	MG	1A	3711	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	3467	1/1	0.98	0.13	44,44,44,44	0
56	MG	1A	3656	1/1	0.98	0.07	56,56,56,56	0
56	MG	1A	3180	1/1	0.98	0.05	50,50,50,50	0
56	MG	1A	3535	1/1	0.98	0.08	24,24,24,24	0
56	MG	1A	3213	1/1	0.98	0.04	23,23,23,23	0
56	MG	1A	3912	1/1	0.98	0.06	49,49,49,49	0
56	MG	1n	502	1/1	0.98	0.03	47,47,47,47	0
56	MG	1A	3913	1/1	0.98	0.04	41,41,41,41	0
56	MG	2A	3421	1/1	0.98	0.04	50,50,50,50	0
56	MG	2A	3298	1/1	0.98	0.04	45,45,45,45	0
56	MG	2a	3161	1/1	0.98	0.09	62,62,62,62	0
56	MG	1A	3914	1/1	0.98	0.10	22,22,22,22	0
56	MG	1A	3608	1/1	0.98	0.08	39,39,39,39	0
56	MG	1A	3719	1/1	0.98	0.05	7,7,7,7	0
56	MG	2A	3546	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3661	1/1	0.98	0.10	51,51,51,51	0
56	MG	1A	3918	1/1	0.98	0.11	25,25,25,25	0
56	MG	1A	3111	1/1	0.98	0.16	39,39,39,39	0
56	MG	1A	3610	1/1	0.98	0.07	33,33,33,33	0
56	MG	1B	220	1/1	0.98	0.05	27,27,27,27	0
56	MG	1a	1831	1/1	0.98	0.09	63,63,63,63	0
56	MG	1A	3087	1/1	0.98	0.10	32,32,32,32	0
56	MG	1A	3094	1/1	0.98	0.10	24,24,24,24	0
56	MG	1A	3614	1/1	0.98	0.06	26,26,26,26	0
56	MG	1a	1835	1/1	0.98	0.11	34,34,34,34	0
56	MG	1A	3995	1/1	0.98	0.13	10,10,10,10	0
56	MG	1A	3996	1/1	0.98	0.06	29,29,29,29	0
56	MG	1a	1744	1/1	0.98	0.05	80,80,80,80	0
56	MG	1A	3997	1/1	0.98	0.04	18,18,18,18	0
56	MG	1A	3026	1/1	0.98	0.25	36,36,36,36	0
56	MG	1A	3617	1/1	0.98	0.11	28,28,28,28	0
56	MG	1a	1656	1/1	0.98	0.06	25,25,25,25	0
56	MG	2A	3564	1/1	0.98	0.31	34,34,34,34	0
56	MG	1a	1844	1/1	0.98	0.05	38,38,38,38	0
56	MG	1A	3729	1/1	0.98	0.06	22,22,22,22	0
56	MG	2A	3445	1/1	0.98	0.06	74,74,74,74	0
56	MG	1A	3542	1/1	0.98	0.07	29,29,29,29	0
56	MG	1A	3577	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3732	1/1	0.98	0.05	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3066	1/1	0.98	0.10	50,50,50,50	0
56	MG	1D	307	1/1	0.98	0.08	39,39,39,39	0
56	MG	1D	308	1/1	0.98	0.04	13,13,13,13	0
56	MG	2A	3329	1/1	0.98	0.06	39,39,39,39	0
56	MG	1D	309	1/1	0.98	0.04	37,37,37,37	0
56	MG	1A	3578	1/1	0.98	0.07	39,39,39,39	0
56	MG	1D	311	1/1	0.98	0.05	49,49,49,49	0
56	MG	1A	3734	1/1	0.98	0.07	27,27,27,27	0
56	MG	1A	3735	1/1	0.98	0.08	27,27,27,27	0
56	MG	2a	3075	1/1	0.98	0.12	60,60,60,60	0
56	MG	1a	1857	1/1	0.98	0.14	47,47,47,47	0
56	MG	1D	314	1/1	0.98	0.04	48,48,48,48	0
56	MG	1A	3736	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3579	1/1	0.98	0.13	49,49,49,49	0
56	MG	2A	3222	1/1	0.98	0.11	45,45,45,45	0
56	MG	1A	3935	1/1	0.98	0.06	20,20,20,20	0
56	MG	1A	3494	1/1	0.98	0.11	58,58,58,58	0
56	MG	2A	3342	1/1	0.98	0.23	46,46,46,46	0
56	MG	1A	3544	1/1	0.98	0.07	30,30,30,30	0
56	MG	1a	1674	1/1	0.98	0.14	57,57,57,57	0
56	MG	2A	3120	1/1	0.98	0.03	23,23,23,23	0
56	MG	1A	3740	1/1	0.98	0.07	13,13,13,13	0
56	MG	2A	3230	1/1	0.98	0.30	51,51,51,51	0
56	MG	2A	3122	1/1	0.98	0.20	43,43,43,43	0
56	MG	1A	3870	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	4014	1/1	0.98	0.07	51,51,51,51	0
56	MG	1A	3626	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3545	1/1	0.98	0.11	31,31,31,31	0
56	MG	2D	304	1/1	0.98	0.17	34,34,34,34	0
56	MG	1A	3138	1/1	0.98	0.11	55,55,55,55	0
56	MG	1A	3078	1/1	0.98	0.09	21,21,21,21	0
56	MG	1A	3202	1/1	0.98	0.11	50,50,50,50	0
56	MG	1A	3187	1/1	0.98	0.05	54,54,54,54	0
56	MG	1A	3382	1/1	0.98	0.08	29,29,29,29	0
56	MG	1a	1685	1/1	0.98	0.06	23,23,23,23	0
56	MG	1A	3948	1/1	0.98	0.05	18,18,18,18	0
56	MG	1a	1687	1/1	0.98	0.12	54,54,54,54	0
56	MG	1A	3750	1/1	0.98	0.04	18,18,18,18	0
56	MG	1A	4024	1/1	0.98	0.06	29,29,29,29	0
56	MG	2A	3248	1/1	0.98	0.11	56,56,56,56	0
56	MG	1a	1880	1/1	0.98	0.08	50,50,50,50	0
56	MG	1A	3551	1/1	0.98	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3490	1/1	0.98	0.05	30,30,30,30	0
56	MG	1A	3500	1/1	0.98	0.05	51,51,51,51	0
56	MG	2A	3142	1/1	0.98	0.15	39,39,39,39	0
56	MG	1A	3553	1/1	0.98	0.04	38,38,38,38	0
56	MG	2A	3376	1/1	0.98	0.11	29,29,29,29	0
56	MG	1A	3636	1/1	0.98	0.06	19,19,19,19	0
56	MG	2A	3255	1/1	0.98	0.06	42,42,42,42	0
56	MG	1A	3555	1/1	0.98	0.05	39,39,39,39	0
56	MG	1H	202	1/1	0.98	0.12	59,59,59,59	0
56	MG	2A	3499	1/1	0.98	0.06	31,31,31,31	0
56	MG	2A	3147	1/1	0.98	0.11	33,33,33,33	0
56	MG	2A	3148	1/1	0.98	0.11	41,41,41,41	0
56	MG	1A	4030	1/1	0.98	0.10	41,41,41,41	0
56	MG	1A	3174	1/1	0.98	0.10	40,40,40,40	0
56	MG	1A	3557	1/1	0.98	0.09	44,44,44,44	0
56	MG	1A	3293	1/1	0.98	0.07	36,36,36,36	0
56	MG	1A	3760	1/1	0.98	0.08	42,42,42,42	0
56	MG	1A	3825	1/1	0.98	0.05	33,33,33,33	0
56	MG	2A	3389	1/1	0.98	0.08	36,36,36,36	0
56	MG	1A	3106	1/1	0.98	0.15	26,26,26,26	0
56	MG	1N	206	1/1	0.98	0.06	34,34,34,34	0
56	MG	1N	207	1/1	0.98	0.22	45,45,45,45	0
56	MG	2n	503	1/1	0.98	0.04	64,64,64,64	0
56	MG	1A	3890	1/1	0.98	0.10	62,62,62,62	0
56	MG	1A	3643	1/1	0.98	0.07	22,22,22,22	0
56	MG	1A	3644	1/1	0.98	0.08	38,38,38,38	0
56	MG	1a	1899	1/1	0.98	0.05	50,50,50,50	0
56	MG	1a	1708	1/1	0.98	0.09	61,61,61,61	0
56	MG	1A	3645	1/1	0.98	0.05	32,32,32,32	0
56	MG	1A	3646	1/1	0.98	0.08	21,21,21,21	0
56	MG	1A	3015	1/1	0.98	0.17	40,40,40,40	0
56	MG	1A	3030	1/1	0.98	0.17	52,52,52,52	0
56	MG	1A	3969	1/1	0.98	0.05	39,39,39,39	0
57	ZN	1n	501	1/1	0.98	0.05	86,86,86,86	0
56	MG	1A	3598	1/1	0.98	0.04	21,21,21,21	0
57	ZN	29	501	1/1	0.98	0.03	65,65,65,65	0
56	MG	1A	3529	1/1	0.98	0.07	62,62,62,62	0
58	SF4	2d	501	8/8	0.98	0.04	58,77,81,90	0
56	MG	1A	3560	1/1	0.99	0.09	24,24,24,24	0
56	MG	2A	3232	1/1	0.99	0.14	38,38,38,38	0
56	MG	1A	3855	1/1	0.99	0.06	15,15,15,15	0
56	MG	1A	3697	1/1	0.99	0.04	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3141	1/1	0.99	0.14	35,35,35,35	0
56	MG	2A	3236	1/1	0.99	0.16	41,41,41,41	0
56	MG	1A	3561	1/1	0.99	0.14	34,34,34,34	0
56	MG	1A	3215	1/1	0.99	0.07	26,26,26,26	0
56	MG	1A	3113	1/1	0.99	0.04	42,42,42,42	0
56	MG	1A	3792	1/1	0.99	0.06	47,47,47,47	0
56	MG	1A	3524	1/1	0.99	0.11	24,24,24,24	0
56	MG	1A	3611	1/1	0.99	0.09	28,28,28,28	0
56	MG	1A	3207	1/1	0.99	0.09	40,40,40,40	0
56	MG	1A	3864	1/1	0.99	0.03	15,15,15,15	0
56	MG	1A	3763	1/1	0.99	0.12	46,46,46,46	0
56	MG	2A	3349	1/1	0.99	0.09	49,49,49,49	0
56	MG	2A	3350	1/1	0.99	0.07	46,46,46,46	0
56	MG	1A	3129	1/1	0.99	0.14	35,35,35,35	0
56	MG	1A	3144	1/1	0.99	0.14	22,22,22,22	0
56	MG	2A	3353	1/1	0.99	0.08	54,54,54,54	0
56	MG	1A	3615	1/1	0.99	0.09	57,57,57,57	0
56	MG	2A	3355	1/1	0.99	0.03	42,42,42,42	0
56	MG	2A	3356	1/1	0.99	0.04	37,37,37,37	0
56	MG	2A	3477	1/1	0.99	0.09	61,61,61,61	0
56	MG	2a	3167	1/1	0.99	0.12	40,40,40,40	0
56	MG	1A	3084	1/1	0.99	0.03	25,25,25,25	0
56	MG	1A	3554	1/1	0.99	0.08	38,38,38,38	0
56	MG	1E	302	1/1	0.99	0.07	19,19,19,19	0
56	MG	2F	302	1/1	0.99	0.07	44,44,44,44	0
56	MG	1A	3082	1/1	0.99	0.10	28,28,28,28	0
56	MG	1A	3683	1/1	0.99	0.07	40,40,40,40	0
56	MG	1A	3908	1/1	0.99	0.05	20,20,20,20	0
56	MG	1A	3909	1/1	0.99	0.03	25,25,25,25	0
56	MG	2A	3306	1/1	0.99	0.06	26,26,26,26	0
56	MG	2A	3365	1/1	0.99	0.06	44,44,44,44	0
56	MG	2A	3307	1/1	0.99	0.07	32,32,32,32	0
56	MG	1A	3639	1/1	0.99	0.05	11,11,11,11	0
56	MG	1A	3059	1/1	0.99	0.03	46,46,46,46	0
56	MG	1A	3773	1/1	0.99	0.05	22,22,22,22	0
56	MG	2A	3370	1/1	0.99	0.03	62,62,62,62	0
56	MG	1a	1841	1/1	0.99	0.04	40,40,40,40	0
56	MG	1A	3774	1/1	0.99	0.08	21,21,21,21	0
56	MG	1A	3713	1/1	0.99	0.03	38,38,38,38	0
56	MG	17	103	1/1	0.99	0.05	53,53,53,53	0
56	MG	1A	3133	1/1	0.99	0.03	32,32,32,32	0
56	MG	1A	3687	1/1	0.99	0.08	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	216	1/1	0.99	0.04	47,47,47,47	0
56	MG	1B	217	1/1	0.99	0.06	36,36,36,36	0
56	MG	1A	3688	1/1	0.99	0.06	23,23,23,23	0
56	MG	1B	219	1/1	0.99	0.06	53,53,53,53	0
56	MG	2A	3269	1/1	0.99	0.11	43,43,43,43	0
56	MG	1A	3621	1/1	0.99	0.03	24,24,24,24	0
56	MG	1A	3622	1/1	0.99	0.06	21,21,21,21	0
56	MG	2A	3506	1/1	0.99	0.04	34,34,34,34	0
56	MG	1A	3748	1/1	0.99	0.05	36,36,36,36	0
56	MG	2A	3325	1/1	0.99	0.06	32,32,32,32	0
56	MG	1A	3603	1/1	0.99	0.07	26,26,26,26	0
56	MG	2A	3224	1/1	0.99	0.04	33,33,33,33	0
57	ZN	1Y	501	1/1	0.99	0.02	63,63,63,63	0
56	MG	1A	3666	1/1	0.99	0.02	9,9,9,9	0
56	MG	2A	3133	1/1	0.99	0.06	40,40,40,40	0
57	ZN	2Y	501	1/1	0.99	0.04	88,88,88,88	0
56	MG	1a	1856	1/1	0.99	0.08	70,70,70,70	0
57	ZN	25	501	1/1	0.99	0.03	49,49,49,49	0
57	ZN	26	102	1/1	0.99	0.05	68,68,68,68	0
56	MG	1A	3721	1/1	0.99	0.05	45,45,45,45	0
56	MG	1A	3096	1/1	0.99	0.05	40,40,40,40	0
58	SF4	1d	301	8/8	0.99	0.05	64,69,73,86	0
56	MG	1A	3235	1/1	0.99	0.04	42,42,42,42	0
56	MG	1A	3962	1/1	1.00	0.03	34,34,34,34	0
57	ZN	15	102	1/1	1.00	0.02	43,43,43,43	0
57	ZN	16	102	1/1	1.00	0.04	45,45,45,45	0
57	ZN	19	501	1/1	1.00	0.04	44,44,44,44	0
56	MG	1A	3756	1/1	1.00	0.04	46,46,46,46	0
56	MG	1A	3539	1/1	1.00	0.04	26,26,26,26	0
56	MG	1A	3676	1/1	1.00	0.02	23,23,23,23	0
56	MG	1A	3746	1/1	1.00	0.07	15,15,15,15	0
56	MG	1A	3795	1/1	1.00	0.06	24,24,24,24	0
56	MG	1A	3689	1/1	1.00	0.05	14,14,14,14	0
56	MG	2A	3485	1/1	1.00	0.02	35,35,35,35	0
56	MG	1A	3947	1/1	1.00	0.02	37,37,37,37	0
56	MG	2a	3095	1/1	1.00	0.02	58,58,58,58	0

6.5 Other polymers

There are no such residues in this entry.