



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 02:42 PM EDT

PDB ID : 8FC5 / pdb_00008fc5
Title : Crystal structure of the A2058-N6-dimethylated *Thermus thermophilus* 70S ribosome in complex with protein Y, hygromycin A, and azithromycin at 2.65Å resolution
Authors : Chen, C.-W.; Syroegin, E.A.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on : 2022-12-01
Resolution : 2.65 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

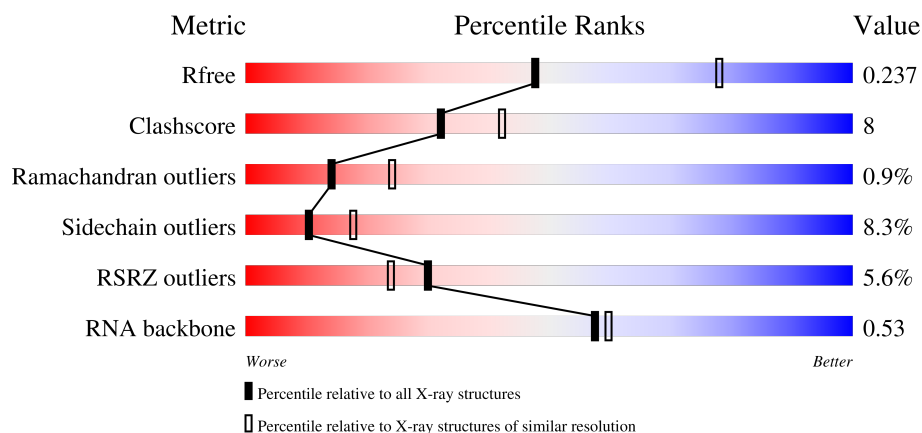
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



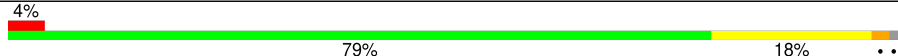
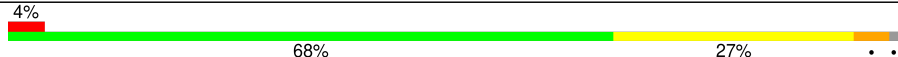
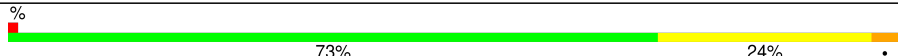
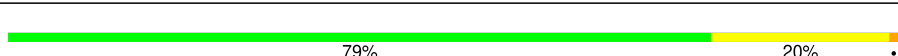
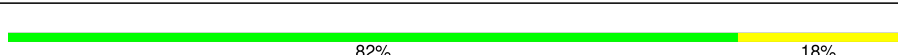
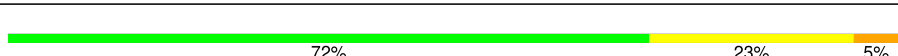
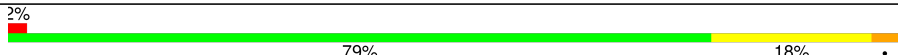
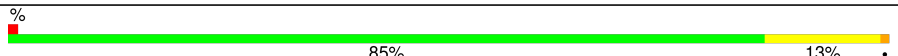
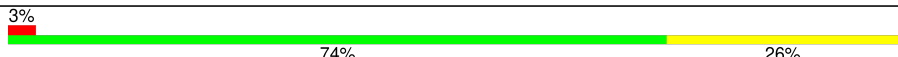
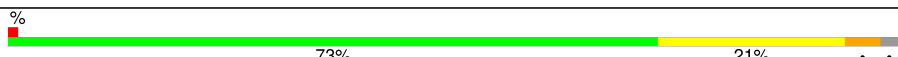
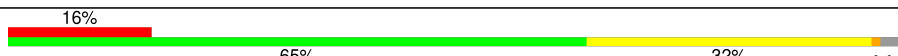
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)
RNA backbone	3983	1090 (2.90-2.42)

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	5% 67% 26% 6%
1	2A	2915	5% 62% 29% 7%
2	1B	121	% 69% 26% • •

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

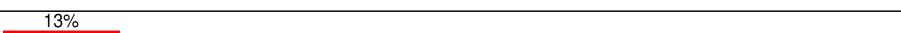
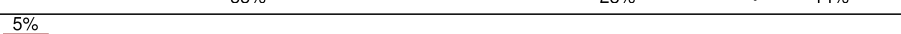
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Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25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

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

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Mol	Chain	Length	Quality of chain
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	

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Mol	Chain	Length	Quality of chain
52	2u	27	
53	1y	113	
53	2y	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3601	-	-	-	X
54	MG	2A	3090	-	-	-	X
54	MG	2A	3206	-	-	-	X
54	MG	2a	3085	-	-	-	X

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 296864 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	2872	Total	C	N	O	P	0	0	0
			61871	27542	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61759	27492	11552	19850	2865			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1031	Total	Mg	0	0
			1031	1031		
54	1B	29	Total	Mg	0	0
			29	29		
54	1D	18	Total	Mg	0	0
			18	18		
54	1E	10	Total	Mg	0	0
			10	10		
54	1F	18	Total	Mg	0	0
			18	18		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	4	Total	Mg	0	0
			4	4		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	7	Total	Mg	0	0
			7	7		
54	1Q	5	Total	Mg	0	0
			5	5		
54	1R	5	Total	Mg	0	0
			5	5		
54	1S	1	Total	Mg	0	0
			1	1		
54	1T	6	Total	Mg	0	0
			6	6		
54	1U	7	Total	Mg	0	0
			7	7		
54	1V	4	Total	Mg	0	0
			4	4		
54	1W	4	Total	Mg	0	0
			4	4		
54	1X	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1Y	1	Total 1	Mg 1	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	10	6	Total 6	Mg 6	0	0
54	11	5	Total 5	Mg 5	0	0
54	13	3	Total 3	Mg 3	0	0
54	15	8	Total 8	Mg 8	0	0
54	17	7	Total 7	Mg 7	0	0
54	18	2	Total 2	Mg 2	0	0
54	19	3	Total 3	Mg 3	0	0
54	1a	281	Total 281	Mg 281	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	2	Total 2	Mg 2	0	0
54	1e	3	Total 3	Mg 3	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1m	1	Total 1	Mg 1	0	0
54	1n	3	Total 3	Mg 3	0	0
54	1o	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1t	1	Total 1	Mg 1	0	0
54	1u	1	Total 1	Mg 1	0	0
54	1y	3	Total 3	Mg 3	0	0
54	2A	711	Total 711	Mg 711	0	0
54	2B	18	Total 18	Mg 18	0	0
54	2D	9	Total 9	Mg 9	0	0
54	2E	5	Total 5	Mg 5	0	0
54	2F	4	Total 4	Mg 4	0	0
54	2G	2	Total 2	Mg 2	0	0
54	2I	1	Total 1	Mg 1	0	0
54	2N	1	Total 1	Mg 1	0	0
54	2O	2	Total 2	Mg 2	0	0
54	2P	1	Total 1	Mg 1	0	0
54	2Q	3	Total 3	Mg 3	0	0
54	2R	1	Total 1	Mg 1	0	0
54	2T	3	Total 3	Mg 3	0	0
54	2V	3	Total 3	Mg 3	0	0
54	2W	3	Total 3	Mg 3	0	0
54	2X	1	Total 1	Mg 1	0	0
54	2Y	1	Total 1	Mg 1	0	0
54	20	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	21	1	Total 1	Mg 1	0	0
54	23	1	Total 1	Mg 1	0	0
54	25	1	Total 1	Mg 1	0	0
54	27	1	Total 1	Mg 1	0	0
54	28	2	Total 2	Mg 2	0	0
54	2a	182	Total 182	Mg 182	0	0
54	2e	2	Total 2	Mg 2	0	0
54	2f	1	Total 1	Mg 1	0	0
54	2j	1	Total 1	Mg 1	0	0
54	2k	1	Total 1	Mg 1	0	0
54	2l	1	Total 1	Mg 1	0	0
54	2n	1	Total 1	Mg 1	0	0
54	2t	1	Total 1	Mg 1	0	0

- Molecule 55 is Hygromycin A (CCD ID: HGR) (formula: $C_{23}H_{29}NO_{12}$) (labeled as "Ligand of Interest" by depositor).



- Molecule 56 is AZITHROMYCIN (CCD ID: ZIT) (formula: $C_{38}H_{72}N_2O_{12}$) (labeled as "Ligand of Interest" by depositor).

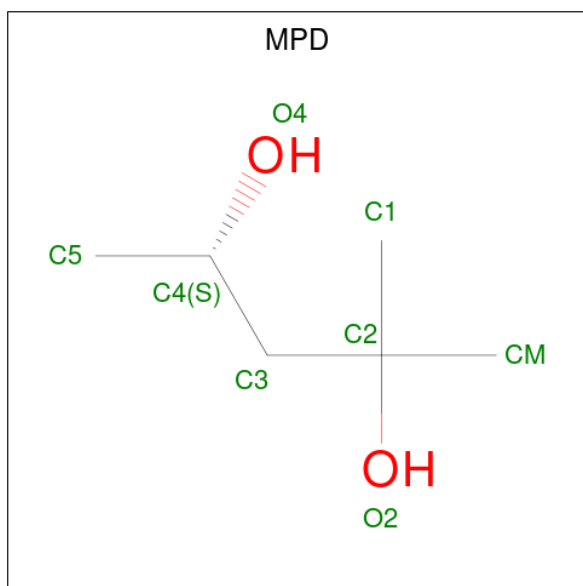


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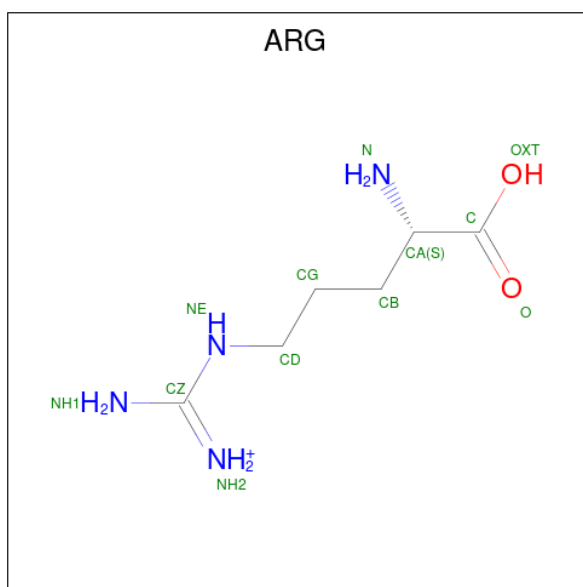
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	2A	1	Total	C	N	O	0	0
			52	38	2	12		

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1A	1	Total	C	O	0	0
			8	6	2		
57	1T	1	Total	C	O	0	0
			8	6	2		
57	18	1	Total	C	O	0	0
			8	6	2		
57	1a	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 58 is ARGinine (CCD ID: ARG) (formula: C₆H₁₅N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1B	1	Total	C	N	O	0	0
			12	6	4	2		
58	1F	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

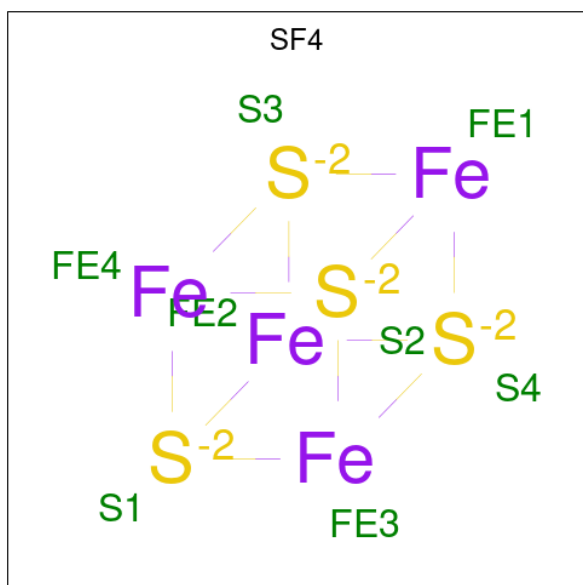
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	29	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	3571	Total	O	0	0
			3571	3571		
61	1B	89	Total	O	0	0
			89	89		
61	1D	109	Total	O	0	0
			109	109		
61	1E	68	Total	O	0	0
			68	68		
61	1F	61	Total	O	0	0
			61	61		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	10	Total	O	0	0
			10	10		
61	1H	15	Total	O	0	0
			15	15		
61	1I	4	Total	O	0	0
			4	4		
61	1N	46	Total	O	0	0
			46	46		
61	1O	17	Total	O	0	0
			17	17		
61	1P	53	Total	O	0	0
			53	53		
61	1Q	30	Total	O	0	0
			30	30		
61	1R	29	Total	O	0	0
			29	29		
61	1S	7	Total	O	0	0
			7	7		
61	1T	32	Total	O	0	0
			32	32		
61	1U	38	Total	O	0	0
			38	38		
61	1V	26	Total	O	0	0
			26	26		
61	1W	28	Total	O	0	0
			28	28		
61	1X	23	Total	O	0	0
			23	23		
61	1Y	13	Total	O	0	0
			13	13		
61	1Z	9	Total	O	0	0
			9	9		
61	10	19	Total	O	0	0
			19	19		
61	11	17	Total	O	0	0
			17	17		
61	12	11	Total	O	0	0
			11	11		
61	13	20	Total	O	0	0
			20	20		
61	15	28	Total	O	0	0
			28	28		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	16	12	Total 12	O 12	0	0
61	17	12	Total 12	O 12	0	0
61	18	24	Total 24	O 24	0	0
61	19	3	Total 3	O 3	0	0
61	1a	388	Total 388	O 388	0	0
61	1d	9	Total 9	O 9	0	0
61	1f	1	Total 1	O 1	0	0
61	1h	2	Total 2	O 2	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	2	Total 2	O 2	0	0
61	1m	1	Total 1	O 1	0	0
61	1n	2	Total 2	O 2	0	0
61	1o	1	Total 1	O 1	0	0
61	1p	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1y	3	Total 3	O 3	0	0
61	2A	2161	Total 2161	O 2161	0	0
61	2B	48	Total 48	O 48	0	0
61	2D	43	Total 43	O 43	0	0
61	2E	22	Total 22	O 22	0	0
61	2F	25	Total 25	O 25	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2G	1	Total	O	0	0
			1	1		
61	2H	1	Total	O	0	0
			1	1		
61	2I	1	Total	O	0	0
			1	1		
61	2N	5	Total	O	0	0
			5	5		
61	2O	17	Total	O	0	0
			17	17		
61	2P	20	Total	O	0	0
			20	20		
61	2Q	19	Total	O	0	0
			19	19		
61	2R	15	Total	O	0	0
			15	15		
61	2S	4	Total	O	0	0
			4	4		
61	2T	11	Total	O	0	0
			11	11		
61	2U	15	Total	O	0	0
			15	15		
61	2V	3	Total	O	0	0
			3	3		
61	2W	16	Total	O	0	0
			16	16		
61	2X	6	Total	O	0	0
			6	6		
61	2Y	2	Total	O	0	0
			2	2		
61	2Z	6	Total	O	0	0
			6	6		
61	20	5	Total	O	0	0
			5	5		
61	21	14	Total	O	0	0
			14	14		
61	23	3	Total	O	0	0
			3	3		
61	25	8	Total	O	0	0
			8	8		
61	26	3	Total	O	0	0
			3	3		

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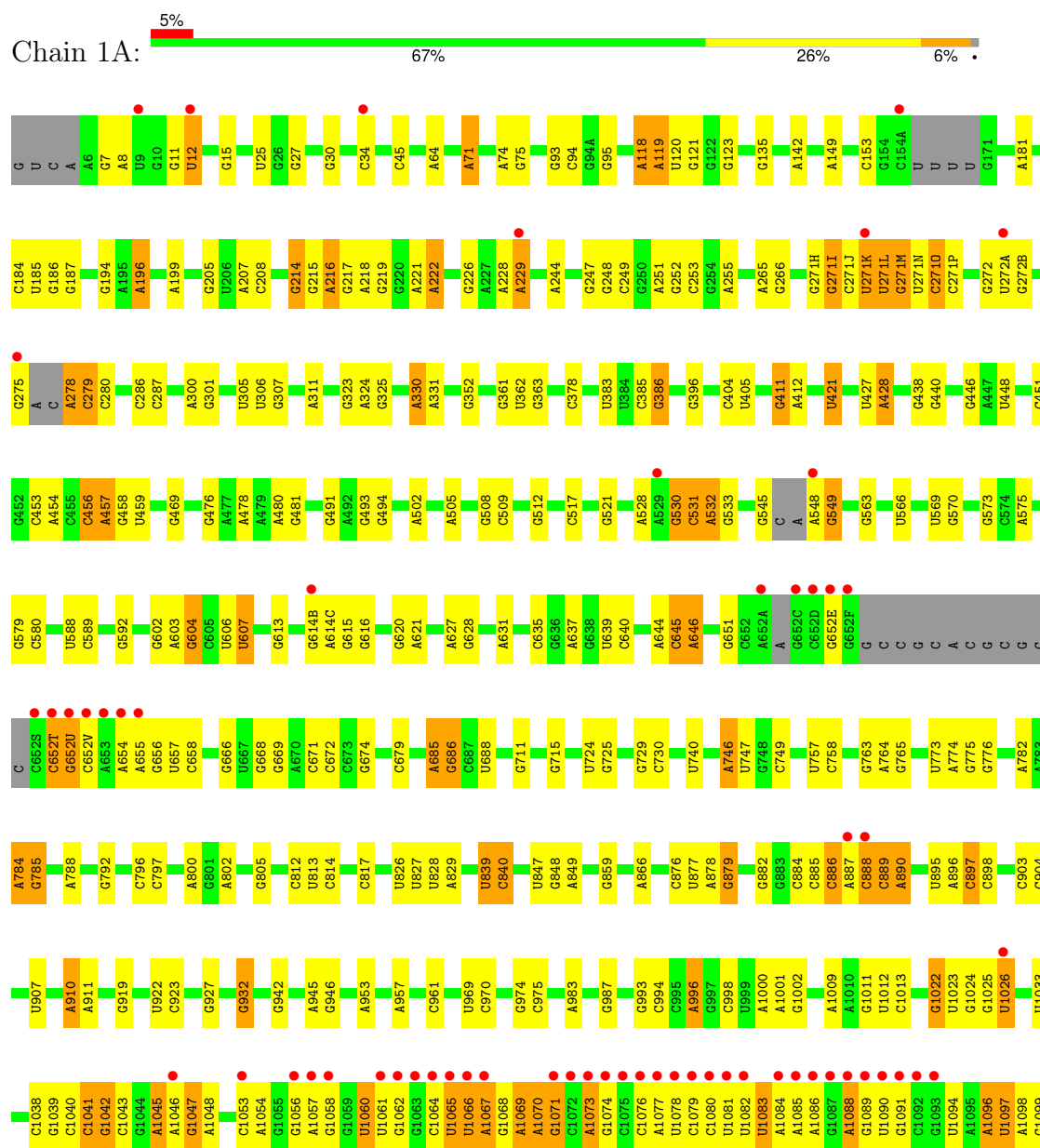
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	27	5	Total 5	O 5	0	0
61	28	8	Total 8	O 8	0	0
61	29	1	Total 1	O 1	0	0
61	2a	394	Total 394	O 394	0	0
61	2d	4	Total 4	O 4	0	0
61	2e	2	Total 2	O 2	0	0
61	2f	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	4	Total 4	O 4	0	0
61	2n	1	Total 1	O 1	0	0
61	2o	3	Total 3	O 3	0	0
61	2p	3	Total 3	O 3	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	5	Total 5	O 5	0	0
61	2t	2	Total 2	O 2	0	0
61	2y	2	Total 2	O 2	0	0

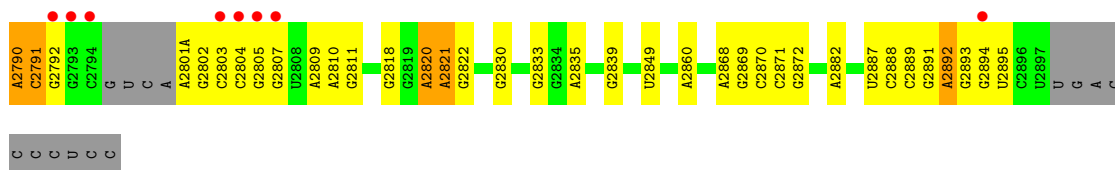
3 Residue-property plots [i](#)

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

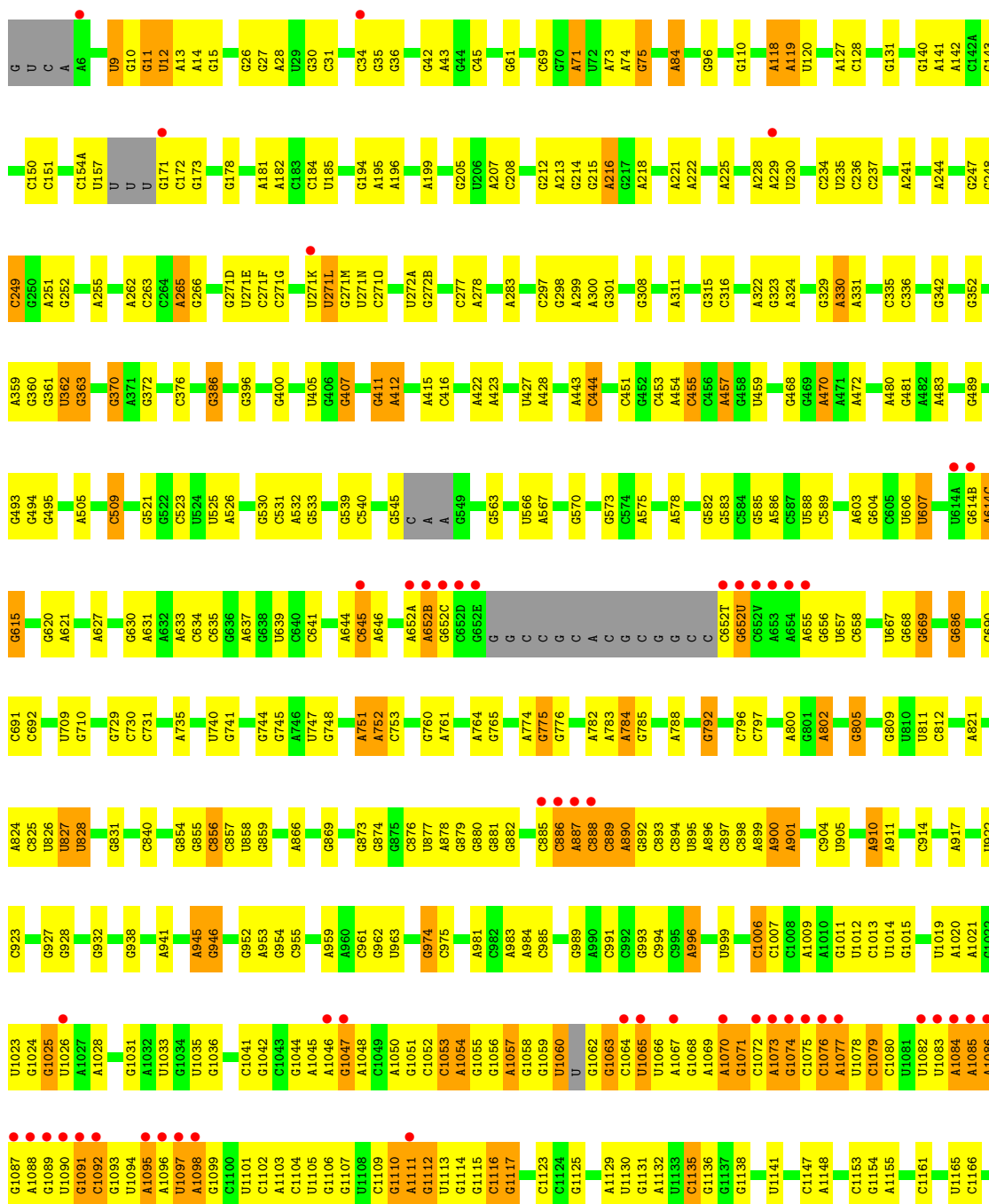
• Molecule 1: 23S Ribosomal RNA



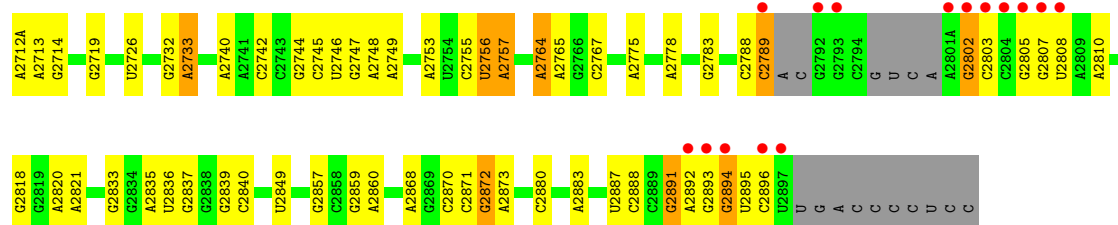




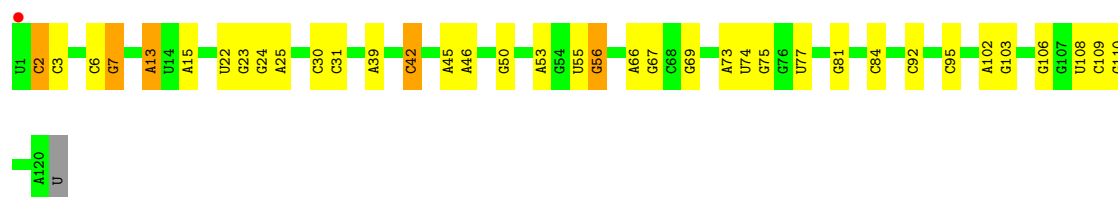
• Molecule 1: 23S Ribosomal RNA



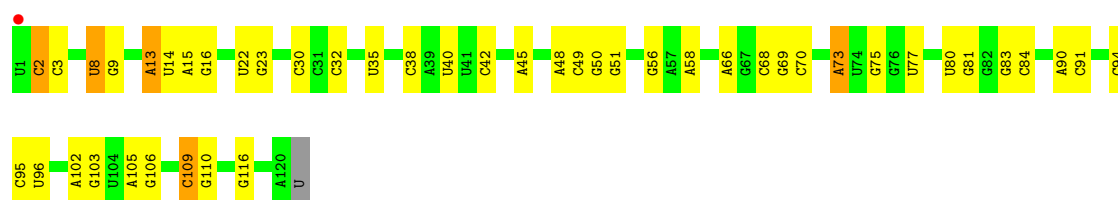




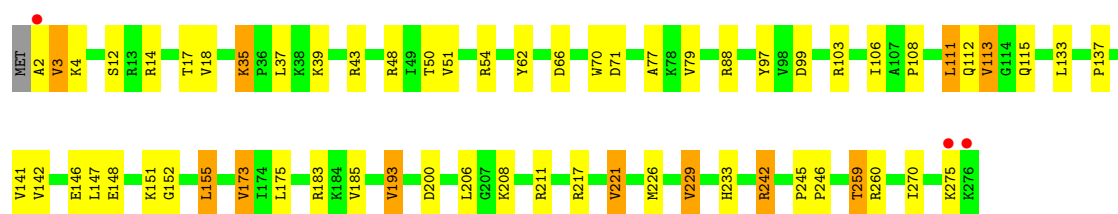
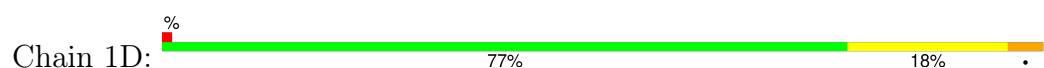
• Molecule 2: 5S Ribosomal RNA



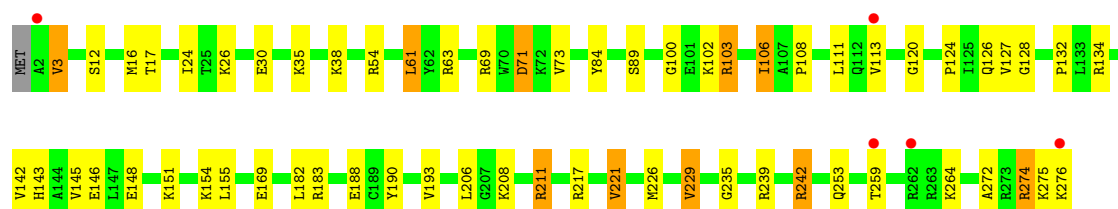
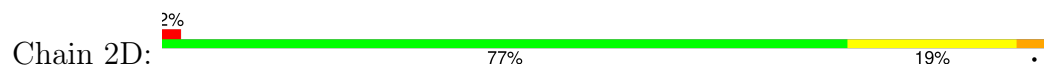
• Molecule 2: 5S Ribosomal RNA



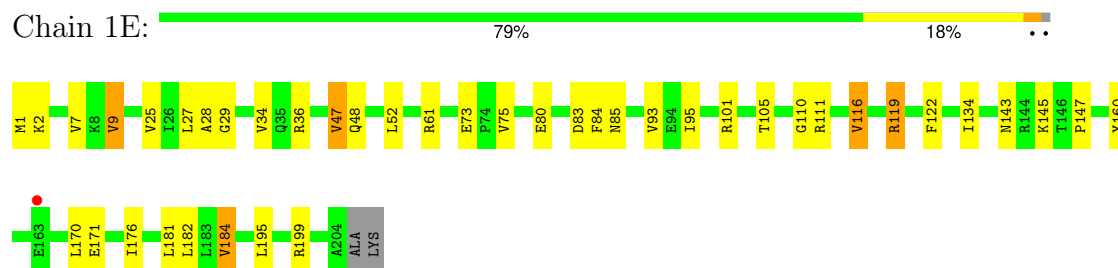
• Molecule 3: 50S ribosomal protein L2



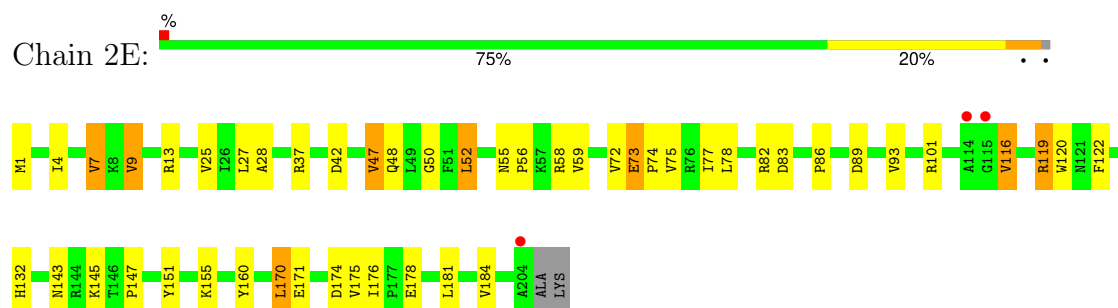
• Molecule 3: 50S ribosomal protein L2



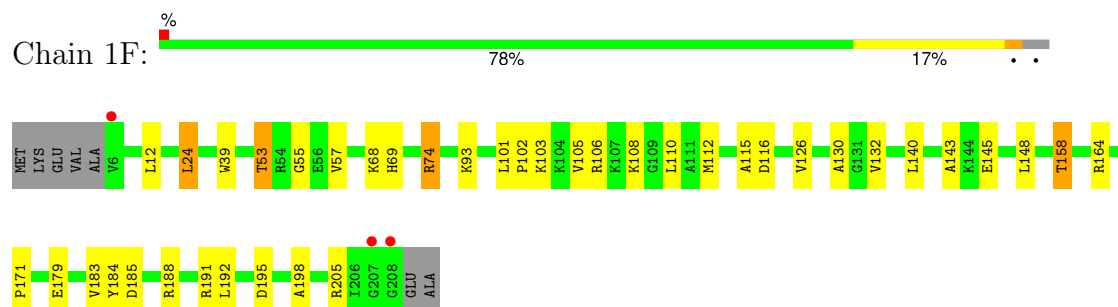
- Molecule 4: 50S ribosomal protein L3



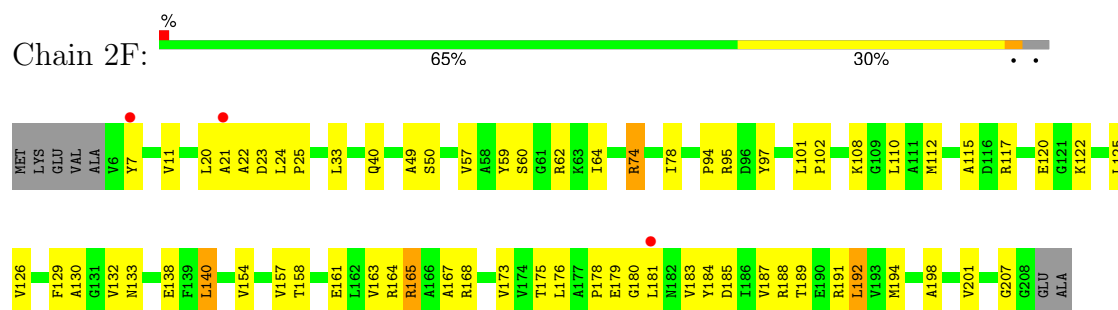
- Molecule 4: 50S ribosomal protein L3



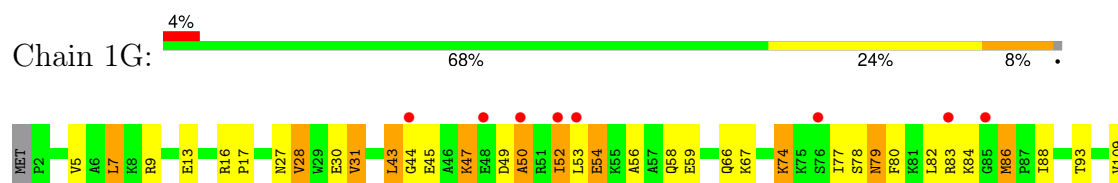
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4



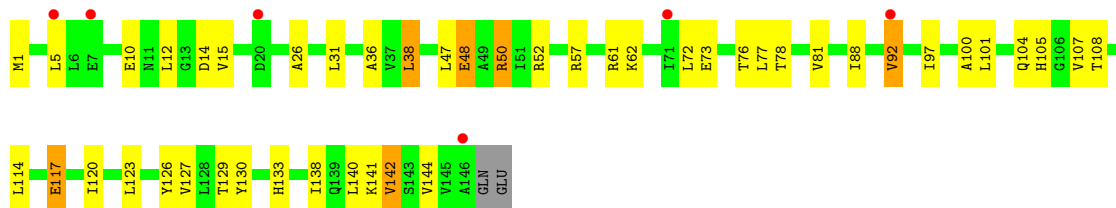
- Molecule 6: 50S ribosomal protein L5



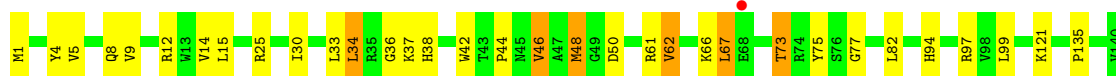
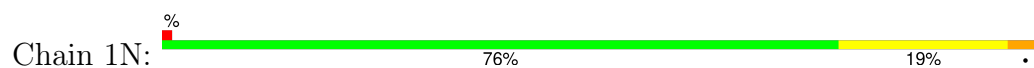




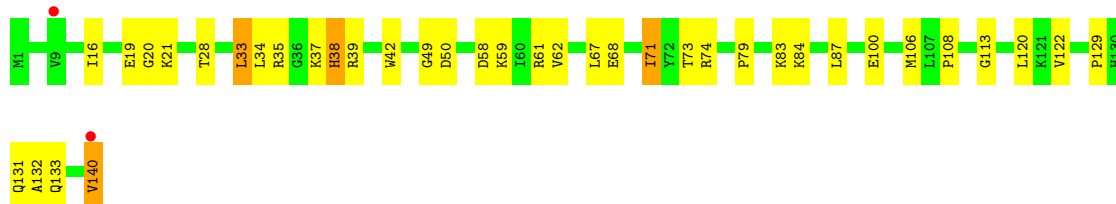
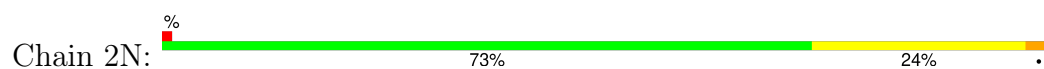
- Molecule 8: 50S ribosomal protein L9



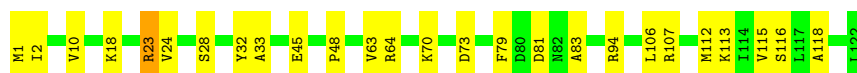
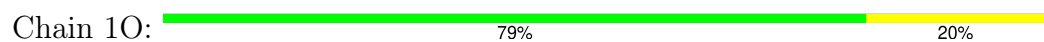
- Molecule 9: 50S ribosomal protein L13



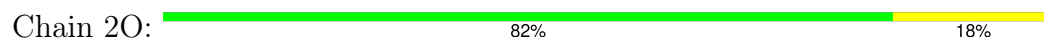
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14

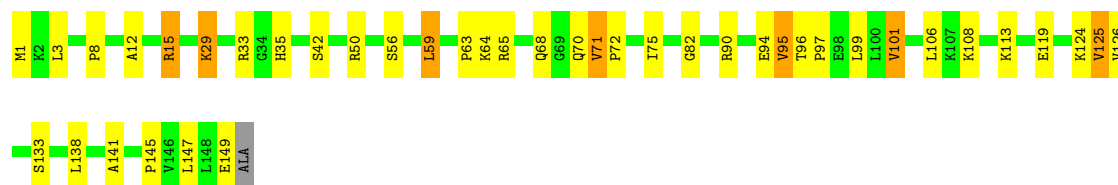


- Molecule 10: 50S ribosomal protein L14

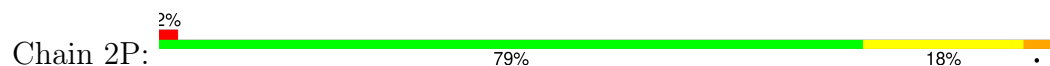


- Molecule 11: 50S ribosomal protein L15

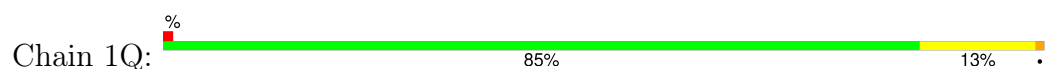




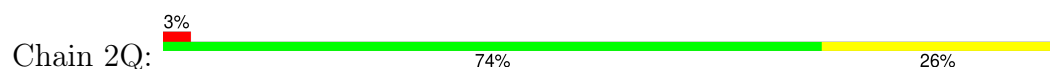
- Molecule 11: 50S ribosomal protein L15



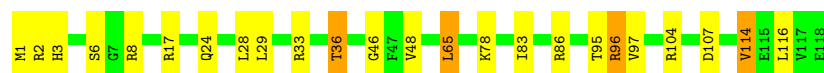
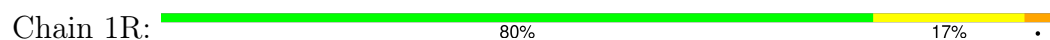
- Molecule 12: 50S ribosomal protein L16



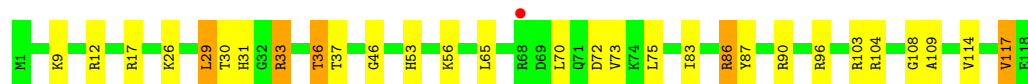
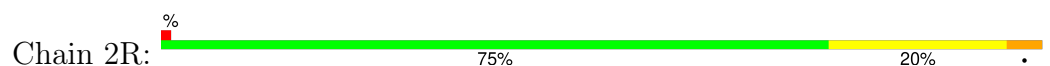
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

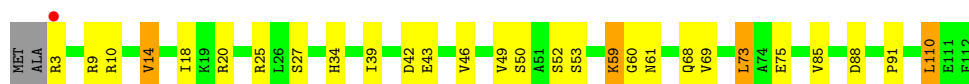


- Molecule 13: 50S ribosomal protein L17

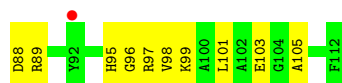
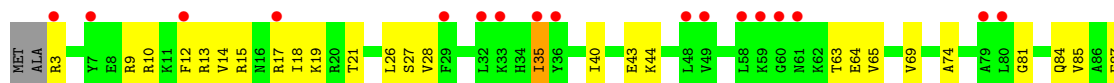


- Molecule 14: 50S ribosomal protein L18

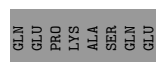
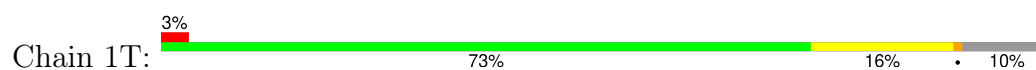




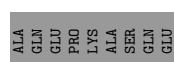
- Molecule 14: 50S ribosomal protein L18



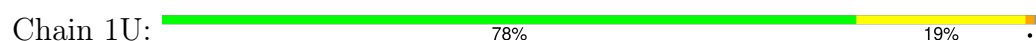
- Molecule 15: 50S ribosomal protein L19



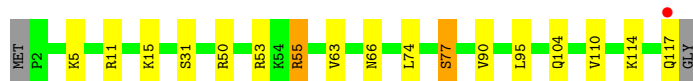
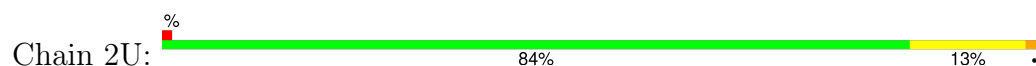
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  74% 24% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  73% 24% ..



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  2% 78% 18% ..



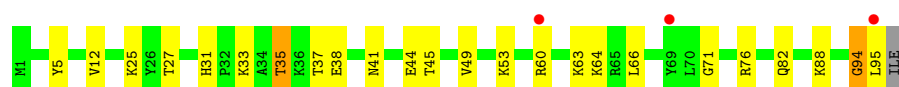
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  % 76% 20% ..



- Molecule 19: 50S ribosomal protein L23

Chain 1X:  3% 74% 23% ..



- Molecule 19: 50S ribosomal protein L23

Chain 2X:  3% 73% 25% ..

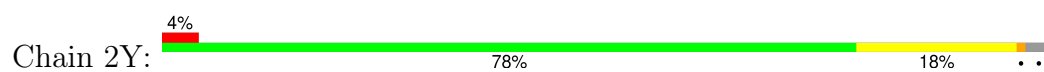


- Molecule 20: 50S ribosomal protein L24

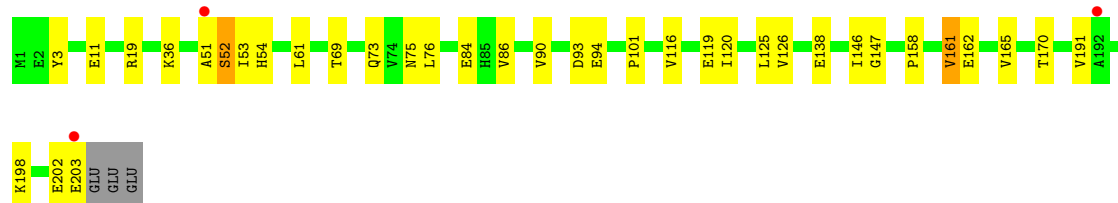
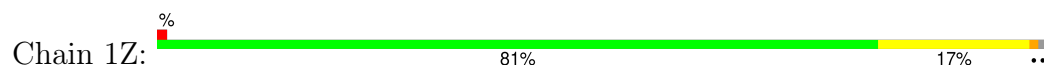
Chain 1Y:  2% 76% 18% ..



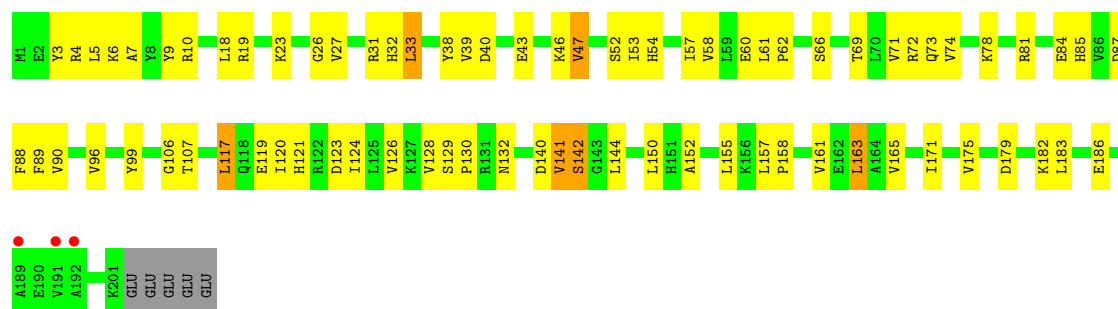
- Molecule 20: 50S ribosomal protein L24



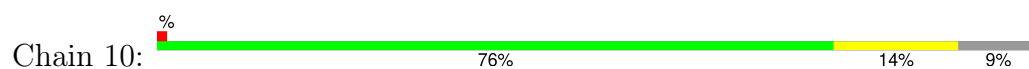
- Molecule 21: 50S ribosomal protein L25



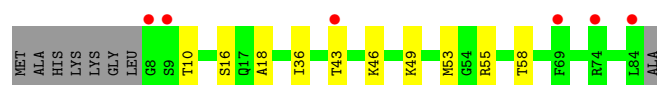
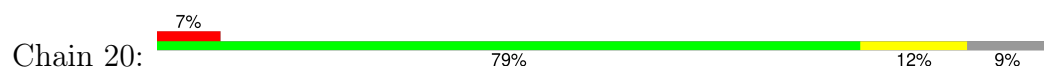
- Molecule 21: 50S ribosomal protein L25



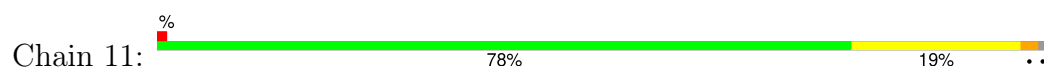
- Molecule 22: 50S ribosomal protein L27

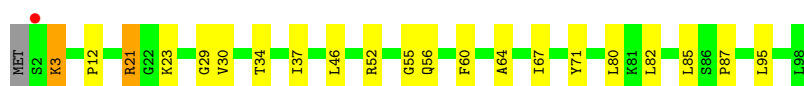


- Molecule 22: 50S ribosomal protein L27

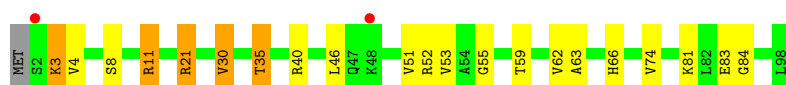
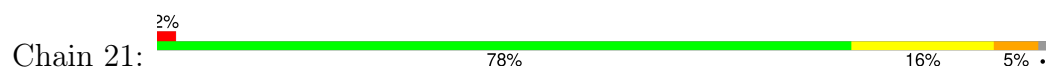


- Molecule 23: 50S ribosomal protein L28

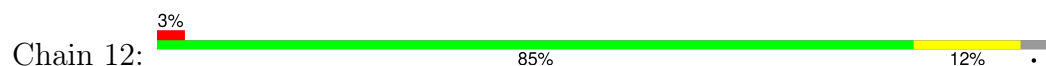




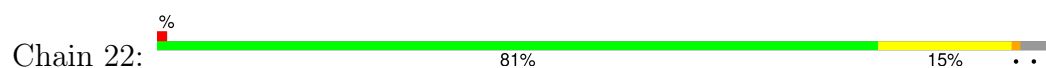
- Molecule 23: 50S ribosomal protein L28



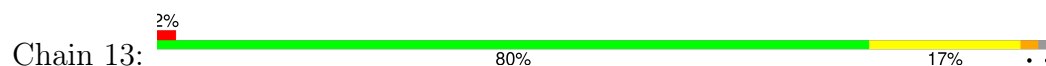
- Molecule 24: 50S ribosomal protein L29



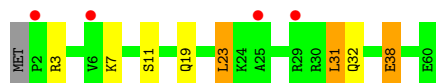
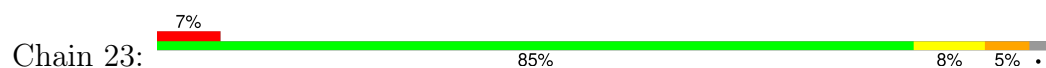
- Molecule 24: 50S ribosomal protein L29



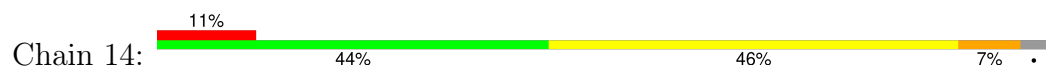
- Molecule 25: 50S ribosomal protein L30



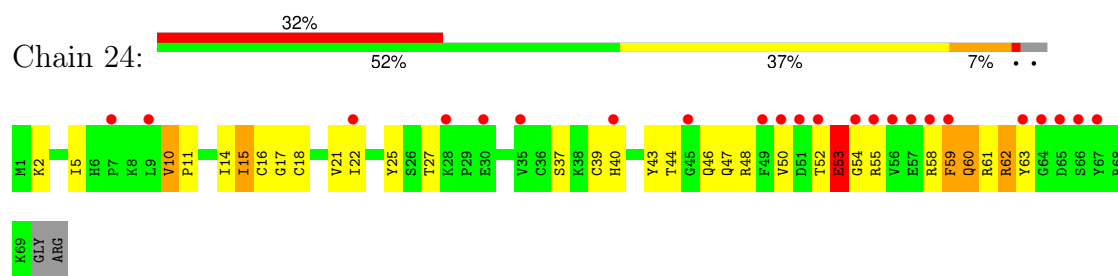
- Molecule 25: 50S ribosomal protein L30



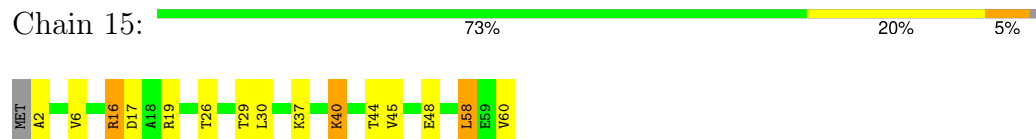
- Molecule 26: 50S ribosomal protein L31



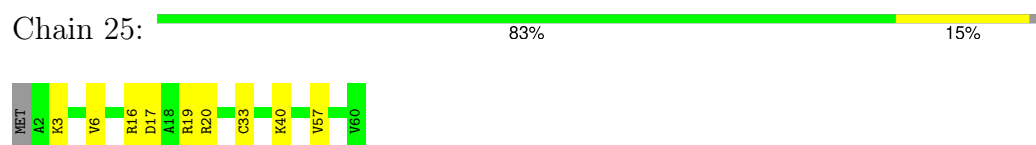
- Molecule 26: 50S ribosomal protein L31



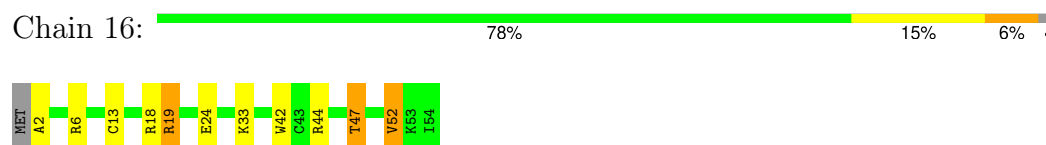
- Molecule 27: 50S ribosomal protein L32



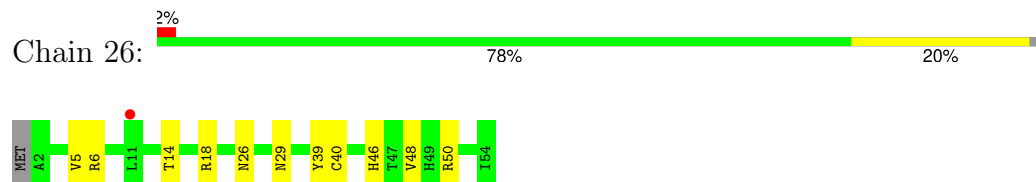
- Molecule 27: 50S ribosomal protein L32



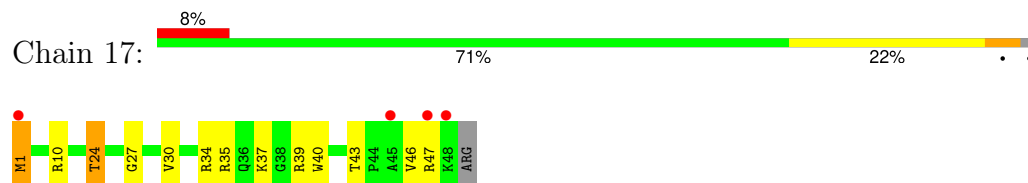
- Molecule 28: 50S ribosomal protein L33



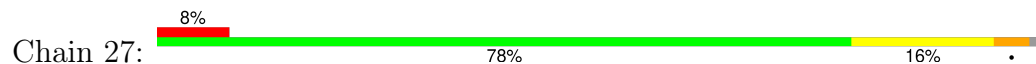
- Molecule 28: 50S ribosomal protein L33

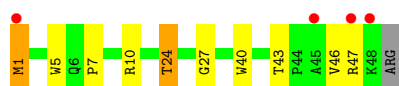


- Molecule 29: 50S ribosomal protein L34



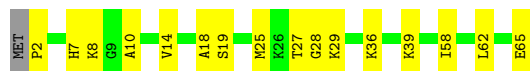
- Molecule 29: 50S ribosomal protein L34





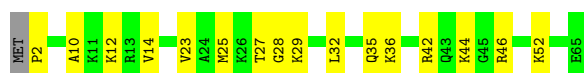
- Molecule 30: 50S ribosomal protein L35

Chain 18: 74% 25% .



- Molecule 30: 50S ribosomal protein L35

Chain 28: 74% 25% .



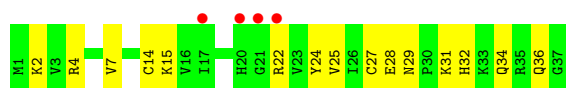
- Molecule 31: 50S ribosomal protein L36

Chain 19: 78% 19% .



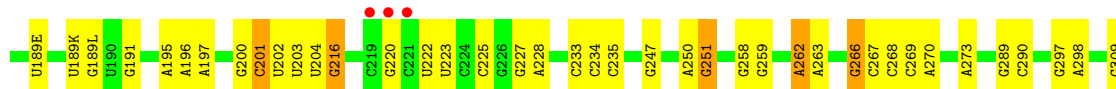
- Molecule 31: 50S ribosomal protein L36

Chain 29: 11% 59% 41% .



- Molecule 32: 16S Ribosomal RNA

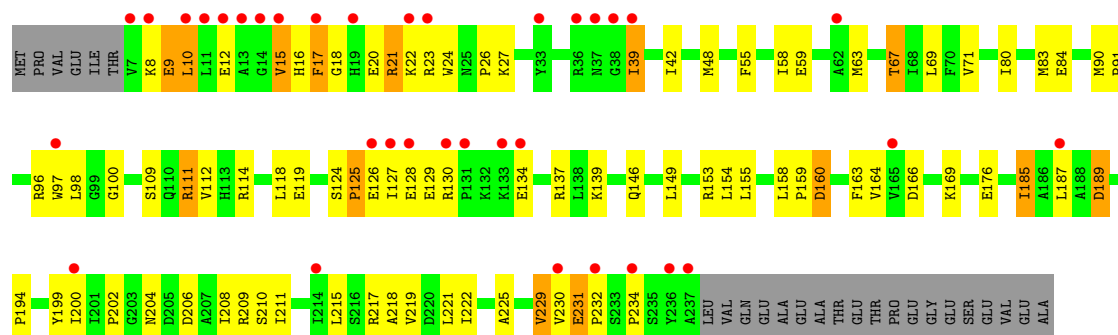
Chain 1a: 3% 59% 33% 7% .



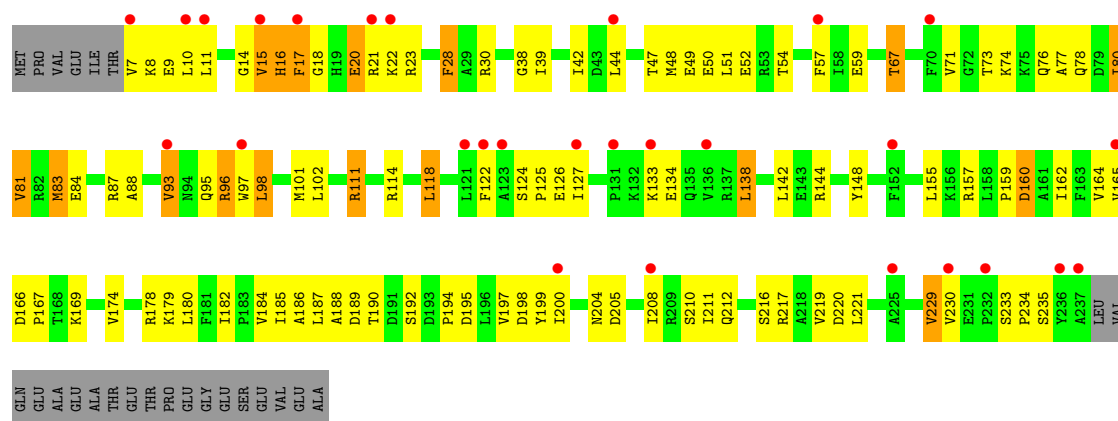
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G1365	G1293	C1128	G1053	G993	A753	U646	U552	A451	C372	U229	G117
G1366	G1294	C1129	C1054	U920	G755	G649	C555	A452	A373	G230	U118
G1367	G1295	A1130	A1055	C995	G756	A653	C556	A453	G376	G231	C121
G1368	A1299	G1133	G1058	C999	U757	A653	G557	C454	G377	G247	G126
G1369	G1300	G1134	C1059	U1000	U758	C656	G558	C458	A382	G251	A130
G1370	U1301	U1135	C1060	A1001	G759	G657	A559	A461	A383	G255	C131
U1372	U1302	U1136	G1061	G1001A	A766	G657	U561	C470	G384	G256	A141
G1373	C1303	U1137	U1062	G1002	G769	G660	C564	C471	G388	G257	A151
A1374	G1304	G1138	C1063	C932	G774	G661	U565	G476	A389	G258	G156
G1375	G1305	G1139	G1064	G933	A777	G662	G566	G482	G391	C267	G157
A1376	A1306	C1140	U1065	C934	G778	A663	G566	G484	G392	A273	A161
U1377	U1307	A1146	C1066	A995	C779	G664	G566	G485	A397	A279	C163
A1378	C1226	C1147	A1067	C936	A780	U677	G577	C501	C398	C280	U164
G1379	A1227	U1150	G1068	A937	G786	U677	G577	C501	G396	A273	C165
U1380	A1238	A1151	C1069	A938	A790	G684	A583	G401	G402	A288	A172
U1381	A1239	A1152	U1070	G939	G791	G685	G584	G403	G403	G289	U173
G1382	U1240	C1153	C1071	G942	A792	U686	G587	U404	U404	U294	C174
G1383	C1244	G1154	C1075	U943	A793	U687	G587	A509	G406	C303	C176
A1384	A1245	G1155	U1077	U944	A794	G688	G587	C511	A510	C304	C177
A1385	C1246	G1156	U1078	U945	G797	G688	C596	C511	A510	C306	U179
C1321	U1247	A1157	G1079	U950	G801	U692	C600	C512	G409	G309	U180
C1322	A1248	C1158	A1080	U951	G802	U692	C601	C513	G410	A313	U182
G1323	U1159	U1159	U1081	U952	G803	U692	G610	A520	G411	A316	C187
A1329	A1251	A1170	G1084	U954	G804	U692	A611	A523	U420	C316	C189D
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G1331	G1255	C1172	U1086	U961	G806	U692	G616	C528	G422	A321	U189F
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G1334	G1258	A1180	A1092	A965	G809	U692	C621	A533	G426	G191	G191
C1259	C1259	G1181	C1028	G966	G810	U692	C622	A533	U427	A327	A195
C1260	C1260	G1182	C1029	C967	G811	U692	C623	A533	U428	A328	A196
C1263	C1263	A1183	C1030	A968	G812	U692	C624	A533	U429	A329	A197
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A1280	A1280	C1195	C1036	A977	G821	U692	C624	A533	U438	G340	G216
U1281	U1281	U1196	C1037	A978	G822	U692	C624	A533	U439	G341	G216
C1282	C1282	U1197	C1038	C979	G823	U692	C624	A533	U440	G342	G216
G1283	G1283	G1202	C1039	C980	G824	U692	C624	A533	U441	G343	G216
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		U1125	C1046	A986	G830	U692	C624	A533	U447	G349	G216
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			U1048	A989	G833	U692	C624	A533	U450	G352	G216
			U1049	A990	G834	U692	C624	A533	U451	G353	G216
			U1050	A991	G835	U692	C624	A533	U452	G354	G216
			U1051	A992	G836	U692	C624	A533	U453	G355	G216
			U1052	A993	G837	U692	C624	A533	U454	G356	G216
			U1053	A994	G838	U692	C624	A533	U455	G357	G216
			U1054	A995	G839	U692	C624	A533	U456	G358	G216
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			U1056	A997	G841	U692	C624	A533	U458	G360	G216
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			U1058	A999	G843	U692	C624	A533	U460	G362	G216
			U1059	A1000	G844	U692	C624	A533	U461	G363	G216
			U1060	A1001	G845	U692	C624	A533	U462	G364	G216
			U1061	A1002	G846	U692	C624	A533	U463	G365	G216
			U1062	A1003	G847	U692	C624	A533	U464	G366	G216
			U1063	A1004	G848	U692	C624	A533	U465	G367	G216
			U1064	A1005	G849	U692	C624	A533	U466	G368	G216
			U1065	A1006	G850	U692	C624	A533	U467	G369	G216
			U1066	A1007	G851	U692	C624	A533	U468	G370	G216
			U1067	A1008	G852	U692	C624	A533	U469	G371	G216
			U1068	A1009	G853	U692	C624	A533	U470	G372	G216
			U1069	A1010	G854	U692	C624	A533	U471	G373	G216
			U1070	A1011	G855	U692	C624	A533	U472	G374	G216
			U1071	A1012	G856	U692	C624	A533	U473	G375	G216
			U1072	A1013	G857	U692	C624	A533	U474	G376	G216
			U1073	A1014	G858	U692	C624	A533	U475	G377	G216
			U1074	A1015	G859	U692	C624	A533	U476	G378	G216
			U1075	A1016	G860	U692	C624	A533	U477	G379	G216
			U1076	A1017	G861	U692	C624	A533	U478	G380	G216
			U1077	A1018	G862	U692	C624	A533	U479	G381	G216
			U1078	A1019	G863	U692	C624	A533	U480	G382	G216
			U1079	A1020	G864	U692	C624	A533	U481	G383	G216
			U1080	A1021	G865	U692	C624	A533	U482	G384	G216
			U1081	A1022	G866	U692	C624	A533	U483	G385	G216
			U1082	A1023	G867	U692	C624	A533	U484	G386	G216
			U1083	A1024	G868	U692	C624	A533	U485	G387	G216
			U1084	A1025	G869	U692	C624	A533	U486	G388	G216
			U1085	A1026	G870	U692	C624	A533	U487	G389	G216
			U1086	A1027	G871	U692	C624	A533	U488	G390	G216
			U1087	A1028	G872	U692	C624	A533	U489	G391	G216
			U1088	A1029	G873	U692	C624	A533	U490	G392	G216
			U1089	A1030	G874	U692	C624	A533	U491	G393	G216
			U1090	A1031	G875	U692	C624	A533	U492	G394	G216
			U1091	A1032	G876	U692	C624	A533	U493	G395	G216
			U1092	A1033	G877	U692	C624	A533	U494	G396	G216
			U1093	A1034	G878	U692	C624	A533	U495	G397	G216
			U1094	A1035	G879	U692	C624	A533	U496	G398	G216
			U1095	A1036	G880	U692	C624	A533	U497	G399	G216
			U1096	A1037	G881	U692	C624	A533	U498	G400	G216
			U1097	A1038	G882	U692	C624	A533	U499	G401	G216
			U1098	A1039	G883	U692	C624	A533	U500	G402	G216
			U1099	A1040	G884	U692	C624	A533	U501	G403	G216
			U1100	A1041	G885	U692	C624	A533	U502	G404	G216
			U1101	A1042	G886	U692	C624	A533	U503	G405	G216
			U1102	A1043	G887	U692	C624	A533	U504	G406	G216
			U1103	A1044	G888	U692	C624	A533	U505	G407	G216
			U1104	A1045	G889	U692	C624	A533	U506	G408	G216
			U1105	A1046	G890	U692	C624	A533	U507	G409	G216
			U1106	A1047	G891	U692	C624	A533	U508	G410	G216
			U1107	A1048	G892	U692	C624	A533	U509	G411	G216
			U1108	A1049	G893	U692	C624	A533	U510	G412	G216
			U1109	A1050	G894	U692	C624	A533	U511	G413	G216
			U1110	A1051	G895	U692	C624	A533	U512	G414	G216
			U1111	A1052	G896	U692	C624	A533	U513	G415	G216
			U1112	A1053	G897	U692	C624	A533	U514	G416	G216
			U1113	A1054	G898	U692	C624	A533	U515	G417	G216
			U1114	A1055	G899	U692	C624	A533	U516	G418	G216
			U1115	A1056	G900	U692	C624	A533	U517	G419	G216
			U1116	A1057	G901	U692	C624	A533	U518	G4	



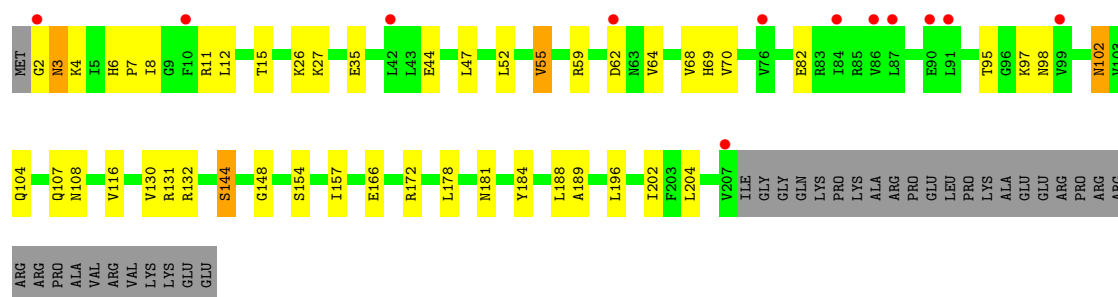
• Molecule 33: 30S ribosomal protein S2



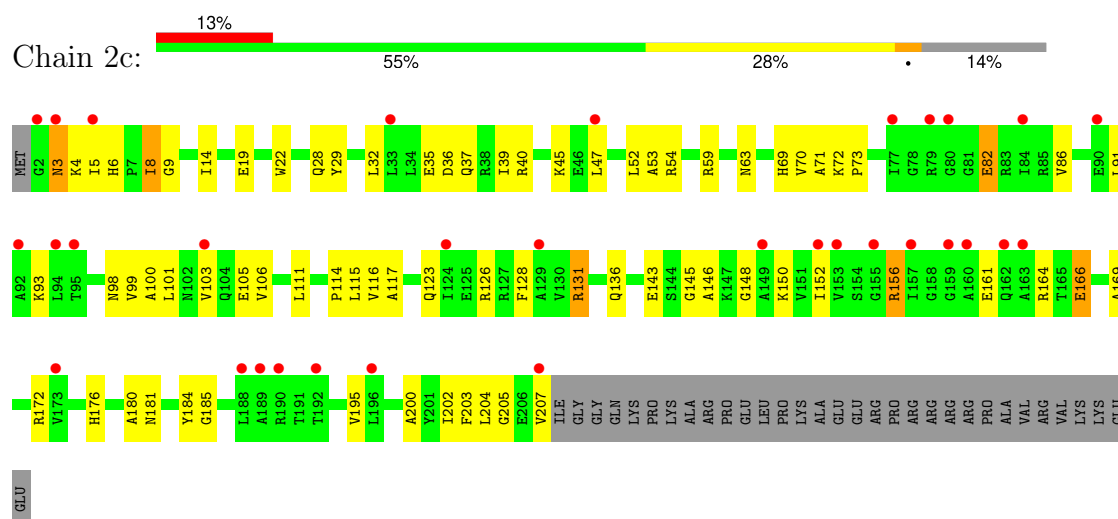
• Molecule 33: 30S ribosomal protein S2



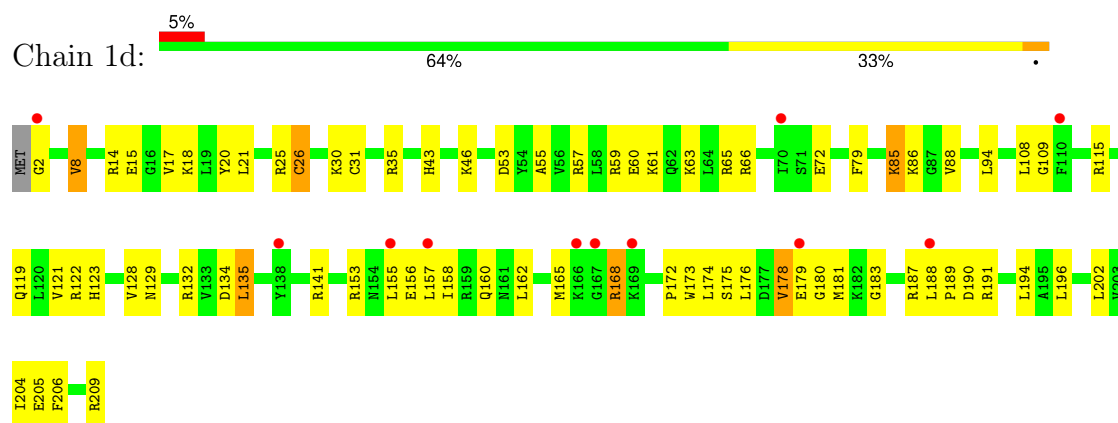
• Molecule 34: 30S ribosomal protein S3



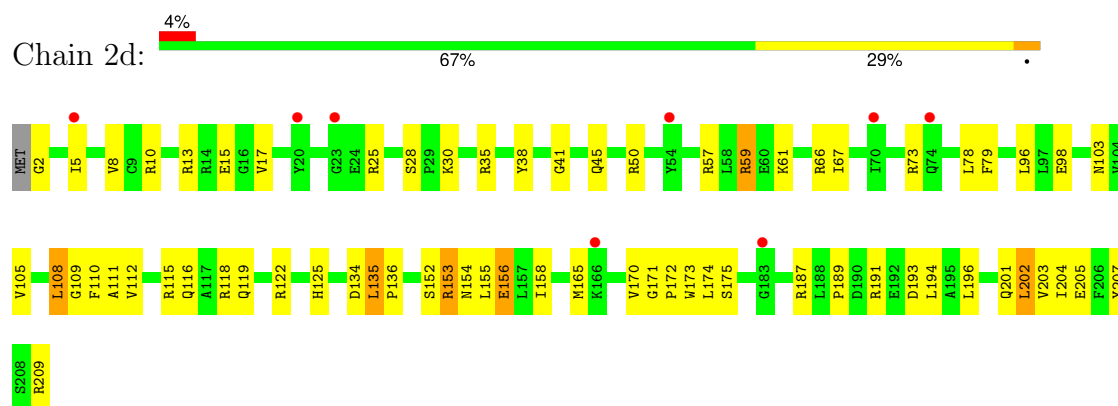
• Molecule 34: 30S ribosomal protein S3



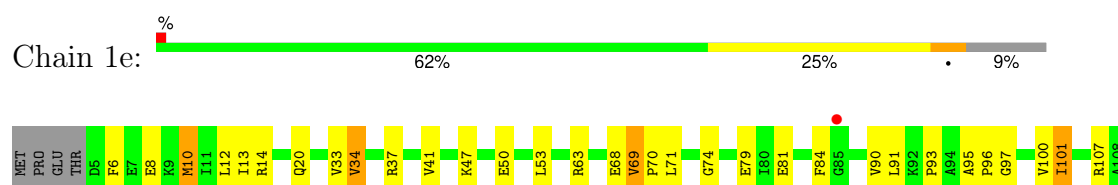
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

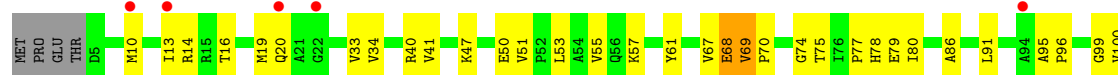


• Molecule 36: 30S ribosomal protein S5

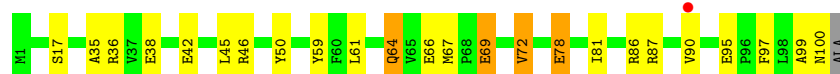
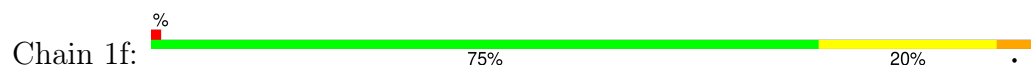




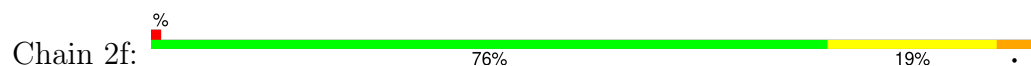
- Molecule 36: 30S ribosomal protein S5



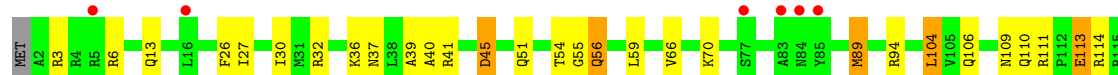
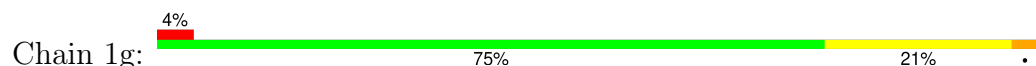
- Molecule 37: 30S ribosomal protein S6



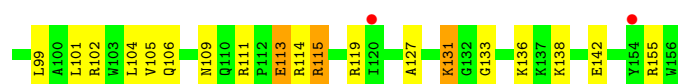
- Molecule 37: 30S ribosomal protein S6



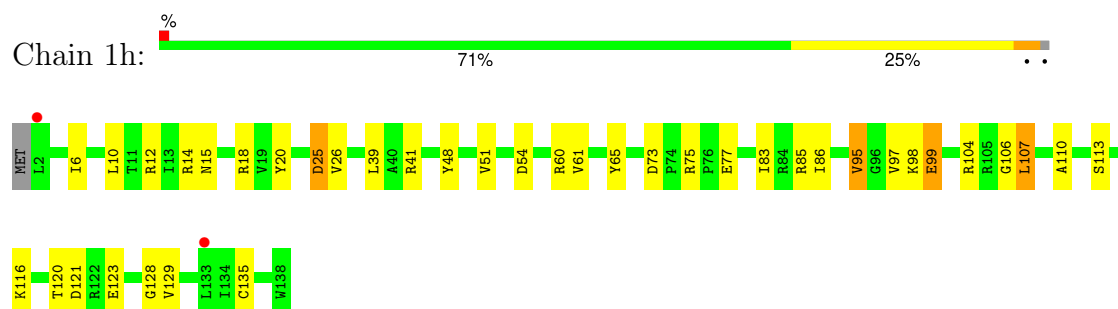
- Molecule 38: 30S ribosomal protein S7



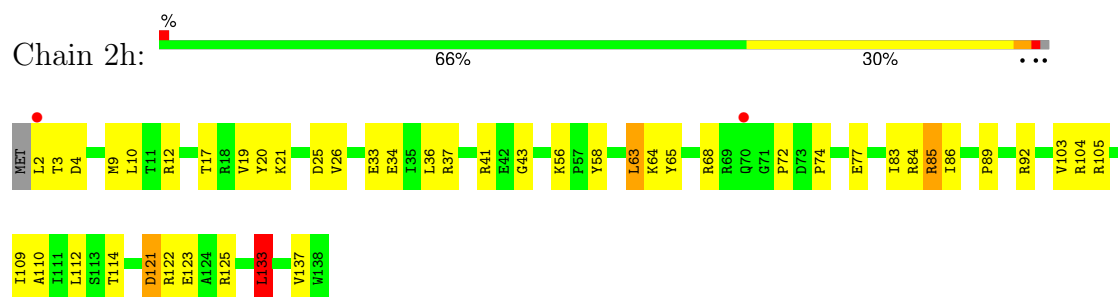
- Molecule 38: 30S ribosomal protein S7



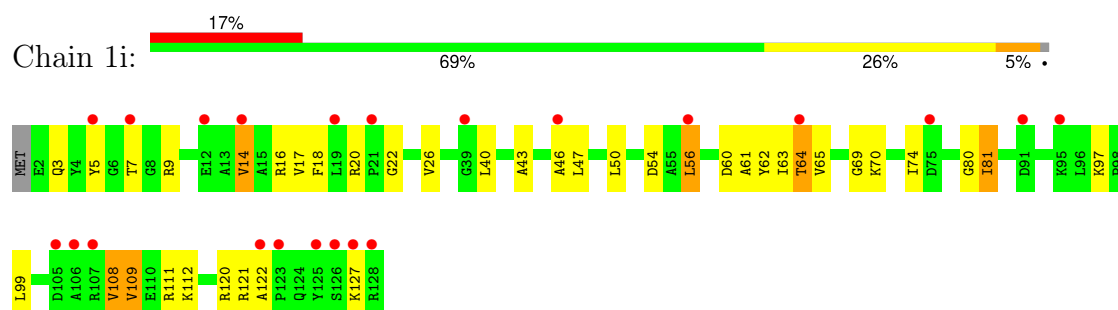
- Molecule 39: 30S ribosomal protein S8



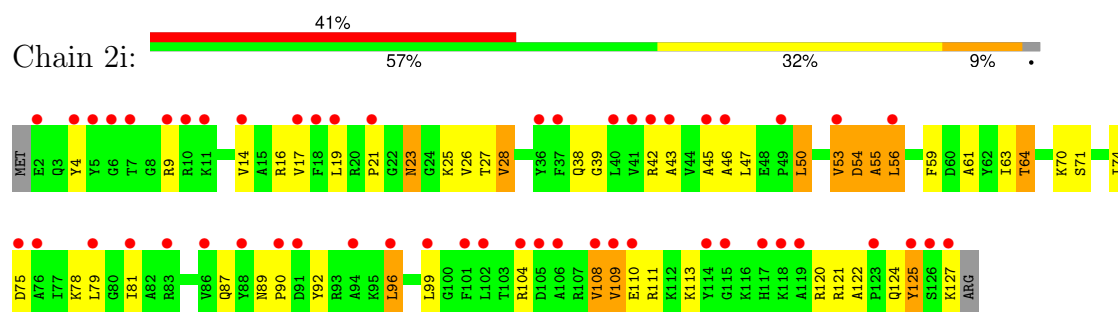
- Molecule 39: 30S ribosomal protein S8



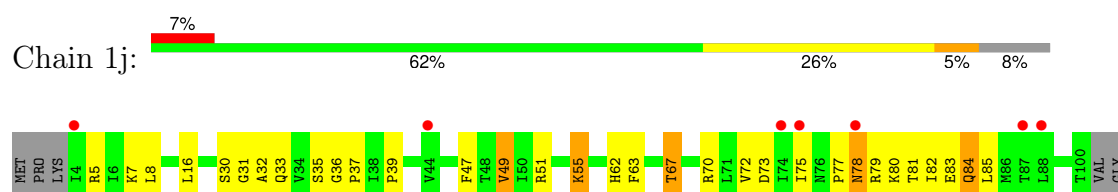
- Molecule 40: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S9

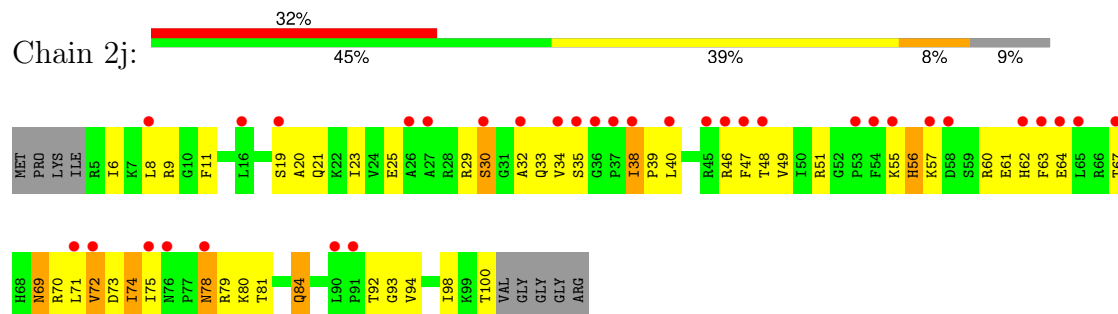


- Molecule 41: 30S ribosomal protein S10

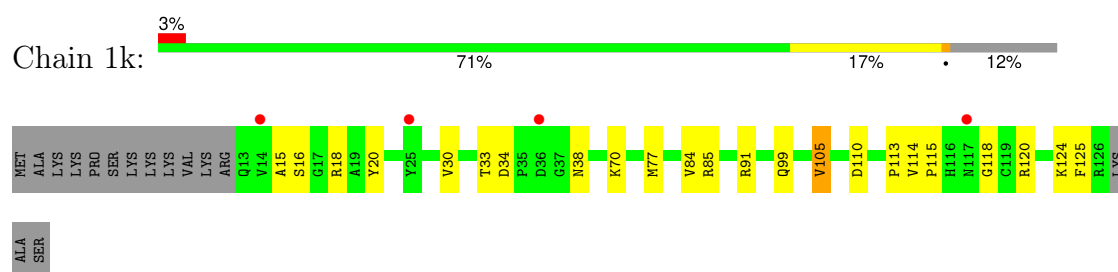


GLY
GLY
ARG

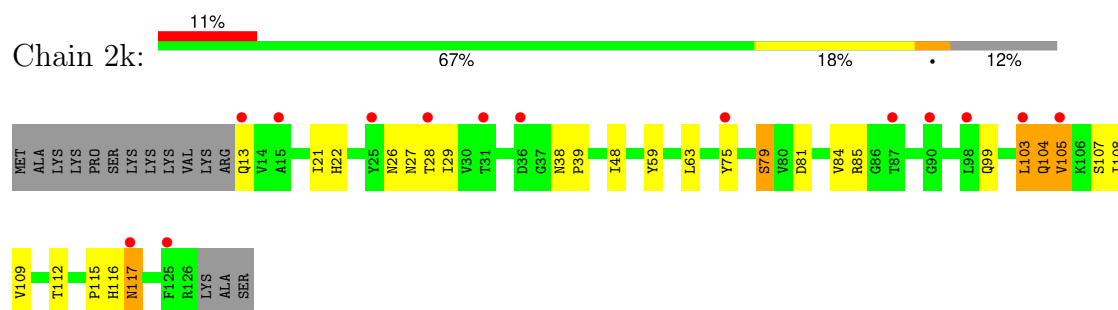
• Molecule 41: 30S ribosomal protein S10



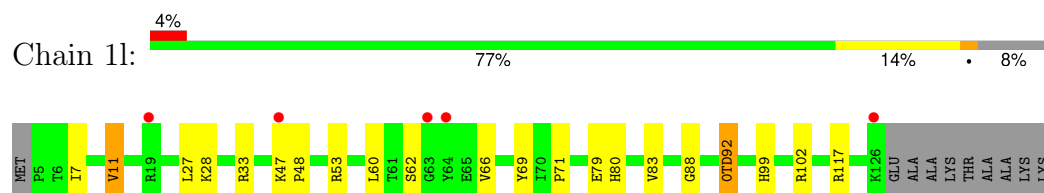
• Molecule 42: 30S ribosomal protein S11



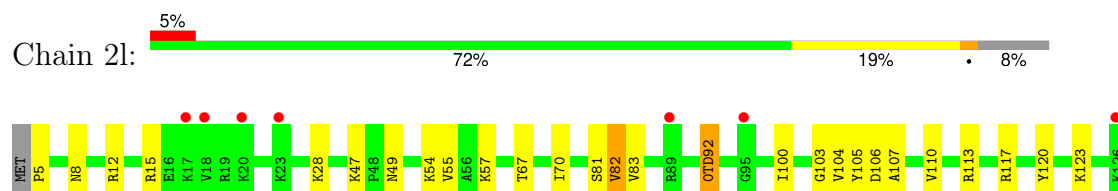
• Molecule 42: 30S ribosomal protein S11



• Molecule 43: 30S ribosomal protein S12



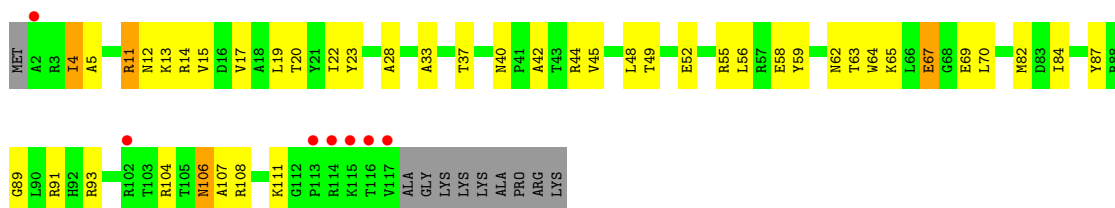
• Molecule 43: 30S ribosomal protein S12



GLU
ALA
ALA
LYS
THR
ALA
ALA
LYS
LYS

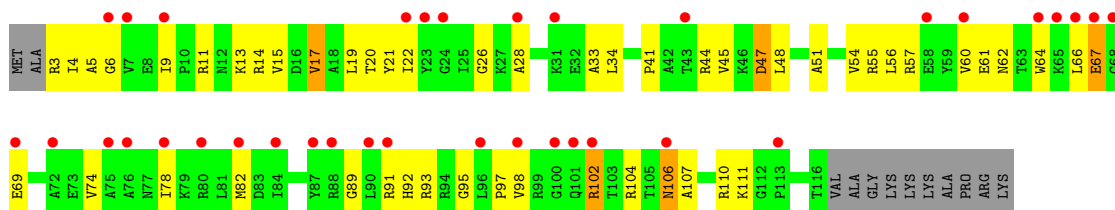
• Molecule 44: 30S ribosomal protein S13

Chain 1m: 



• Molecule 44: 30S ribosomal protein S13

Chain 2m: 

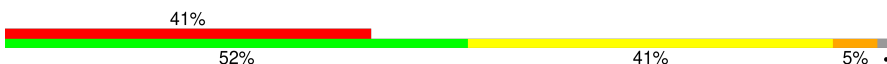


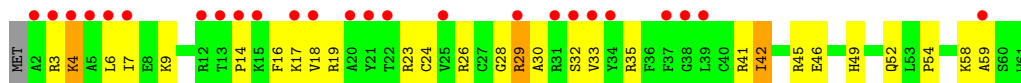
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n: 



• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n: 



• Molecule 46: 30S ribosomal protein S15

Chain 1o: 

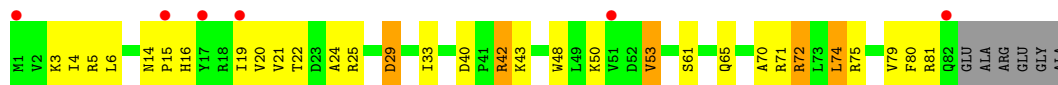


• Molecule 46: 30S ribosomal protein S15

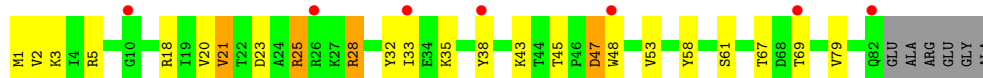
Chain 2o: 



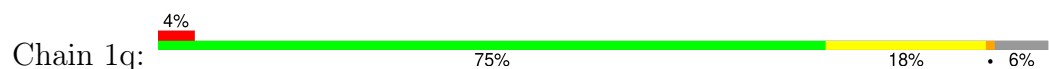
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



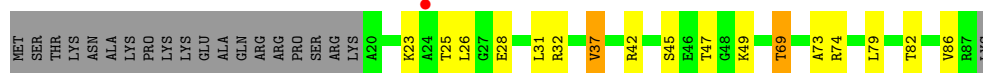
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



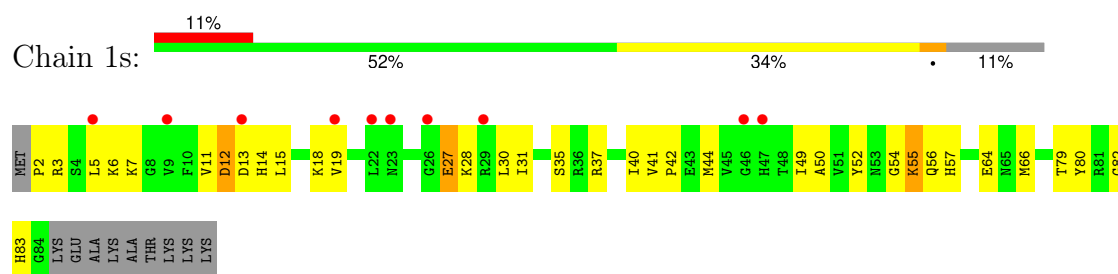
- Molecule 49: 30S ribosomal protein S18



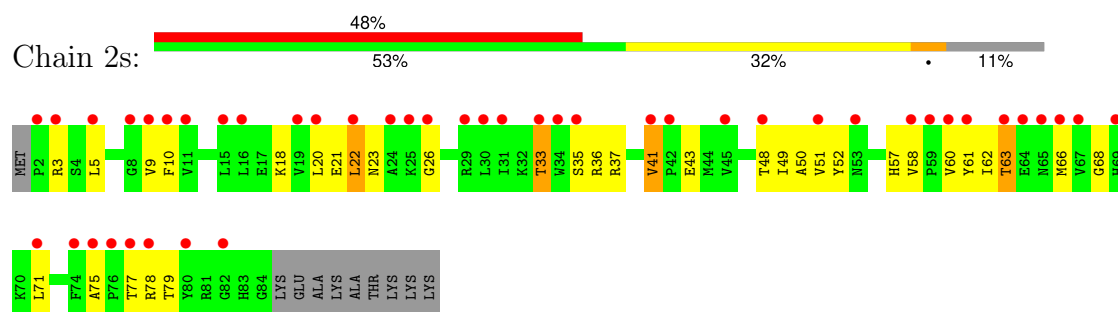
- Molecule 49: 30S ribosomal protein S18



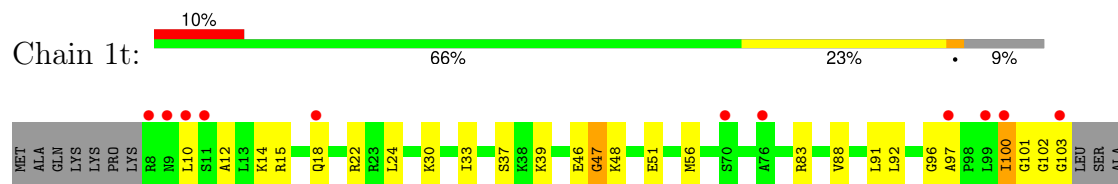
- Molecule 50: 30S ribosomal protein S19



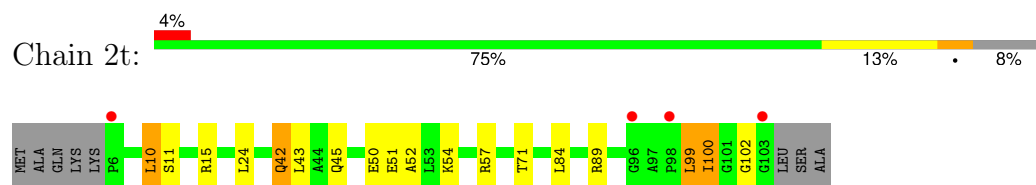
- Molecule 50: 30S ribosomal protein S19



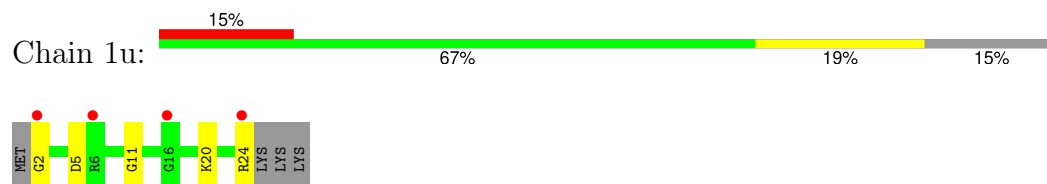
- Molecule 51: 30S ribosomal protein S20



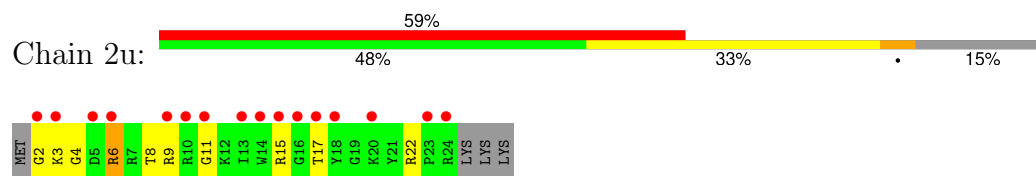
- Molecule 51: 30S ribosomal protein S20



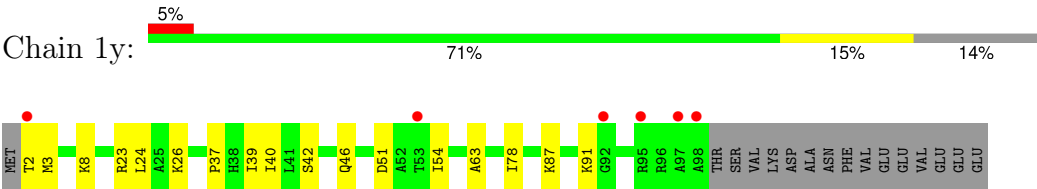
- Molecule 52: 30S ribosomal protein Thx



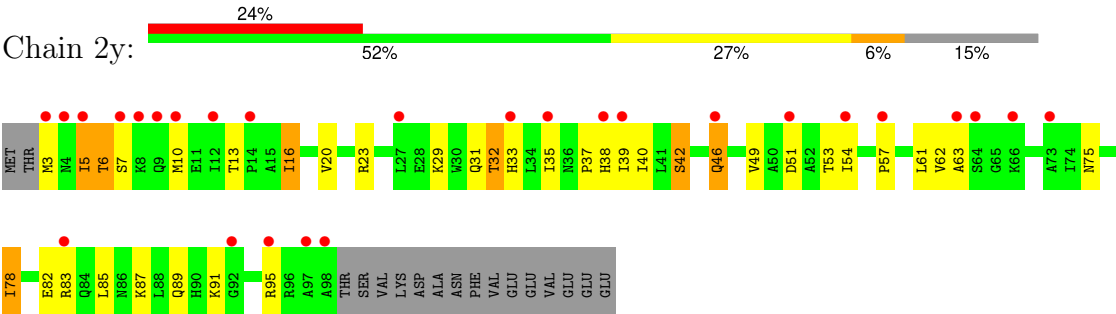
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



• Molecule 53: Ribosome-associated inhibitor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.55Å 449.77Å 619.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.31 – 2.65 153.31 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (153.31-2.65) 99.8 (153.31-2.65)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.194 , 0.236 0.197 , 0.237	Depositor DCC
R_{free} test set	83721 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	296864	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: MPD, UR3, ZIT, ZN, OMG, HGR, MG, G7M, 4OC, SF4, 2MG, OMC, 0TD, 2MA, OMU, PSU, MA6, 5MC, 5MU, M2G

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	0.30	1/69005 (0.0%)	0.48	2/107711 (0.0%)
1	2A	0.24	0/68875	0.43	1/107505 (0.0%)
2	1B	0.23	0/2876	0.42	0/4486
2	2B	0.19	0/2878	0.36	0/4490
3	1D	0.29	0/2181	0.54	2/2940 (0.1%)
3	2D	0.24	0/2186	0.49	0/2944
4	1E	0.28	0/1592	0.51	0/2149
4	2E	0.22	0/1592	0.47	0/2149
5	1F	0.27	0/1619	0.48	0/2193
5	2F	0.22	0/1615	0.47	0/2188
6	1G	0.19	0/1451	0.42	0/1961
6	2G	0.20	0/1449	0.42	0/1957
7	1H	0.23	0/1356	0.40	0/1834
7	2H	0.18	0/1350	0.40	0/1826
8	1I	0.22	0/1109	0.48	0/1512
8	2I	0.21	0/1091	0.38	0/1490
9	1N	0.26	0/1148	0.46	0/1547
9	2N	0.20	0/1144	0.43	0/1543
10	1O	0.27	0/943	0.52	0/1269
10	2O	0.23	0/943	0.48	0/1269
11	1P	0.27	0/1152	0.60	4/1533 (0.3%)
11	2P	0.23	0/1152	0.47	0/1533
12	1Q	0.27	0/1143	0.49	0/1527
12	2Q	0.20	0/1143	0.41	0/1527
13	1R	0.28	0/982	0.51	0/1312
13	2R	0.23	0/982	0.47	0/1312
14	1S	0.24	0/887	0.58	1/1180 (0.1%)
14	2S	0.22	0/880	0.46	0/1172
15	1T	0.27	0/1105	0.48	0/1477
15	2T	0.23	0/1097	0.44	0/1468
16	1U	0.29	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.40	0/1301
17	1V	0.26	0/786	0.47	0/1053
17	2V	0.19	0/782	0.42	0/1049
18	1W	0.29	0/897	0.49	0/1205
18	2W	0.23	0/897	0.42	0/1205
19	1X	0.26	0/764	0.47	0/1025
19	2X	0.20	0/764	0.44	0/1025
20	1Y	0.26	0/823	0.50	0/1099
20	2Y	0.20	0/823	0.46	0/1100
21	1Z	0.22	0/1620	0.43	0/2200
21	2Z	0.20	0/1590	0.42	0/2162
22	10	0.27	0/616	0.51	0/821
22	20	0.21	0/616	0.47	0/821
23	11	0.26	0/761	0.47	0/1013
23	21	0.25	0/766	0.43	0/1018
24	12	0.26	0/590	0.48	0/781
24	22	0.20	0/594	0.38	0/785
25	13	0.27	0/474	0.48	0/635
25	23	0.19	0/469	0.39	0/630
26	14	0.27	0/559	0.65	0/754
26	24	0.29	0/549	0.63	2/741 (0.3%)
27	15	0.29	0/473	0.55	0/639
27	25	0.29	0/469	0.48	0/635
28	16	0.28	0/460	0.46	0/613
28	26	0.22	0/456	0.44	0/608
29	17	0.31	0/426	0.53	0/561
29	27	0.25	0/426	0.48	0/561
30	18	0.28	0/525	0.49	0/691
30	28	0.22	0/525	0.40	0/691
31	19	0.28	0/310	0.51	0/407
31	29	0.22	0/310	0.48	0/407
32	1a	0.21	0/35795	0.40	1/55864 (0.0%)
32	2a	0.20	1/35890 (0.0%)	0.39	2/56012 (0.0%)
33	1b	0.21	0/1876	0.49	1/2533 (0.0%)
33	2b	0.23	0/1860	0.45	0/2518
34	1c	0.19	0/1582	0.39	0/2137
34	2c	0.22	0/1566	0.42	0/2119
35	1d	0.21	0/1695	0.44	0/2274
35	2d	0.20	0/1698	0.44	0/2277
36	1e	0.20	0/1149	0.44	0/1548
36	2e	0.20	0/1149	0.42	0/1548
37	1f	0.21	0/827	0.40	0/1120
37	2f	0.20	0/829	0.44	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1254	0.36	0/1683
38	2g	0.20	0/1248	0.40	0/1676
39	1h	0.19	0/1118	0.42	0/1506
39	2h	0.18	0/1108	0.42	0/1494
40	1i	0.20	0/1005	0.46	0/1351
40	2i	0.21	0/985	0.47	0/1329
41	1j	0.22	0/732	0.39	0/993
41	2j	0.23	0/723	0.47	0/984
42	1k	0.19	0/849	0.42	0/1150
42	2k	0.22	0/848	0.45	0/1149
43	1l	0.20	0/937	0.43	0/1260
43	2l	0.18	0/937	0.41	0/1260
44	1m	0.20	0/924	0.45	0/1242
44	2m	0.24	0/905	0.49	0/1217
45	1n	0.20	0/501	0.45	0/664
45	2n	0.21	0/501	0.41	0/664
46	1o	0.21	0/739	0.39	0/985
46	2o	0.19	0/739	0.39	0/985
47	1p	0.20	0/697	0.51	0/939
47	2p	0.19	0/693	0.45	0/935
48	1q	0.19	0/836	0.40	0/1117
48	2q	0.19	0/836	0.39	0/1117
49	1r	0.18	0/560	0.39	0/746
49	2r	0.20	0/560	0.42	0/746
50	1s	0.18	0/663	0.44	0/895
50	2s	0.20	0/660	0.38	0/893
51	1t	0.21	0/734	0.45	0/969
51	2t	0.20	0/736	0.42	0/976
52	1u	0.18	0/203	0.43	0/266
52	2u	0.18	0/203	0.46	0/266
53	1y	0.19	0/776	0.39	0/1048
53	2y	0.18	0/761	0.36	0/1030
All	All	0.24	2/309887 (0.0%)	0.44	16/463149 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
26	14	0	1
33	1b	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	O3'-P	5.38	1.61	1.56
32	2a	527	G7M	O3'-P	5.21	1.61	1.56

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1S	60	GLY	N-CA-C	9.98	119.29	110.21
1	2A	1992	G	C2'-C3'-O3'	6.63	119.45	109.50
11	1P	33	ARG	CA-C-N	-6.18	110.27	121.32
11	1P	33	ARG	C-N-CA	-6.18	110.27	121.32
32	2a	266	G	C2'-C3'-O3'	6.16	118.74	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	52	THR	Peptide
33	1b	231	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61871	0	31210	574	0
1	2A	61759	0	31157	664	0
2	1B	2572	0	1305	24	0
2	2B	2573	0	1306	29	0
3	1D	2131	0	2207	45	0
3	2D	2136	0	2218	51	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	33	0
5	1F	1584	0	1625	24	0
5	2F	1580	0	1619	43	0
6	1G	1426	0	1445	35	0
6	2G	1424	0	1441	64	0
7	1H	1330	0	1407	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	2H	1324	0	1402	37	0
8	1I	1094	0	1127	19	0
8	2I	1076	0	1094	24	0
9	1N	1121	0	1195	19	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	18	0
10	2O	933	0	996	14	0
11	1P	1135	0	1212	31	0
11	2P	1135	0	1212	24	0
12	1Q	1122	0	1179	12	0
12	2Q	1122	0	1179	23	0
13	1R	968	0	1033	18	0
13	2R	968	0	1033	21	0
14	1S	877	0	938	18	0
14	2S	870	0	923	24	0
15	1T	1091	0	1151	16	0
15	2T	1083	0	1136	19	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	9	0
17	1V	775	0	841	17	0
17	2V	771	0	830	15	0
18	1W	886	0	940	14	0
18	2W	886	0	940	14	0
19	1X	750	0	814	18	0
19	2X	750	0	814	18	0
20	1Y	810	0	892	16	0
20	2Y	810	0	887	16	0
21	1Z	1587	0	1598	17	0
21	2Z	1557	0	1564	49	0
22	10	608	0	622	10	0
22	20	608	0	622	9	0
23	11	754	0	823	12	0
23	21	759	0	837	12	0
24	12	588	0	643	5	0
24	22	592	0	654	6	0
25	13	469	0	518	5	0
25	23	464	0	514	6	0
26	14	546	0	522	25	0
26	24	536	0	514	22	0
27	15	459	0	476	11	0
27	25	455	0	465	6	0
28	16	453	0	473	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	26	449	0	469	5	0
29	17	418	0	467	10	0
29	27	418	0	467	8	0
30	18	517	0	582	11	0
30	28	517	0	582	12	0
31	19	307	0	335	5	0
31	29	307	0	335	11	0
32	1a	32246	0	16293	387	0
32	2a	32331	0	16338	441	0
33	1b	1842	0	1862	55	0
33	2b	1825	0	1828	70	0
34	1c	1558	0	1557	26	0
34	2c	1542	0	1517	51	0
35	1d	1665	0	1687	50	0
35	2d	1668	0	1703	52	0
36	1e	1133	0	1191	27	0
36	2e	1133	0	1191	36	0
37	1f	814	0	808	18	0
37	2f	816	0	808	15	0
38	1g	1235	0	1249	24	0
38	2g	1229	0	1238	26	0
39	1h	1098	0	1143	27	0
39	2h	1088	0	1126	30	0
40	1i	986	0	990	31	0
40	2i	966	0	953	44	0
41	1j	719	0	672	22	0
41	2j	710	0	661	33	0
42	1k	834	0	838	13	0
42	2k	833	0	836	17	0
43	1l	932	0	981	11	0
43	2l	932	0	981	12	0
44	1m	914	0	954	33	0
44	2m	895	0	920	41	0
45	1n	492	0	529	16	0
45	2n	492	0	529	30	0
46	1o	728	0	760	12	0
46	2o	728	0	760	17	0
47	1p	681	0	697	22	0
47	2p	677	0	686	14	0
48	1q	823	0	891	13	0
48	2q	823	0	891	16	0
49	1r	555	0	618	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	2r	555	0	618	10	0
50	1s	648	0	658	25	0
50	2s	645	0	635	24	0
51	1t	732	0	809	18	0
51	2t	733	0	795	12	0
52	1u	199	0	208	3	0
52	2u	199	0	208	6	0
53	1y	764	0	786	16	0
53	2y	749	0	757	25	0
54	10	6	0	0	0	0
54	11	5	0	0	0	0
54	13	3	0	0	0	0
54	15	8	0	0	0	0
54	17	7	0	0	0	0
54	18	2	0	0	0	0
54	19	3	0	0	0	0
54	1A	1031	0	0	0	0
54	1B	29	0	0	0	0
54	1D	18	0	0	0	0
54	1E	10	0	0	0	0
54	1F	18	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	4	0	0	0	0
54	1O	1	0	0	0	0
54	1P	7	0	0	0	0
54	1Q	5	0	0	0	0
54	1R	5	0	0	0	0
54	1S	1	0	0	0	0
54	1T	6	0	0	0	0
54	1U	7	0	0	0	0
54	1V	4	0	0	0	0
54	1W	4	0	0	0	0
54	1X	1	0	0	0	0
54	1Y	1	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	281	0	0	0	0
54	1b	1	0	0	0	0
54	1d	2	0	0	0	0
54	1e	3	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	1	0	0	0	0
54	1n	3	0	0	0	0
54	1o	1	0	0	0	0
54	1t	1	0	0	0	0
54	1u	1	0	0	0	0
54	1y	3	0	0	0	0
54	20	1	0	0	0	0
54	21	1	0	0	0	0
54	23	1	0	0	0	0
54	25	1	0	0	0	0
54	27	1	0	0	0	0
54	28	2	0	0	0	0
54	2A	711	0	0	0	0
54	2B	18	0	0	0	0
54	2D	9	0	0	0	0
54	2E	5	0	0	0	0
54	2F	4	0	0	0	0
54	2G	2	0	0	0	0
54	2I	1	0	0	0	0
54	2N	1	0	0	0	0
54	2O	2	0	0	0	0
54	2P	1	0	0	0	0
54	2Q	3	0	0	0	0
54	2R	1	0	0	0	0
54	2T	3	0	0	0	0
54	2V	3	0	0	0	0
54	2W	3	0	0	0	0
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	182	0	0	0	0
54	2e	2	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2k	1	0	0	0	0
54	2l	1	0	0	0	0
54	2n	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	36	0	29	2	0
55	2A	36	0	29	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1A	52	0	72	6	0
56	2A	52	0	72	2	0
57	18	8	0	14	0	0
57	1A	8	0	14	1	0
57	1T	8	0	14	0	0
57	1a	8	0	12	5	0
57	2A	16	0	28	0	0
57	2B	8	0	14	0	0
58	1B	12	0	12	3	0
58	1F	12	0	12	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	1	0
60	2d	8	0	0	0	0
61	10	19	0	0	1	0
61	11	17	0	0	0	0
61	12	11	0	0	0	0
61	13	20	0	0	1	0
61	15	28	0	0	2	0
61	16	12	0	0	1	0
61	17	12	0	0	1	0
61	18	24	0	0	1	0
61	19	3	0	0	0	0
61	1A	3571	0	0	95	0
61	1B	89	0	0	8	0
61	1D	109	0	0	5	0
61	1E	68	0	0	1	0
61	1F	61	0	0	1	0
61	1G	10	0	0	0	0
61	1H	15	0	0	0	0
61	1I	4	0	0	0	0
61	1N	46	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1O	17	0	0	0	0
61	1P	53	0	0	2	0
61	1Q	30	0	0	2	0
61	1R	29	0	0	2	0
61	1S	7	0	0	0	0
61	1T	32	0	0	0	0
61	1U	38	0	0	2	0
61	1V	26	0	0	2	0
61	1W	28	0	0	1	0
61	1X	23	0	0	2	0
61	1Y	13	0	0	1	0
61	1Z	9	0	0	1	0
61	1a	388	0	0	20	0
61	1d	9	0	0	0	0
61	1f	1	0	0	0	0
61	1h	2	0	0	0	0
61	1j	1	0	0	0	0
61	1l	2	0	0	0	0
61	1m	1	0	0	0	0
61	1n	2	0	0	0	0
61	1o	1	0	0	0	0
61	1p	3	0	0	0	0
61	1u	1	0	0	0	0
61	1y	3	0	0	0	0
61	20	5	0	0	0	0
61	21	14	0	0	1	0
61	23	3	0	0	0	0
61	25	8	0	0	0	0
61	26	3	0	0	0	0
61	27	5	0	0	0	0
61	28	8	0	0	0	0
61	29	1	0	0	0	0
61	2A	2161	0	0	79	0
61	2B	48	0	0	7	0
61	2D	43	0	0	3	0
61	2E	22	0	0	0	0
61	2F	25	0	0	2	0
61	2G	1	0	0	0	0
61	2H	1	0	0	0	0
61	2I	1	0	0	0	0
61	2N	5	0	0	1	0
61	2O	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2P	20	0	0	1	0
61	2Q	19	0	0	0	0
61	2R	15	0	0	0	0
61	2S	4	0	0	1	0
61	2T	11	0	0	0	0
61	2U	15	0	0	0	0
61	2V	3	0	0	0	0
61	2W	16	0	0	0	0
61	2X	6	0	0	0	0
61	2Y	2	0	0	0	0
61	2Z	6	0	0	1	0
61	2a	394	0	0	20	0
61	2d	4	0	0	0	0
61	2e	2	0	0	0	0
61	2f	1	0	0	0	0
61	2j	2	0	0	1	0
61	2l	4	0	0	1	0
61	2n	1	0	0	0	0
61	2o	3	0	0	0	0
61	2p	3	0	0	0	0
61	2q	1	0	0	0	0
61	2r	5	0	0	0	0
61	2t	2	0	0	0	0
61	2y	2	0	0	0	0
All	All	296864	0	194726	3732	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 8.

The worst 5 of 3732 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.47	1.11
1:1A:2137:C:N4	1:1A:2154:G:H1	1.54	1.05
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.19	1.03
1:2A:2139:C:N4	1:2A:2152:G:H1	1.60	0.98
1:2A:2107:C:H42	1:2A:2182:G:H1	1.06	0.97

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%)	260 (95%)	13 (5%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	39
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24	39
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	39
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	39
6	1G	179/182 (98%)	161 (90%)	12 (7%)	6 (3%)	3	4
6	2G	179/182 (98%)	159 (89%)	15 (8%)	5 (3%)	4	6
7	1H	172/180 (96%)	161 (94%)	11 (6%)	0	100	100
7	2H	171/180 (95%)	152 (89%)	16 (9%)	3 (2%)	6	11
8	1I	145/148 (98%)	131 (90%)	14 (10%)	0	100	100
8	2I	144/148 (97%)	132 (92%)	10 (7%)	2 (1%)	9	14
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	134 (97%)	2 (1%)	2 (1%)	9	14
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	27
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	30
11	2P	147/150 (98%)	138 (94%)	6 (4%)	3 (2%)	6	10
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	104 (96%)	2 (2%)	2 (2%)	6	10
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	20
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	20
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%)	2 (2%)	1 (1%)	11	19
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	19
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
21	1Z	201/206 (98%)	185 (92%)	14 (7%)	2 (1%)	12	20
21	2Z	199/206 (97%)	179 (90%)	20 (10%)	0	100	100
22	10	75/85 (88%)	71 (95%)	4 (5%)	0	100	100
22	20	75/85 (88%)	71 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	19
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	19
24	12	68/72 (94%)	67 (98%)	1 (2%)	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%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	0
26	24	67/71 (94%)	41 (61%)	21 (31%)	5 (8%)	1	0
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	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%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	197 (86%)	25 (11%)	7 (3%)	3	5
33	2b	229/256 (90%)	197 (86%)	26 (11%)	6 (3%)	4	6
34	1c	204/239 (85%)	184 (90%)	19 (9%)	1 (0%)	24	39
34	2c	204/239 (85%)	169 (83%)	33 (16%)	2 (1%)	12	20
35	1d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	24	39
35	2d	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	12	20
36	1e	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
36	2e	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	18	30
38	2g	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	6	10
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
39	2h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	18	30
40	1i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
40	2i	124/128 (97%)	106 (86%)	14 (11%)	4 (3%)	3	4
41	1j	95/105 (90%)	83 (87%)	7 (7%)	5 (5%)	1	2
41	2j	94/105 (90%)	77 (82%)	12 (13%)	5 (5%)	1	2
42	1k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	24
42	2k	112/129 (87%)	100 (89%)	12 (11%)	0	100	100
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16	27
44	1m	114/126 (90%)	106 (93%)	5 (4%)	3 (3%)	4	6
44	2m	112/126 (89%)	96 (86%)	14 (12%)	2 (2%)	6	11
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	79 (92%)	4 (5%)	3 (4%)	3	4
46	2o	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	8
47	1p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	81/93 (87%)	70 (86%)	9 (11%)	2 (2%)	4	7
50	2s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	10	17
51	1t	94/106 (89%)	84 (89%)	8 (8%)	2 (2%)	5	9
51	2t	96/106 (91%)	88 (92%)	6 (6%)	2 (2%)	5	9
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	2
53	1y	95/113 (84%)	93 (98%)	2 (2%)	0	100	100
53	2y	94/113 (83%)	93 (99%)	1 (1%)	0	100	100
All	All	11629/12354 (94%)	10830 (93%)	694 (6%)	105 (1%)	14	24

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
21	1Z	53	ILE
26	14	55	ARG
33	1b	17	PHE

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	214/218 (98%)	197 (92%)	17 (8%)	11	19
3	2D	215/218 (99%)	198 (92%)	17 (8%)	11	19
4	1E	164/166 (99%)	156 (95%)	8 (5%)	22	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	155 (94%)	9 (6%)	19	33
5	1F	160/166 (96%)	146 (91%)	14 (9%)	9	15
5	2F	159/166 (96%)	146 (92%)	13 (8%)	10	18
6	1G	144/156 (92%)	127 (88%)	17 (12%)	5	7
6	2G	142/156 (91%)	124 (87%)	18 (13%)	4	6
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	14
7	2H	143/148 (97%)	125 (87%)	18 (13%)	4	6
8	1I	111/124 (90%)	101 (91%)	10 (9%)	9	14
8	2I	108/124 (87%)	95 (88%)	13 (12%)	5	7
9	1N	119/119 (100%)	105 (88%)	14 (12%)	5	7
9	2N	118/119 (99%)	107 (91%)	11 (9%)	8	13
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	47
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36	57
11	1P	115/116 (99%)	102 (89%)	13 (11%)	5	8
11	2P	115/116 (99%)	110 (96%)	5 (4%)	26	44
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	16	29
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9	14
13	1R	101/101 (100%)	93 (92%)	8 (8%)	11	19
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9	15
14	1S	87/88 (99%)	75 (86%)	12 (14%)	3	5
14	2S	85/88 (97%)	76 (89%)	9 (11%)	6	10
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	24
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16	29
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15	27
16	2U	93/94 (99%)	85 (91%)	8 (9%)	10	16
17	1V	81/82 (99%)	77 (95%)	4 (5%)	22	38
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9	15
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	20
18	2W	90/92 (98%)	83 (92%)	7 (8%)	11	20
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	48
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	86/91 (94%)	81 (94%)	5 (6%)	18	31
20	2Y	86/91 (94%)	82 (95%)	4 (5%)	23	40
21	1Z	169/179 (94%)	155 (92%)	14 (8%)	10	18
21	2Z	165/179 (92%)	152 (92%)	13 (8%)	11	19
22	10	61/67 (91%)	58 (95%)	3 (5%)	22	38
22	20	61/67 (91%)	59 (97%)	2 (3%)	33	55
23	11	79/83 (95%)	75 (95%)	4 (5%)	21	36
23	21	81/83 (98%)	73 (90%)	8 (10%)	7	11
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	56
24	22	66/67 (98%)	61 (92%)	5 (8%)	12	21
25	13	51/52 (98%)	48 (94%)	3 (6%)	18	30
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	30
26	14	58/63 (92%)	55 (95%)	3 (5%)	21	36
26	24	54/63 (86%)	47 (87%)	7 (13%)	4	6
27	15	51/52 (98%)	46 (90%)	5 (10%)	7	11
27	25	50/52 (96%)	49 (98%)	1 (2%)	48	69
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	20
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	11
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	11
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	22
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	32
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	32
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	58
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	30
33	1b	191/220 (87%)	173 (91%)	18 (9%)	8	13
33	2b	187/220 (85%)	159 (85%)	28 (15%)	3	4
34	1c	144/188 (77%)	131 (91%)	13 (9%)	9	14
34	2c	140/188 (74%)	124 (89%)	16 (11%)	5	8
35	1d	171/181 (94%)	159 (93%)	12 (7%)	14	24
35	2d	172/181 (95%)	158 (92%)	14 (8%)	11	18
36	1e	114/123 (93%)	104 (91%)	10 (9%)	9	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	12
37	1f	85/90 (94%)	77 (91%)	8 (9%)	8	13
37	2f	85/90 (94%)	75 (88%)	10 (12%)	5	7
38	1g	120/127 (94%)	111 (92%)	9 (8%)	12	21
38	2g	119/127 (94%)	103 (87%)	16 (13%)	4	5
39	1h	116/119 (98%)	108 (93%)	8 (7%)	14	24
39	2h	114/119 (96%)	101 (89%)	13 (11%)	5	8
40	1i	91/99 (92%)	83 (91%)	8 (9%)	9	15
40	2i	88/99 (89%)	74 (84%)	14 (16%)	2	3
41	1j	68/92 (74%)	65 (96%)	3 (4%)	25	43
41	2j	68/92 (74%)	56 (82%)	12 (18%)	2	2
42	1k	83/99 (84%)	81 (98%)	2 (2%)	43	65
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10	17
43	1l	96/108 (89%)	94 (98%)	2 (2%)	47	69
43	2l	96/108 (89%)	87 (91%)	9 (9%)	8	13
44	1m	90/101 (89%)	85 (94%)	5 (6%)	19	32
44	2m	87/101 (86%)	82 (94%)	5 (6%)	18	32
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	7
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	10
46	1o	78/80 (98%)	72 (92%)	6 (8%)	12	20
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	28
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3	4
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2	3
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20	35
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16	28
49	1r	59/77 (77%)	52 (88%)	7 (12%)	5	7
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	53
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7	10
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	5
51	1t	71/82 (87%)	68 (96%)	3 (4%)	26	45
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	32
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	32
53	1y	82/98 (84%)	81 (99%)	1 (1%)	63	79
53	2y	79/98 (81%)	67 (85%)	12 (15%)	3	4
All	All	9524/10260 (93%)	8730 (92%)	794 (8%)	10	18

5 of 794 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	2P	35	HIS
28	26	50	ARG
12	2Q	135	ASP
11	2P	15	ARG
18	2W	23	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
33	2b	146	GLN
44	2m	12	ASN
34	2c	139	GLN
37	2f	100	ASN
48	2q	16	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	399 (13%)	33 (1%)
1	2A	2858/2915 (98%)	464 (16%)	35 (1%)
2	1B	119/121 (98%)	13 (10%)	0
2	2B	119/121 (98%)	15 (12%)	0
32	1a	1497/1521 (98%)	242 (16%)	0
32	2a	1501/1521 (98%)	240 (15%)	0
All	All	8959/9114 (98%)	1373 (15%)	68 (0%)

5 of 1373 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	71	A

5 of 68 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1992	G
1	2A	2171	A
1	2A	2602	A
1	1A	1653	G
1	1A	1608	A

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

50 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	$\# Z > 2$
1	5MC	2A	1942	1	19,22,23	1.62	3 (15%)	26,32,35	1.28	3 (11%)
1	5MC	1A	1942	1,54	19,22,23	1.54	3 (15%)	26,32,35	1.12	3 (11%)
32	5MC	1a	967	32	19,22,23	1.66	3 (15%)	26,32,35	1.07	2 (7%)
43	0TD	1l	92	43	8,9,10	4.50	1 (12%)	6,11,13	5.92	3 (50%)
32	4OC	2a	1402	32	20,23,24	0.76	1 (5%)	25,32,35	0.95	1 (4%)
1	PSU	1A	2605	1	18,21,22	1.35	3 (16%)	21,30,33	2.08	4 (19%)
32	2MG	1a	1207	32	23,26,27	1.26	2 (8%)	33,38,41	2.44	9 (27%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.02	3 (14%)
32	UR3	2a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.76	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.60	3 (15%)	26,32,35	1.14	2 (7%)
1	5MC	1A	1962	1,54	19,22,23	1.51	3 (15%)	26,32,35	1.06	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.36	3 (16%)	21,30,33	2.17	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	0TD	2l	92	43	8,9,10	4.42	1 (12%)	6,11,13	2.32	3 (50%)
1	5MU	1A	1915	1,54	19,22,23	1.46	5 (26%)	27,32,35	2.29	8 (29%)
32	5MC	1a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.16	2 (7%)
1	5MU	2A	1915	1	19,22,23	1.49	4 (21%)	27,32,35	2.27	9 (33%)
32	5MC	2a	967	32	19,22,23	2.01	3 (15%)	26,32,35	1.15	3 (11%)
1	5MU	2A	1939	1,54	19,22,23	1.47	6 (31%)	27,32,35	2.28	6 (22%)
32	G7M	2a	527	32	23,26,27	2.39	5 (21%)	34,39,42	3.05	10 (29%)
32	M2G	2a	966	32,54	24,27,28	1.27	3 (12%)	33,40,43	1.82	5 (15%)
32	4OC	1a	1402	32	20,23,24	0.75	1 (5%)	25,32,35	1.03	1 (4%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.11	9 (27%)
32	G7M	1a	527	32,54	23,26,27	2.33	5 (21%)	34,39,42	3.02	10 (29%)
32	2MG	2a	1207	32	23,26,27	1.25	4 (17%)	33,38,41	2.15	9 (27%)
1	5MC	2A	1962	1,54	19,22,23	1.57	3 (15%)	26,32,35	1.09	2 (7%)
32	5MC	2a	1400	32	19,22,23	1.60	3 (15%)	26,32,35	1.21	3 (11%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.85	6 (18%)
1	OMG	2A	2251	1,54	23,26,27	1.22	3 (13%)	32,38,41	1.95	5 (15%)
1	OMC	1A	1920	1,54	19,22,23	0.79	0	25,31,34	0.94	1 (4%)
32	MA6	1a	1518	32	23,26,27	0.40	0	33,38,41	1.93	8 (24%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.98	1 (4%)
32	UR3	1a	1498	32	19,22,23	0.94	1 (5%)	26,32,35	1.83	3 (11%)
1	2MA	2A	2503	1,54	22,25,26	1.44	4 (18%)	32,37,40	2.41	9 (28%)
1	OMU	2A	2552	1,54	19,22,23	1.30	2 (10%)	25,31,34	1.89	6 (24%)
1	MA6	1A	2058	1,54	23,26,27	0.40	0	33,38,41	2.04	9 (27%)
1	5MU	1A	1939	1	19,22,23	1.41	5 (26%)	27,32,35	2.19	6 (22%)
32	PSU	1a	516	32,54	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)
32	PSU	2a	516	32,54	18,21,22	1.34	2 (11%)	21,30,33	2.08	5 (23%)
32	5MC	2a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.24	4 (15%)
1	PSU	2A	1911	1	18,21,22	1.41	3 (16%)	21,30,33	2.06	5 (23%)
32	MA6	2a	1518	32	23,26,27	0.41	0	33,38,41	2.02	9 (27%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	1.86	4 (19%)
1	OMG	1A	2251	1,54	23,26,27	1.26	3 (13%)	32,38,41	1.99	6 (18%)
1	2MA	1A	2503	1,54	22,25,26	1.50	5 (22%)	32,37,40	2.38	10 (31%)
32	5MC	1a	1407	32	19,22,23	1.71	3 (15%)	26,32,35	1.19	4 (15%)
1	OMU	1A	2552	1,54	19,22,23	1.33	4 (21%)	25,31,34	1.81	6 (24%)
1	MA6	2A	2058	1	23,26,27	0.38	0	33,38,41	1.95	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	1407	32	19,22,23	1.53	2 (10%)	26,32,35	1.09	3 (11%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.13	5 (23%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.17	9 (27%)

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
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,54	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
1	5MU	1A	1915	1,54	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,54	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	0/7/25/26	0/3/3/3
32	M2G	2a	966	32,54	-	0/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
32	MA6	1a	1519	32	-	1/11/29/30	0/3/3/3
32	G7M	1a	527	32,54	-	1/7/25/26	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	5MC	2A	1962	1,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	OMG	2A	2251	1,54	-	0/9/27/28	0/3/3/3
1	OMC	1A	1920	1,54	-	1/9/27/28	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	OMC	2A	1920	1	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,54	-	1/7/25/26	0/3/3/3
1	OMU	2A	2552	1,54	-	0/9/27/28	0/2/2/2
1	MA6	1A	2058	1,54	-	0/11/29/30	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,54	-	0/9/27/28	0/3/3/3
1	2MA	1A	2503	1,54	-	1/7/25/26	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,54	-	0/9/27/28	0/2/2/2
1	MA6	2A	2058	1	-	0/11/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	1/11/29/30	0/3/3/3

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.18	1.70	1.82
43	2l	92	0TD	CB-SB	-12.14	1.70	1.82
32	2a	527	G7M	C8-N7	7.77	1.46	1.33
32	2a	967	5MC	C5-C4	7.62	1.49	1.44
32	1a	527	G7M	C8-N7	7.31	1.45	1.33

The worst 5 of 256 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	13.66	126.92	102.36
1	2A	2503	2MA	C5-C4-N3	-8.38	118.35	127.18
32	2a	527	G7M	CN7-N7-C8	-8.36	112.13	124.79
32	1a	527	G7M	CN7-N7-C8	-8.34	112.16	124.79
1	1A	2503	2MA	C5-C4-N3	-8.31	118.42	127.18

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6

There are no ring outliers.

21 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	1l	92	0TD	1	0
32	2a	1402	4OC	3	0
43	2l	92	0TD	1	0
32	1a	1400	5MC	2	0
32	2a	967	5MC	1	0
1	2A	1939	5MU	1	0
32	1a	1402	4OC	1	0
32	1a	1519	MA6	3	0
32	2a	1207	2MG	3	0
32	2a	1400	5MC	2	0
1	1A	1920	OMC	1	0
32	1a	1518	MA6	2	0
1	2A	1920	OMC	1	0
32	1a	1498	UR3	1	0
1	2A	2503	2MA	1	0
1	1A	2058	MA6	3	0
32	2a	1518	MA6	1	0
1	1A	1917	PSU	1	0
1	1A	2251	OMG	1	0
1	2A	2058	MA6	1	0
32	2a	1519	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2493 ligands modelled in this entry, 2478 are monoatomic - leaving 15 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
56	ZIT	2A	3713	-	54,54,54	0.91	1 (1%)	82,83,83	1.66	16 (19%)
55	HGR	2A	3712	-	39,39,39	2.39	8 (20%)	48,58,58	1.66	13 (27%)
57	MPD	2A	3714	-	7,7,7	0.36	0	9,10,10	0.35	0
57	MPD	2B	219	-	7,7,7	0.33	0	9,10,10	0.24	0
57	MPD	1A	4034	-	7,7,7	0.36	0	9,10,10	0.38	0
58	ARG	1F	319	54	10,11,11	0.71	1 (10%)	9,13,13	0.99	1 (11%)
55	HGR	1A	4032	-	39,39,39	2.42	9 (23%)	48,58,58	1.70	13 (27%)
56	ZIT	1A	4033	-	54,54,54	0.90	1 (1%)	82,83,83	1.45	11 (13%)
58	ARG	1B	230	-	10,11,11	0.76	1 (10%)	9,13,13	1.10	1 (11%)
57	MPD	18	103	-	7,7,7	0.32	0	9,10,10	0.37	0
57	MPD	2A	3715	-	7,7,7	0.32	0	9,10,10	0.25	0
57	MPD	1T	207	-	7,7,7	0.35	0	9,10,10	0.30	0
57	MPD	1a	1882	32	7,7,7	0.41	0	9,10,10	0.61	0
60	SF4	2d	501	35	0,12,12	-	-	-	-	-
60	SF4	1d	303	35	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	ZIT	2A	3713	-	-	15/72/107/107	0/3/3/3
55	HGR	2A	3712	-	-	5/20/79/79	0/4/4/4
57	MPD	2A	3714	-	-	0/5/5/5	-
57	MPD	2B	219	-	-	5/5/5/5	-
57	MPD	1A	4034	-	-	2/5/5/5	-
58	ARG	1F	319	54	-	5/11/11/11	-
55	HGR	1A	4032	-	-	5/20/79/79	0/4/4/4
56	ZIT	1A	4033	-	-	9/72/107/107	0/3/3/3
58	ARG	1B	230	-	-	5/11/11/11	-
57	MPD	18	103	-	-	3/5/5/5	-
57	MPD	2A	3715	-	-	5/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	1T	207	-	-	1/5/5/5	-
57	MPD	1a	1882	32	-	3/5/5/5	-
60	SF4	2d	501	35	-	-	0/6/5/5
60	SF4	1d	303	35	-	-	0/6/5/5

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4032	HGR	C12-C14	9.06	1.55	1.33
55	2A	3712	HGR	C12-C14	8.98	1.54	1.33
55	1A	4032	HGR	C5-C4	-5.56	1.39	1.49
55	2A	3712	HGR	C5-C4	-5.54	1.39	1.49
56	2A	3713	ZIT	O14-C1	5.35	1.46	1.34

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	4033	ZIT	O1A-C5-C6	4.82	112.14	106.40
56	2A	3713	ZIT	O3B-C3B-C2B	-4.47	106.07	112.95
55	2A	3712	HGR	C4-C5-C6	4.31	121.56	112.35
55	1A	4032	HGR	C4-C5-C6	4.30	121.53	112.35
56	1A	4033	ZIT	O3B-C3B-C4B	4.27	110.05	103.86

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	1A	4033	ZIT	C19-C6-C7-C8
56	1A	4033	ZIT	O6-C6-C7-C8
56	1A	4033	ZIT	C12-C11-N10-C21
56	1A	4033	ZIT	C22-C11-N10-C21
56	1A	4033	ZIT	C4B-C3B-O3B-C8B

There are no ring outliers.

9 monomers are involved in 23 short contacts:

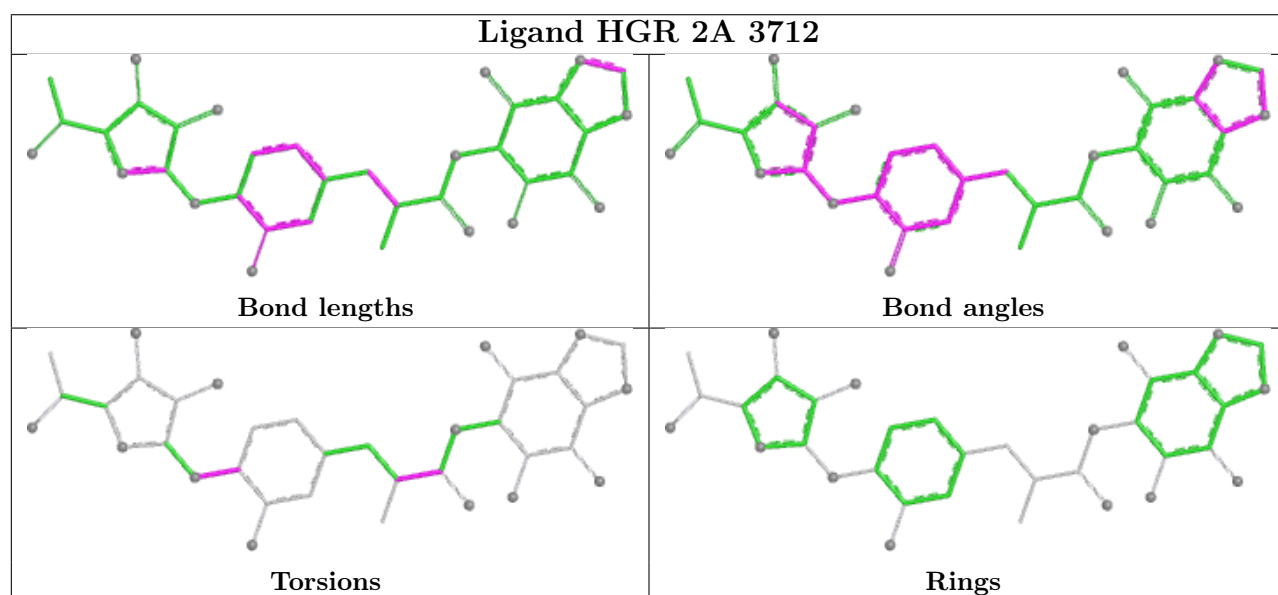
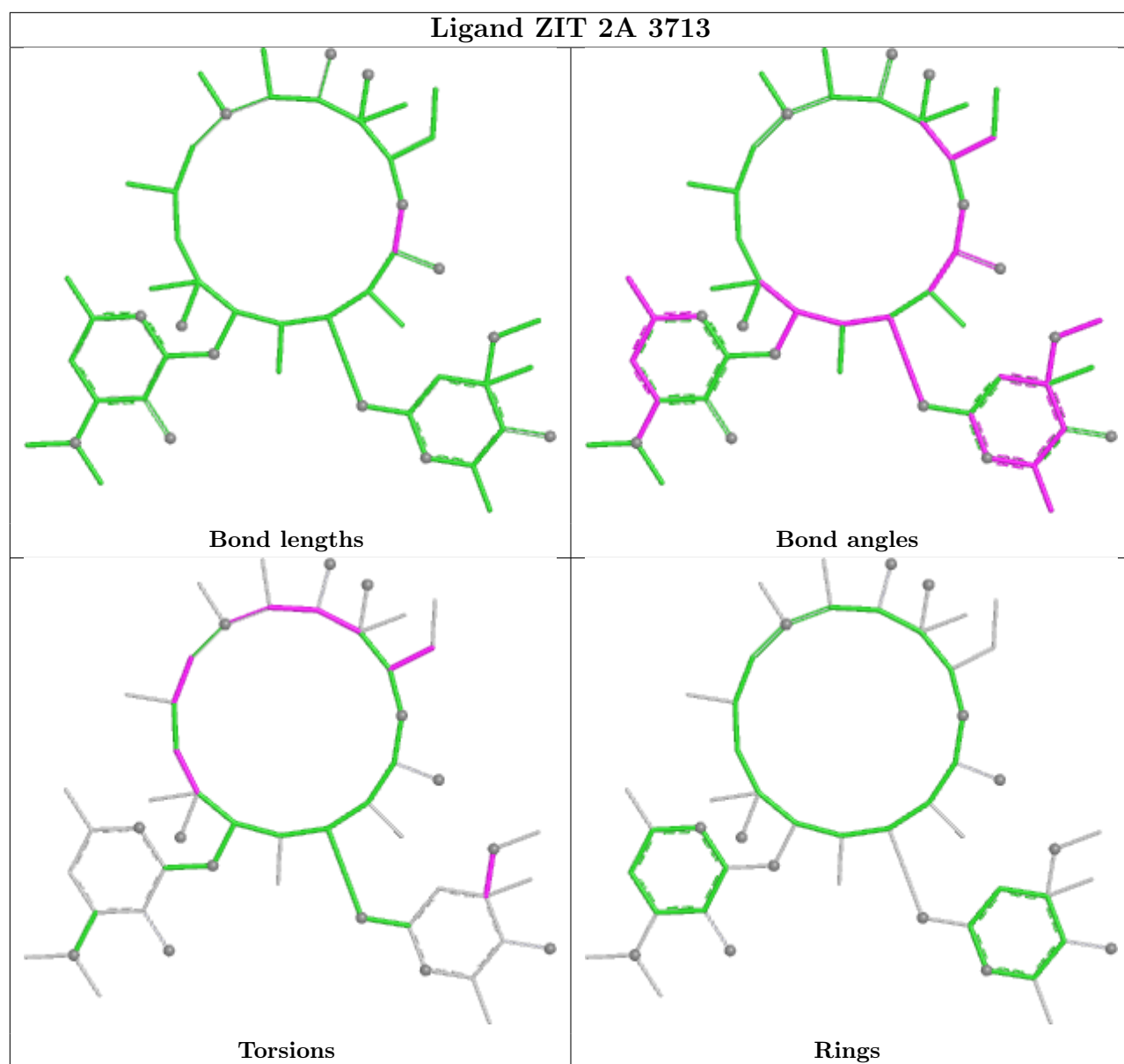
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	2A	3713	ZIT	2	0
55	2A	3712	HGR	2	0
57	1A	4034	MPD	1	0
58	1F	319	ARG	1	0

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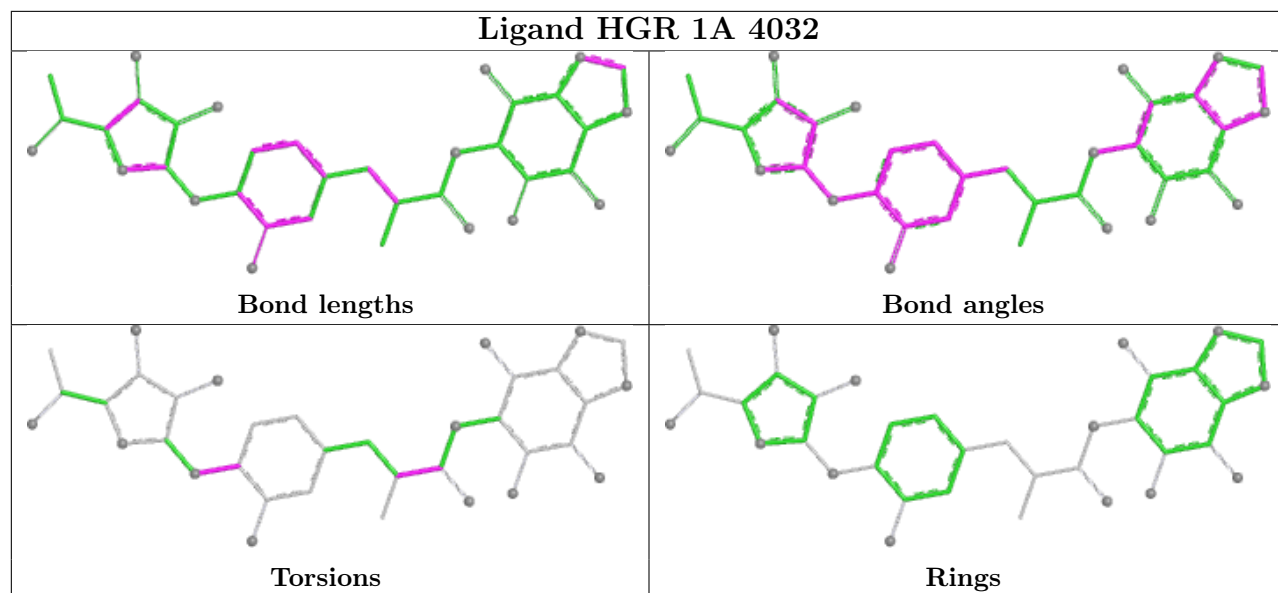
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1A	4032	HGR	2	0
56	1A	4033	ZIT	6	0
58	1B	230	ARG	3	0
57	1a	1882	MPD	5	0
60	1d	303	SF4	1	0

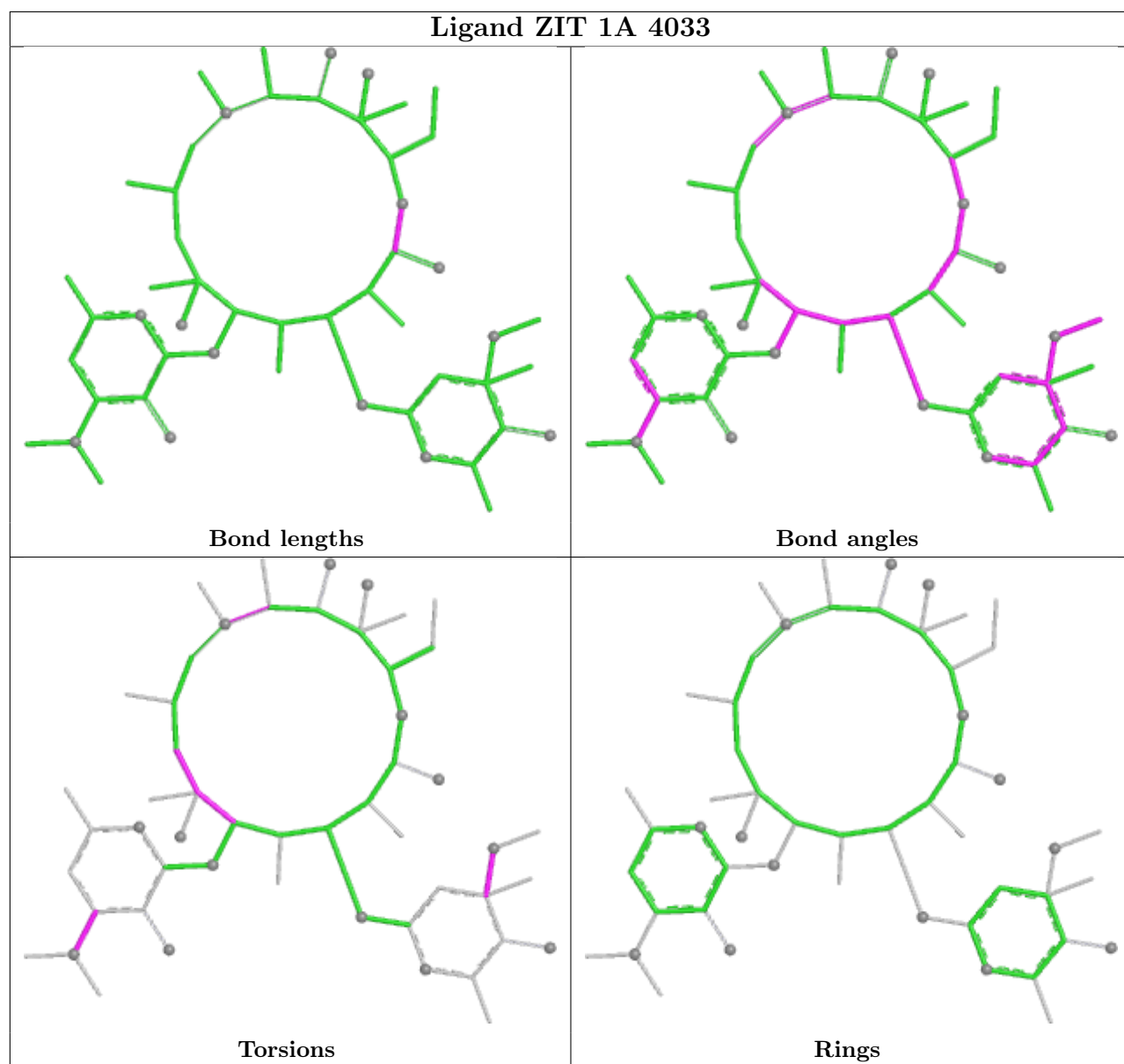
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand HGR 1A 4032



Ligand ZIT 1A 4033



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	1A	2860/2915 (98%)	-0.58	133 (4%)	36	28	24, 40, 101, 113	0
1	2A	2855/2915 (97%)	-0.17	150 (5%)	32	25	34, 57, 103, 114	0
2	1B	120/121 (99%)	-0.41	1 (0%)	82	79	36, 56, 70, 89	0
2	2B	120/121 (99%)	0.35	1 (0%)	82	79	63, 82, 90, 100	0
3	1D	275/276 (99%)	-0.17	3 (1%)	78	75	24, 40, 55, 81	0
3	2D	275/276 (99%)	0.09	5 (1%)	67	63	32, 51, 64, 87	0
4	1E	204/206 (99%)	-0.19	1 (0%)	87	85	23, 43, 66, 79	0
4	2E	204/206 (99%)	0.16	3 (1%)	72	67	34, 57, 74, 86	0
5	1F	203/210 (96%)	-0.05	3 (1%)	72	67	24, 46, 72, 89	0
5	2F	203/210 (96%)	0.38	3 (1%)	72	67	35, 68, 82, 91	0
6	1G	181/182 (99%)	0.48	8 (4%)	39	31	54, 73, 85, 93	0
6	2G	181/182 (99%)	1.64	58 (32%)	1	0	77, 89, 96, 99	0
7	1H	174/180 (96%)	0.17	2 (1%)	78	75	39, 56, 70, 75	0
7	2H	173/180 (96%)	0.92	13 (7%)	20	15	71, 84, 91, 95	0
8	1I	147/148 (99%)	0.63	6 (4%)	41	33	46, 74, 84, 90	0
8	2I	146/148 (98%)	0.74	6 (4%)	41	33	58, 77, 88, 92	0
9	1N	140/140 (100%)	-0.16	1 (0%)	84	82	30, 43, 65, 81	0
9	2N	140/140 (100%)	0.51	2 (1%)	73	69	47, 65, 78, 87	0
10	1O	122/122 (100%)	-0.28	0	100	100	33, 43, 63, 69	0
10	2O	122/122 (100%)	0.23	0	100	100	45, 57, 70, 77	0
11	1P	149/150 (99%)	0.05	0	100	100	25, 50, 70, 88	0
11	2P	149/150 (99%)	0.34	3 (2%)	65	59	40, 68, 84, 91	0
12	1Q	141/141 (100%)	-0.20	1 (0%)	84	82	30, 44, 56, 71	0
12	2Q	141/141 (100%)	0.60	4 (2%)	55	48	48, 67, 79, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.24	0 100 100	30, 40, 57, 65	0
13	2R	118/118 (100%)	0.10	1 (0%) 82 79	39, 53, 66, 71	0
14	1S	110/112 (98%)	0.07	1 (0%) 81 78	45, 57, 71, 75	0
14	2S	110/112 (98%)	1.15	18 (16%) 4 3	66, 77, 84, 87	0
15	1T	131/146 (89%)	0.06	4 (3%) 51 43	36, 48, 71, 86	0
15	2T	131/146 (89%)	0.31	4 (3%) 51 43	50, 60, 78, 86	0
16	1U	116/118 (98%)	-0.38	0 100 100	28, 35, 52, 67	0
16	2U	116/118 (98%)	0.32	1 (0%) 81 78	42, 61, 76, 85	0
17	1V	101/101 (100%)	-0.29	0 100 100	25, 46, 62, 76	0
17	2V	101/101 (100%)	0.44	0 100 100	43, 73, 81, 87	0
18	1W	112/113 (99%)	-0.21	2 (1%) 67 63	28, 36, 56, 86	0
18	2W	112/113 (99%)	-0.01	1 (0%) 81 78	39, 51, 71, 93	0
19	1X	95/96 (98%)	0.01	3 (3%) 50 42	33, 45, 70, 78	0
19	2X	95/96 (98%)	0.41	3 (3%) 50 42	46, 62, 77, 85	0
20	1Y	107/110 (97%)	0.10	2 (1%) 66 61	40, 53, 69, 78	0
20	2Y	107/110 (97%)	0.61	4 (3%) 45 37	59, 71, 82, 87	0
21	1Z	203/206 (98%)	0.37	3 (1%) 72 67	47, 63, 77, 87	0
21	2Z	201/206 (97%)	0.75	3 (1%) 72 67	66, 79, 88, 94	0
22	10	77/85 (90%)	-0.09	1 (1%) 75 71	34, 42, 62, 69	0
22	20	77/85 (90%)	0.64	6 (7%) 19 14	53, 66, 77, 81	0
23	11	97/98 (98%)	0.09	1 (1%) 79 76	31, 50, 74, 84	0
23	21	97/98 (98%)	0.29	2 (2%) 63 57	43, 56, 75, 84	0
24	12	70/72 (97%)	0.11	2 (2%) 53 46	41, 53, 65, 89	0
24	22	70/72 (97%)	0.48	1 (1%) 73 69	61, 72, 79, 80	0
25	13	59/60 (98%)	-0.09	1 (1%) 69 64	32, 41, 68, 76	0
25	23	59/60 (98%)	0.75	4 (6%) 23 17	53, 64, 78, 85	0
26	14	69/71 (97%)	0.77	8 (11%) 9 8	66, 85, 95, 98	0
26	24	69/71 (97%)	1.89	23 (33%) 1 0	86, 95, 100, 103	0
27	15	59/60 (98%)	-0.30	0 100 100	27, 39, 61, 71	0
27	25	59/60 (98%)	-0.15	0 100 100	36, 53, 70, 77	0
28	16	53/54 (98%)	-0.23	0 100 100	37, 47, 61, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.26	1 (1%) 66 61	53, 62, 73, 77	0
29	17	48/49 (97%)	-0.10	4 (8%) 17 12	26, 33, 57, 66	0
29	27	48/49 (97%)	-0.05	4 (8%) 17 12	36, 41, 64, 75	0
30	18	64/65 (98%)	-0.23	0 100 100	33, 40, 46, 60	0
30	28	64/65 (98%)	0.41	0 100 100	48, 57, 64, 71	0
31	19	37/37 (100%)	-0.03	0 100 100	36, 45, 63, 64	0
31	29	37/37 (100%)	1.13	4 (10%) 11 9	59, 70, 78, 80	0
32	1a	1488/1521 (97%)	0.21	49 (3%) 49 40	39, 73, 98, 112	0
32	2a	1492/1521 (98%)	0.41	56 (3%) 44 36	47, 78, 101, 113	0
33	1b	231/256 (90%)	0.94	35 (15%) 5 4	69, 83, 92, 96	0
33	2b	231/256 (90%)	1.22	28 (12%) 8 7	77, 87, 94, 98	0
34	1c	206/239 (86%)	0.81	12 (5%) 29 22	65, 78, 89, 94	0
34	2c	206/239 (86%)	1.28	32 (15%) 5 4	77, 88, 93, 97	0
35	1d	208/209 (99%)	0.75	11 (5%) 32 25	57, 73, 82, 92	0
35	2d	208/209 (99%)	0.77	8 (3%) 44 36	61, 74, 82, 87	0
36	1e	148/162 (91%)	0.37	1 (0%) 84 82	49, 67, 77, 91	0
36	2e	148/162 (91%)	0.77	6 (4%) 41 33	60, 75, 85, 92	0
37	1f	100/101 (99%)	0.43	1 (1%) 79 76	53, 70, 79, 85	0
37	2f	100/101 (99%)	0.44	1 (1%) 79 76	58, 71, 81, 85	0
38	1g	155/156 (99%)	0.66	7 (4%) 38 31	70, 78, 85, 90	0
38	2g	155/156 (99%)	0.92	15 (9%) 13 10	78, 85, 90, 94	0
39	1h	137/138 (99%)	0.59	2 (1%) 72 67	57, 70, 78, 83	0
39	2h	137/138 (99%)	0.65	2 (1%) 72 67	65, 76, 82, 87	0
40	1i	127/128 (99%)	1.38	22 (17%) 4 3	70, 85, 91, 93	0
40	2i	126/128 (98%)	1.91	53 (42%) 0 0	80, 90, 95, 97	0
41	1j	97/105 (92%)	1.11	7 (7%) 21 16	68, 85, 91, 95	0
41	2j	96/105 (91%)	1.81	34 (35%) 1 0	81, 90, 95, 97	0
42	1k	114/129 (88%)	0.40	4 (3%) 47 38	46, 67, 78, 85	0
42	2k	114/129 (88%)	0.97	14 (12%) 8 7	59, 75, 84, 88	0
43	1l	121/132 (91%)	0.44	5 (4%) 41 33	49, 62, 74, 80	0
43	2l	121/132 (91%)	0.58	7 (5%) 29 22	57, 68, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.74	7 (6%) 27 21	66, 80, 86, 90	0
44	2m	114/126 (90%)	1.62	35 (30%) 1 0	82, 90, 95, 98	0
45	1n	60/61 (98%)	1.06	9 (15%) 5 4	71, 76, 85, 89	0
45	2n	60/61 (98%)	1.99	25 (41%) 0 0	82, 89, 94, 99	0
46	1o	88/89 (98%)	0.74	4 (4%) 38 31	49, 70, 81, 86	0
46	2o	88/89 (98%)	0.92	7 (7%) 18 14	60, 74, 82, 89	0
47	1p	82/88 (93%)	1.13	6 (7%) 21 15	63, 74, 83, 88	0
47	2p	82/88 (93%)	1.06	7 (8%) 16 12	63, 72, 82, 88	0
48	1q	99/105 (94%)	0.95	4 (4%) 42 34	55, 71, 81, 84	0
48	2q	99/105 (94%)	0.75	3 (3%) 52 45	59, 73, 81, 87	0
49	1r	68/88 (77%)	0.40	1 (1%) 72 67	61, 68, 83, 87	0
49	2r	68/88 (77%)	0.70	3 (4%) 39 31	65, 73, 83, 86	0
50	1s	83/93 (89%)	1.08	10 (12%) 9 7	74, 82, 89, 92	0
50	2s	83/93 (89%)	1.99	45 (54%) 0 0	84, 92, 96, 100	0
51	1t	96/106 (90%)	0.96	11 (11%) 9 8	65, 75, 87, 92	0
51	2t	98/106 (92%)	0.63	4 (4%) 41 33	59, 73, 84, 86	0
52	1u	23/27 (85%)	1.11	4 (17%) 4 3	77, 79, 83, 84	0
52	2u	23/27 (85%)	2.54	16 (69%) 0 0	84, 88, 91, 93	0
53	1y	97/113 (85%)	0.59	6 (6%) 26 20	59, 69, 79, 82	0
53	2y	96/113 (84%)	1.59	27 (28%) 1 1	70, 83, 90, 92	0
All	All	20764/21468 (96%)	0.25	1165 (5%) 30 24	23, 66, 93, 114	0

The worst 5 of 1165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	653	A	9.5
1	2A	653	A	9.1
1	2A	652(U)	G	9.1
45	2n	2	ALA	8.1
1	2A	652(T)	C	8.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MU	2A	1915	21/22	0.83	0.11	82,90,98,107	0
1	5MU	1A	1915	21/22	0.85	0.12	75,82,90,97	0
32	2MG	2a	1207	24/25	0.86	0.13	88,95,99,101	0
32	M2G	2a	966	25/26	0.89	0.16	72,77,93,104	0
32	5MC	2a	967	21/22	0.89	0.14	75,79,87,92	0
32	2MG	1a	1207	24/25	0.89	0.11	71,78,82,89	0
1	PSU	2A	1917	20/21	0.90	0.08	77,83,93,95	0
43	0TD	2l	92	10/11	0.90	0.12	66,69,72,88	0
1	PSU	1A	1917	20/21	0.91	0.10	68,76,83,84	0
1	PSU	2A	1911	20/21	0.91	0.08	72,77,88,89	0
32	PSU	2a	516	20/21	0.93	0.08	79,82,86,86	0
32	G7M	2a	527	24/25	0.93	0.10	64,74,76,79	0
32	5MC	1a	967	21/22	0.94	0.11	65,73,82,86	0
1	PSU	1A	1911	20/21	0.94	0.07	65,71,77,77	0
43	0TD	1l	92	10/11	0.94	0.09	53,60,63,71	0
32	5MC	1a	1407	21/22	0.95	0.10	47,54,61,64	0
32	PSU	1a	516	20/21	0.95	0.08	64,68,72,78	0
1	OMC	2A	1920	21/22	0.95	0.08	69,73,78,82	0
1	5MC	2A	1942	21/22	0.95	0.09	51,55,60,64	0
32	4OC	2a	1402	22/23	0.95	0.10	63,70,73,79	0
32	5MC	2a	1404	21/22	0.95	0.09	61,65,69,70	0
32	5MC	2a	1407	21/22	0.95	0.09	61,67,72,78	0
32	UR3	2a	1498	21/22	0.95	0.09	56,62,68,71	0
32	MA6	2a	1518	24/25	0.95	0.11	57,70,75,76	0
32	MA6	2a	1519	24/25	0.95	0.13	58,67,72,75	0
32	M2G	1a	966	25/26	0.95	0.10	61,67,71,75	0
32	G7M	1a	527	24/25	0.96	0.09	48,57,62,71	0
1	OMC	1A	1920	21/22	0.96	0.09	49,61,65,67	0
1	5MU	2A	1939	21/22	0.96	0.09	36,41,45,48	0
32	4OC	1a	1402	22/23	0.96	0.09	52,58,61,71	0
32	5MC	2a	1400	21/22	0.96	0.12	71,78,80,84	0
32	5MC	1a	1404	21/22	0.96	0.08	48,51,55,58	0
1	5MC	2A	1962	21/22	0.97	0.07	44,49,54,68	0
1	MA6	2A	2058	24/25	0.97	0.09	33,40,45,49	0
1	2MA	2A	2503	23/24	0.97	0.08	34,38,40,43	0
32	UR3	1a	1498	21/22	0.97	0.07	47,51,55,64	0
32	MA6	1a	1518	24/25	0.97	0.09	46,49,56,56	0
32	MA6	1a	1519	24/25	0.97	0.08	42,52,56,57	0
32	5MC	1a	1400	21/22	0.97	0.08	47,58,62,67	0
1	5MC	1A	1942	21/22	0.97	0.07	36,42,47,48	0
1	2MA	1A	2503	23/24	0.98	0.06	21,28,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OMU	1A	2552	21/22	0.98	0.06	30,34,38,43	0
1	PSU	1A	2605	20/21	0.98	0.07	28,32,35,37	0
1	OMG	2A	2251	24/25	0.98	0.09	39,43,46,49	0
1	5MU	1A	1939	21/22	0.98	0.06	28,33,37,38	0
1	OMU	2A	2552	21/22	0.98	0.08	38,43,49,51	0
1	PSU	2A	2605	20/21	0.98	0.07	35,41,46,46	0
1	5MC	1A	1962	21/22	0.98	0.07	28,36,42,49	0
1	MA6	1A	2058	24/25	0.98	0.06	19,27,36,43	0
1	OMG	1A	2251	24/25	0.98	0.06	23,29,31,33	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
54	MG	2a	3085	1/1	0.21	0.66	97,97,97,97	0
54	MG	2a	3045	1/1	0.22	0.21	91,91,91,91	0
54	MG	2A	3414	1/1	0.39	0.20	82,82,82,82	0
54	MG	1A	3656	1/1	0.46	0.29	85,85,85,85	0
54	MG	2G	201	1/1	0.46	0.25	90,90,90,90	0
54	MG	1A	3854	1/1	0.51	0.27	76,76,76,76	0
54	MG	1A	3657	1/1	0.54	0.30	74,74,74,74	0
54	MG	1A	3983	1/1	0.55	0.16	61,61,61,61	0
54	MG	2G	202	1/1	0.55	0.20	88,88,88,88	0
54	MG	2A	3108	1/1	0.57	0.17	78,78,78,78	0
54	MG	1A	3984	1/1	0.57	0.18	41,41,41,41	0
54	MG	1A	3685	1/1	0.58	0.29	74,74,74,74	0
54	MG	2A	3206	1/1	0.62	0.41	81,81,81,81	0
54	MG	1A	3282	1/1	0.63	0.10	91,91,91,91	0
54	MG	1B	227	1/1	0.64	0.11	79,79,79,79	0
54	MG	2B	206	1/1	0.64	0.40	85,85,85,85	0
54	MG	2A	3355	1/1	0.64	0.17	92,92,92,92	0
54	MG	2n	3101	1/1	0.64	0.30	88,88,88,88	0
54	MG	2B	213	1/1	0.65	0.16	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3027	1/1	0.65	0.16	75,75,75,75	0
54	MG	1a	1877	1/1	0.66	0.16	90,90,90,90	0
54	MG	2a	3066	1/1	0.66	0.22	81,81,81,81	0
54	MG	1a	1791	1/1	0.66	0.20	80,80,80,80	0
54	MG	1a	1813	1/1	0.66	0.28	80,80,80,80	0
54	MG	1A	4026	1/1	0.67	0.27	84,84,84,84	0
54	MG	1A	3556	1/1	0.67	0.21	43,43,43,43	0
54	MG	2A	3529	1/1	0.67	0.17	77,77,77,77	0
54	MG	2a	3055	1/1	0.67	0.35	89,89,89,89	0
54	MG	2A	3607	1/1	0.67	0.15	80,80,80,80	0
54	MG	1a	1744	1/1	0.67	0.15	97,97,97,97	0
54	MG	1A	3875	1/1	0.67	0.20	76,76,76,76	0
54	MG	1S	201	1/1	0.68	0.20	68,68,68,68	0
54	MG	2A	3347	1/1	0.68	0.21	82,82,82,82	0
54	MG	1a	1685	1/1	0.68	0.22	76,76,76,76	0
54	MG	1a	1874	1/1	0.68	0.16	79,79,79,79	0
54	MG	1a	1714	1/1	0.68	0.22	81,81,81,81	0
54	MG	2A	3085	1/1	0.68	0.36	79,79,79,79	0
54	MG	2B	204	1/1	0.68	0.21	85,85,85,85	0
54	MG	1A	3895	1/1	0.68	0.19	64,64,64,64	0
54	MG	2a	3008	1/1	0.69	0.29	81,81,81,81	0
54	MG	2A	3471	1/1	0.69	0.17	84,84,84,84	0
54	MG	2A	3359	1/1	0.69	0.27	71,71,71,71	0
54	MG	2A	3556	1/1	0.69	0.23	68,68,68,68	0
54	MG	2A	3601	1/1	0.69	0.21	88,88,88,88	0
54	MG	2A	3449	1/1	0.69	0.20	75,75,75,75	0
54	MG	1A	3863	1/1	0.70	0.20	76,76,76,76	0
54	MG	1A	3963	1/1	0.70	0.25	72,72,72,72	0
54	MG	2A	3439	1/1	0.70	0.26	65,65,65,65	0
54	MG	1A	3988	1/1	0.70	0.22	82,82,82,82	0
57	MPD	2B	219	8/8	0.70	0.30	70,79,82,82	0
54	MG	1n	103	1/1	0.71	0.19	85,85,85,85	0
54	MG	2a	3056	1/1	0.71	0.30	74,74,74,74	0
54	MG	1A	3910	1/1	0.71	0.15	61,61,61,61	0
54	MG	1A	3887	1/1	0.72	0.15	64,64,64,64	0
54	MG	1A	3998	1/1	0.72	0.30	66,66,66,66	0
54	MG	2a	3113	1/1	0.72	0.23	79,79,79,79	0
54	MG	2a	3164	1/1	0.72	0.15	97,97,97,97	0
54	MG	1A	4000	1/1	0.72	0.32	83,83,83,83	0
54	MG	2A	3430	1/1	0.72	0.15	77,77,77,77	0
54	MG	2A	3089	1/1	0.73	0.20	80,80,80,80	0
54	MG	2a	3061	1/1	0.73	0.13	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3090	1/1	0.73	0.43	75,75,75,75	0
54	MG	1A	4020	1/1	0.73	0.19	79,79,79,79	0
54	MG	2A	3572	1/1	0.73	0.13	59,59,59,59	0
54	MG	1a	1850	1/1	0.73	0.22	86,86,86,86	0
54	MG	2A	3267	1/1	0.73	0.34	66,66,66,66	0
54	MG	1A	3300	1/1	0.73	0.14	93,93,93,93	0
54	MG	1A	3165	1/1	0.74	0.23	62,62,62,62	0
54	MG	1A	3542	1/1	0.74	0.15	66,66,66,66	0
54	MG	1a	1693	1/1	0.74	0.29	79,79,79,79	0
54	MG	2A	3470	1/1	0.74	0.18	70,70,70,70	0
54	MG	2A	3185	1/1	0.74	0.21	84,84,84,84	0
54	MG	2A	3371	1/1	0.74	0.17	51,51,51,51	0
54	MG	2A	3409	1/1	0.74	0.13	85,85,85,85	0
54	MG	2I	201	1/1	0.74	0.12	80,80,80,80	0
54	MG	2N	201	1/1	0.74	0.11	75,75,75,75	0
54	MG	1A	3727	1/1	0.74	0.26	57,57,57,57	0
54	MG	1a	1708	1/1	0.75	0.13	98,98,98,98	0
54	MG	2A	3209	1/1	0.75	0.32	80,80,80,80	0
54	MG	1A	3651	1/1	0.75	0.31	36,36,36,36	0
54	MG	2A	3493	1/1	0.75	0.14	74,74,74,74	0
54	MG	2A	3502	1/1	0.75	0.17	51,51,51,51	0
54	MG	1A	3759	1/1	0.75	0.15	70,70,70,70	0
54	MG	2A	3051	1/1	0.75	0.28	68,68,68,68	0
54	MG	1a	1638	1/1	0.75	0.27	72,72,72,72	0
54	MG	1a	1794	1/1	0.75	0.26	79,79,79,79	0
54	MG	1A	3272	1/1	0.75	0.16	57,57,57,57	0
54	MG	1a	1814	1/1	0.75	0.20	81,81,81,81	0
54	MG	2a	3117	1/1	0.75	0.22	74,74,74,74	0
54	MG	2A	3424	1/1	0.75	0.16	56,56,56,56	0
54	MG	2A	3124	1/1	0.75	0.27	76,76,76,76	0
54	MG	1A	3693	1/1	0.75	0.29	79,79,79,79	0
54	MG	2A	3254	1/1	0.76	0.18	59,59,59,59	0
54	MG	1A	3979	1/1	0.76	0.21	74,74,74,74	0
54	MG	1A	3385	1/1	0.76	0.15	70,70,70,70	0
54	MG	2a	3065	1/1	0.76	0.26	78,78,78,78	0
54	MG	1A	3840	1/1	0.76	0.19	61,61,61,61	0
54	MG	2a	3067	1/1	0.76	0.20	80,80,80,80	0
54	MG	1A	3601	1/1	0.76	0.43	50,50,50,50	0
54	MG	2A	3462	1/1	0.76	0.16	56,56,56,56	0
54	MG	1B	224	1/1	0.76	0.14	64,64,64,64	0
54	MG	2a	3016	1/1	0.76	0.14	94,94,94,94	0
54	MG	2A	3219	1/1	0.76	0.18	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MPD	1T	207	8/8	0.76	0.23	73,77,81,82	0
54	MG	2a	3047	1/1	0.76	0.34	72,72,72,72	0
58	ARG	1F	319	12/12	0.76	0.22	60,72,89,89	0
54	MG	1H	201	1/1	0.77	0.17	76,76,76,76	0
54	MG	1A	3237	1/1	0.77	0.29	79,79,79,79	0
54	MG	2A	3153	1/1	0.77	0.18	77,77,77,77	0
54	MG	2A	3376	1/1	0.77	0.21	60,60,60,60	0
54	MG	1a	1879	1/1	0.77	0.15	90,90,90,90	0
54	MG	2a	3103	1/1	0.77	0.12	73,73,73,73	0
54	MG	1n	101	1/1	0.77	0.17	72,72,72,72	0
54	MG	1A	3731	1/1	0.77	0.13	48,48,48,48	0
54	MG	1a	1642	1/1	0.77	0.16	76,76,76,76	0
54	MG	1A	3736	1/1	0.77	0.09	74,74,74,74	0
54	MG	1A	3975	1/1	0.77	0.19	63,63,63,63	0
54	MG	1A	3978	1/1	0.77	0.20	67,67,67,67	0
54	MG	2a	3059	1/1	0.77	0.34	85,85,85,85	0
54	MG	2A	3512	1/1	0.78	0.11	79,79,79,79	0
54	MG	1A	3562	1/1	0.78	0.15	58,58,58,58	0
54	MG	1A	3797	1/1	0.78	0.24	73,73,73,73	0
54	MG	1a	1647	1/1	0.78	0.30	71,71,71,71	0
54	MG	15	106	1/1	0.78	0.19	58,58,58,58	0
54	MG	2a	3180	1/1	0.78	0.16	86,86,86,86	0
54	MG	2A	3398	1/1	0.78	0.16	70,70,70,70	0
54	MG	2A	3675	1/1	0.78	0.20	55,55,55,55	0
54	MG	2A	3448	1/1	0.78	0.22	67,67,67,67	0
54	MG	2a	3033	1/1	0.78	0.18	84,84,84,84	0
54	MG	1A	3476	1/1	0.79	0.13	58,58,58,58	0
54	MG	2A	3597	1/1	0.79	0.20	48,48,48,48	0
54	MG	2A	3415	1/1	0.79	0.23	71,71,71,71	0
54	MG	1a	1747	1/1	0.79	0.17	78,78,78,78	0
54	MG	1A	3341	1/1	0.79	0.14	49,49,49,49	0
54	MG	1D	318	1/1	0.79	0.19	68,68,68,68	0
54	MG	1a	1652	1/1	0.79	0.25	81,81,81,81	0
54	MG	2a	3080	1/1	0.79	0.20	70,70,70,70	0
54	MG	2A	3282	1/1	0.79	0.17	61,61,61,61	0
54	MG	2A	3292	1/1	0.79	0.14	65,65,65,65	0
54	MG	2A	3465	1/1	0.79	0.18	80,80,80,80	0
54	MG	1A	3733	1/1	0.79	0.22	68,68,68,68	0
54	MG	1a	1821	1/1	0.79	0.17	88,88,88,88	0
54	MG	1A	3814	1/1	0.79	0.24	68,68,68,68	0
54	MG	1T	202	1/1	0.79	0.17	59,59,59,59	0
54	MG	1a	1875	1/1	0.79	0.18	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3964	1/1	0.79	0.15	70,70,70,70	0
54	MG	2A	3186	1/1	0.79	0.29	59,59,59,59	0
54	MG	1g	202	1/1	0.80	0.14	69,69,69,69	0
54	MG	1A	3696	1/1	0.80	0.15	71,71,71,71	0
54	MG	2a	3032	1/1	0.80	0.24	74,74,74,74	0
54	MG	1A	3396	1/1	0.80	0.26	71,71,71,71	0
54	MG	1A	3614	1/1	0.80	0.18	75,75,75,75	0
54	MG	2A	3334	1/1	0.80	0.15	83,83,83,83	0
54	MG	2A	3345	1/1	0.80	0.22	81,81,81,81	0
54	MG	1a	1793	1/1	0.80	0.13	71,71,71,71	0
54	MG	2A	3517	1/1	0.80	0.12	61,61,61,61	0
54	MG	1A	3675	1/1	0.80	0.14	34,34,34,34	0
54	MG	1a	1671	1/1	0.80	0.21	81,81,81,81	0
54	MG	1a	1679	1/1	0.80	0.28	71,71,71,71	0
54	MG	1A	3626	1/1	0.80	0.15	85,85,85,85	0
54	MG	1A	3749	1/1	0.80	0.15	59,59,59,59	0
54	MG	2A	3162	1/1	0.80	0.21	68,68,68,68	0
54	MG	2A	3671	1/1	0.80	0.14	67,67,67,67	0
54	MG	2a	3111	1/1	0.80	0.23	75,75,75,75	0
54	MG	2A	3171	1/1	0.80	0.15	80,80,80,80	0
54	MG	1a	1865	1/1	0.80	0.25	85,85,85,85	0
54	MG	1a	1706	1/1	0.80	0.44	81,81,81,81	0
54	MG	2A	3195	1/1	0.80	0.22	67,67,67,67	0
54	MG	1A	3445	1/1	0.80	0.14	78,78,78,78	0
54	MG	1a	1618	1/1	0.80	0.15	66,66,66,66	0
54	MG	1a	1723	1/1	0.80	0.27	79,79,79,79	0
54	MG	2A	3452	1/1	0.80	0.18	70,70,70,70	0
54	MG	2a	3028	1/1	0.81	0.26	87,87,87,87	0
54	MG	2A	3498	1/1	0.81	0.21	46,46,46,46	0
54	MG	1A	3236	1/1	0.81	0.28	74,74,74,74	0
54	MG	2a	3035	1/1	0.81	0.26	74,74,74,74	0
54	MG	1A	3150	1/1	0.81	0.23	76,76,76,76	0
54	MG	1A	3751	1/1	0.81	0.12	55,55,55,55	0
54	MG	2A	3194	1/1	0.81	0.16	64,64,64,64	0
54	MG	1A	3701	1/1	0.81	0.14	74,74,74,74	0
54	MG	2a	3058	1/1	0.81	0.20	92,92,92,92	0
54	MG	1a	1756	1/1	0.81	0.11	84,84,84,84	0
54	MG	2A	3593	1/1	0.81	0.14	50,50,50,50	0
54	MG	2A	3208	1/1	0.81	0.21	65,65,65,65	0
54	MG	1a	1660	1/1	0.81	0.38	79,79,79,79	0
54	MG	1a	1666	1/1	0.81	0.12	77,77,77,77	0
54	MG	2A	3240	1/1	0.81	0.37	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3445	1/1	0.81	0.11	84,84,84,84	0
54	MG	1A	3304	1/1	0.81	0.18	51,51,51,51	0
54	MG	1A	3319	1/1	0.81	0.17	74,74,74,74	0
54	MG	1A	3185	1/1	0.81	0.15	71,71,71,71	0
54	MG	1a	1816	1/1	0.81	0.13	76,76,76,76	0
54	MG	1l	102	1/1	0.81	0.31	63,63,63,63	0
54	MG	1A	3845	1/1	0.81	0.11	53,53,53,53	0
54	MG	2e	202	1/1	0.81	0.34	79,79,79,79	0
54	MG	1A	3972	1/1	0.81	0.13	51,51,51,51	0
54	MG	2A	3477	1/1	0.81	0.27	75,75,75,75	0
54	MG	2a	3011	1/1	0.81	0.33	77,77,77,77	0
54	MG	1a	1871	1/1	0.81	0.15	76,76,76,76	0
54	MG	1A	3856	1/1	0.82	0.16	61,61,61,61	0
54	MG	1A	3318	1/1	0.82	0.19	69,69,69,69	0
54	MG	2A	3043	1/1	0.82	0.32	80,80,80,80	0
54	MG	1a	1798	1/1	0.82	0.31	72,72,72,72	0
54	MG	2A	3264	1/1	0.82	0.19	75,75,75,75	0
54	MG	2A	3052	1/1	0.82	0.28	68,68,68,68	0
54	MG	2A	3084	1/1	0.82	0.18	80,80,80,80	0
54	MG	13	102	1/1	0.82	0.21	67,67,67,67	0
54	MG	2A	3293	1/1	0.82	0.18	56,56,56,56	0
54	MG	1A	3870	1/1	0.82	0.20	45,45,45,45	0
54	MG	2A	3506	1/1	0.82	0.20	92,92,92,92	0
54	MG	2A	3510	1/1	0.82	0.18	79,79,79,79	0
54	MG	1A	3457	1/1	0.82	0.13	53,53,53,53	0
54	MG	2a	3057	1/1	0.82	0.30	86,86,86,86	0
54	MG	1B	203	1/1	0.82	0.25	67,67,67,67	0
54	MG	1a	1827	1/1	0.82	0.19	88,88,88,88	0
54	MG	1a	1836	1/1	0.82	0.29	74,74,74,74	0
54	MG	2A	3161	1/1	0.82	0.20	83,83,83,83	0
54	MG	1A	3377	1/1	0.82	0.15	61,61,61,61	0
54	MG	2A	3392	1/1	0.82	0.21	78,78,78,78	0
54	MG	1A	3591	1/1	0.82	0.14	76,76,76,76	0
54	MG	2A	3179	1/1	0.82	0.23	82,82,82,82	0
54	MG	1A	3509	1/1	0.82	0.12	29,29,29,29	0
54	MG	2a	3104	1/1	0.82	0.10	85,85,85,85	0
54	MG	1A	3713	1/1	0.82	0.33	54,54,54,54	0
54	MG	2A	3680	1/1	0.82	0.18	64,64,64,64	0
54	MG	2A	3689	1/1	0.82	0.25	70,70,70,70	0
54	MG	1a	1662	1/1	0.82	0.14	70,70,70,70	0
54	MG	2a	3167	1/1	0.82	0.24	89,89,89,89	0
54	MG	1a	1773	1/1	0.82	0.22	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2B	208	1/1	0.82	0.29	85,85,85,85	0
54	MG	2B	209	1/1	0.82	0.29	80,80,80,80	0
54	MG	2A	3203	1/1	0.82	0.30	72,72,72,72	0
54	MG	1a	1788	1/1	0.82	0.12	86,86,86,86	0
54	MG	1A	3992	1/1	0.82	0.25	55,55,55,55	0
54	MG	2A	3291	1/1	0.83	0.14	59,59,59,59	0
54	MG	2a	3018	1/1	0.83	0.42	74,74,74,74	0
54	MG	1A	3574	1/1	0.83	0.27	46,46,46,46	0
54	MG	1A	3540	1/1	0.83	0.14	66,66,66,66	0
54	MG	1a	1795	1/1	0.83	0.15	66,66,66,66	0
54	MG	2A	3106	1/1	0.83	0.20	62,62,62,62	0
54	MG	1A	3592	1/1	0.83	0.27	52,52,52,52	0
54	MG	1a	1684	1/1	0.83	0.31	76,76,76,76	0
54	MG	1A	3970	1/1	0.83	0.19	51,51,51,51	0
54	MG	1A	4009	1/1	0.83	0.10	84,84,84,84	0
54	MG	1a	1704	1/1	0.83	0.20	74,74,74,74	0
54	MG	1A	3336	1/1	0.83	0.16	63,63,63,63	0
54	MG	1a	1707	1/1	0.83	0.20	75,75,75,75	0
54	MG	1a	1615	1/1	0.83	0.10	79,79,79,79	0
54	MG	2A	3612	1/1	0.83	0.20	72,72,72,72	0
54	MG	1A	4024	1/1	0.83	0.17	61,61,61,61	0
54	MG	2A	3187	1/1	0.83	0.25	74,74,74,74	0
54	MG	1a	1717	1/1	0.83	0.33	80,80,80,80	0
54	MG	2A	3686	1/1	0.83	0.18	82,82,82,82	0
54	MG	2a	3099	1/1	0.83	0.13	78,78,78,78	0
54	MG	1a	1720	1/1	0.83	0.41	77,77,77,77	0
54	MG	2A	3691	1/1	0.83	0.20	83,83,83,83	0
54	MG	1a	1626	1/1	0.83	0.09	66,66,66,66	0
54	MG	1a	1727	1/1	0.83	0.16	70,70,70,70	0
54	MG	1A	3551	1/1	0.83	0.30	62,62,62,62	0
54	MG	2a	3145	1/1	0.83	0.16	88,88,88,88	0
54	MG	1A	3621	1/1	0.83	0.14	46,46,46,46	0
54	MG	1B	210	1/1	0.83	0.15	65,65,65,65	0
54	MG	2a	3173	1/1	0.83	0.23	72,72,72,72	0
54	MG	1a	1765	1/1	0.83	0.19	67,67,67,67	0
54	MG	1A	3261	1/1	0.83	0.22	81,81,81,81	0
54	MG	1a	1777	1/1	0.83	0.10	69,69,69,69	0
54	MG	1A	3331	1/1	0.83	0.32	81,81,81,81	0
54	MG	2A	3268	1/1	0.83	0.17	78,78,78,78	0
54	MG	1A	3725	1/1	0.83	0.18	26,26,26,26	0
54	MG	1A	3799	1/1	0.84	0.16	34,34,34,34	0
54	MG	1a	1680	1/1	0.84	0.14	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1B	226	1/1	0.84	0.10	78,78,78,78	0
54	MG	1A	3405	1/1	0.84	0.14	51,51,51,51	0
54	MG	1A	3834	1/1	0.84	0.21	47,47,47,47	0
54	MG	1a	1698	1/1	0.84	0.24	78,78,78,78	0
54	MG	1A	3443	1/1	0.84	0.29	82,82,82,82	0
54	MG	1N	203	1/1	0.84	0.14	70,70,70,70	0
54	MG	1A	3707	1/1	0.84	0.15	70,70,70,70	0
54	MG	2A	3227	1/1	0.84	0.27	65,65,65,65	0
54	MG	2A	3234	1/1	0.84	0.26	73,73,73,73	0
54	MG	1A	3981	1/1	0.84	0.25	59,59,59,59	0
54	MG	1A	3145	1/1	0.84	0.17	69,69,69,69	0
54	MG	1A	3454	1/1	0.84	0.23	65,65,65,65	0
54	MG	1d	302	1/1	0.84	0.20	74,74,74,74	0
54	MG	1A	3986	1/1	0.84	0.10	75,75,75,75	0
54	MG	19	103	1/1	0.84	0.21	67,67,67,67	0
54	MG	2A	3548	1/1	0.84	0.14	37,37,37,37	0
54	MG	1a	1603	1/1	0.84	0.22	77,77,77,77	0
54	MG	1a	1612	1/1	0.84	0.20	79,79,79,79	0
54	MG	1A	3325	1/1	0.84	0.18	66,66,66,66	0
54	MG	2a	3072	1/1	0.84	0.36	67,67,67,67	0
54	MG	1A	3061	1/1	0.84	0.23	64,64,64,64	0
54	MG	2A	3053	1/1	0.84	0.28	69,69,69,69	0
54	MG	1A	3667	1/1	0.84	0.17	65,65,65,65	0
54	MG	2a	3101	1/1	0.84	0.14	71,71,71,71	0
54	MG	1a	1769	1/1	0.84	0.18	63,63,63,63	0
54	MG	1A	3491	1/1	0.84	0.12	60,60,60,60	0
54	MG	1A	4008	1/1	0.84	0.14	61,61,61,61	0
54	MG	1a	1782	1/1	0.84	0.12	76,76,76,76	0
54	MG	1A	3676	1/1	0.84	0.12	49,49,49,49	0
54	MG	2a	3119	1/1	0.84	0.13	65,65,65,65	0
54	MG	1A	3898	1/1	0.84	0.27	40,40,40,40	0
54	MG	2A	3406	1/1	0.84	0.20	92,92,92,92	0
54	MG	2B	202	1/1	0.84	0.16	73,73,73,73	0
54	MG	1A	3107	1/1	0.84	0.15	36,36,36,36	0
54	MG	2a	3178	1/1	0.84	0.19	81,81,81,81	0
54	MG	1A	3931	1/1	0.84	0.17	64,64,64,64	0
54	MG	1a	1665	1/1	0.84	0.17	76,76,76,76	0
54	MG	1A	3530	1/1	0.84	0.12	79,79,79,79	0
54	MG	1a	1809	1/1	0.84	0.28	74,74,74,74	0
54	MG	2A	3438	1/1	0.84	0.37	64,64,64,64	0
54	MG	1A	3694	1/1	0.84	0.23	78,78,78,78	0
54	MG	1a	1869	1/1	0.85	0.13	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1729	1/1	0.85	0.19	74,74,74,74	0
54	MG	2A	3228	1/1	0.85	0.16	66,66,66,66	0
54	MG	1a	1872	1/1	0.85	0.11	89,89,89,89	0
54	MG	2A	3632	1/1	0.85	0.12	87,87,87,87	0
54	MG	1A	3699	1/1	0.85	0.16	41,41,41,41	0
54	MG	1A	3926	1/1	0.85	0.15	30,30,30,30	0
54	MG	2A	3259	1/1	0.85	0.20	57,57,57,57	0
54	MG	1a	1749	1/1	0.85	0.13	65,65,65,65	0
54	MG	1a	1750	1/1	0.85	0.20	73,73,73,73	0
54	MG	1d	301	1/1	0.85	0.26	74,74,74,74	0
54	MG	2A	3707	1/1	0.85	0.12	73,73,73,73	0
54	MG	2A	3708	1/1	0.85	0.21	64,64,64,64	0
54	MG	2A	3269	1/1	0.85	0.18	39,39,39,39	0
54	MG	2B	203	1/1	0.85	0.27	74,74,74,74	0
54	MG	1a	1752	1/1	0.85	0.33	71,71,71,71	0
54	MG	1e	201	1/1	0.85	0.21	72,72,72,72	0
54	MG	1A	3479	1/1	0.85	0.12	50,50,50,50	0
54	MG	1h	201	1/1	0.85	0.16	71,71,71,71	0
54	MG	2A	3297	1/1	0.85	0.21	82,82,82,82	0
54	MG	2E	305	1/1	0.85	0.21	62,62,62,62	0
54	MG	2A	3333	1/1	0.85	0.10	36,36,36,36	0
54	MG	1i	3100	1/1	0.85	0.14	80,80,80,80	0
54	MG	1a	1757	1/1	0.85	0.20	50,50,50,50	0
54	MG	1A	3035	1/1	0.85	0.34	68,68,68,68	0
54	MG	2a	3002	1/1	0.85	0.13	66,66,66,66	0
54	MG	1t	201	1/1	0.85	0.14	70,70,70,70	0
54	MG	1y	203	1/1	0.85	0.11	75,75,75,75	0
54	MG	2A	3012	1/1	0.85	0.14	71,71,71,71	0
54	MG	2A	3024	1/1	0.85	0.24	77,77,77,77	0
54	MG	2a	3020	1/1	0.85	0.28	66,66,66,66	0
54	MG	2a	3021	1/1	0.85	0.20	76,76,76,76	0
54	MG	2a	3022	1/1	0.85	0.22	60,60,60,60	0
54	MG	2A	3036	1/1	0.85	0.20	57,57,57,57	0
54	MG	1A	3189	1/1	0.85	0.13	76,76,76,76	0
54	MG	1A	4019	1/1	0.85	0.12	66,66,66,66	0
54	MG	2A	3408	1/1	0.85	0.18	59,59,59,59	0
54	MG	1a	1774	1/1	0.85	0.14	73,73,73,73	0
54	MG	1A	3583	1/1	0.85	0.12	63,63,63,63	0
54	MG	2a	3049	1/1	0.85	0.34	69,69,69,69	0
54	MG	2A	3073	1/1	0.85	0.28	65,65,65,65	0
54	MG	1a	1682	1/1	0.85	0.12	69,69,69,69	0
54	MG	1a	1601	1/1	0.85	0.15	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3659	1/1	0.85	0.23	42,42,42,42	0
54	MG	1A	3079	1/1	0.85	0.18	60,60,60,60	0
54	MG	1A	3538	1/1	0.85	0.10	62,62,62,62	0
54	MG	1A	3866	1/1	0.85	0.12	56,56,56,56	0
54	MG	2A	3120	1/1	0.85	0.23	63,63,63,63	0
54	MG	1a	1796	1/1	0.85	0.18	90,90,90,90	0
54	MG	1A	3600	1/1	0.85	0.18	65,65,65,65	0
54	MG	2A	3160	1/1	0.85	0.14	72,72,72,72	0
54	MG	1a	1630	1/1	0.85	0.16	63,63,63,63	0
54	MG	2a	3086	1/1	0.85	0.28	81,81,81,81	0
54	MG	1A	3455	1/1	0.85	0.14	34,34,34,34	0
54	MG	1a	1710	1/1	0.85	0.25	71,71,71,71	0
54	MG	2A	3486	1/1	0.85	0.15	74,74,74,74	0
54	MG	2A	3491	1/1	0.85	0.09	76,76,76,76	0
54	MG	1a	1641	1/1	0.85	0.17	79,79,79,79	0
54	MG	2A	3180	1/1	0.85	0.19	71,71,71,71	0
54	MG	2a	3116	1/1	0.85	0.22	82,82,82,82	0
54	MG	1A	3610	1/1	0.85	0.30	74,74,74,74	0
54	MG	1A	3402	1/1	0.85	0.17	72,72,72,72	0
54	MG	2a	3143	1/1	0.85	0.17	70,70,70,70	0
54	MG	1a	1829	1/1	0.85	0.24	74,74,74,74	0
54	MG	2a	3158	1/1	0.85	0.15	88,88,88,88	0
54	MG	1a	1831	1/1	0.85	0.13	62,62,62,62	0
54	MG	2A	3515	1/1	0.85	0.21	82,82,82,82	0
54	MG	1A	3363	1/1	0.85	0.12	71,71,71,71	0
54	MG	2A	3202	1/1	0.85	0.24	63,63,63,63	0
54	MG	2A	3531	1/1	0.85	0.12	87,87,87,87	0
54	MG	1a	1841	1/1	0.85	0.22	79,79,79,79	0
54	MG	2j	201	1/1	0.85	0.08	84,84,84,84	0
54	MG	1a	1849	1/1	0.85	0.15	66,66,66,66	0
57	MPD	1A	4034	8/8	0.85	0.26	54,59,62,65	0
54	MG	1a	1724	1/1	0.85	0.18	64,64,64,64	0
54	MG	2A	3591	1/1	0.85	0.13	55,55,55,55	0
54	MG	1a	1657	1/1	0.85	0.21	84,84,84,84	0
54	MG	2D	308	1/1	0.86	0.10	37,37,37,37	0
54	MG	1A	3036	1/1	0.86	0.10	51,51,51,51	0
54	MG	1a	1867	1/1	0.86	0.12	87,87,87,87	0
54	MG	1a	1659	1/1	0.86	0.24	47,47,47,47	0
54	MG	1a	1870	1/1	0.86	0.17	69,69,69,69	0
54	MG	1A	3152	1/1	0.86	0.19	50,50,50,50	0
54	MG	2O	202	1/1	0.86	0.14	76,76,76,76	0
54	MG	2O	101	1/1	0.86	0.16	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3524	1/1	0.86	0.16	56,56,56,56	0
54	MG	1A	3646	1/1	0.86	0.13	30,30,30,30	0
54	MG	2A	3451	1/1	0.86	0.15	67,67,67,67	0
54	MG	1A	3787	1/1	0.86	0.09	24,24,24,24	0
54	MG	1a	1668	1/1	0.86	0.25	82,82,82,82	0
54	MG	1A	3648	1/1	0.86	0.20	55,55,55,55	0
54	MG	1a	1673	1/1	0.86	0.17	61,61,61,61	0
54	MG	1a	1770	1/1	0.86	0.12	68,68,68,68	0
54	MG	1A	3398	1/1	0.86	0.13	53,53,53,53	0
54	MG	2a	3030	1/1	0.86	0.34	72,72,72,72	0
54	MG	2A	3482	1/1	0.86	0.17	65,65,65,65	0
54	MG	2A	3204	1/1	0.86	0.15	67,67,67,67	0
54	MG	2a	3034	1/1	0.86	0.23	92,92,92,92	0
54	MG	2A	3205	1/1	0.86	0.16	74,74,74,74	0
54	MG	1A	3809	1/1	0.86	0.24	59,59,59,59	0
54	MG	1A	3587	1/1	0.86	0.14	57,57,57,57	0
54	MG	2A	3499	1/1	0.86	0.12	67,67,67,67	0
54	MG	2a	3052	1/1	0.86	0.20	59,59,59,59	0
54	MG	1A	3941	1/1	0.86	0.18	53,53,53,53	0
54	MG	1A	3947	1/1	0.86	0.13	48,48,48,48	0
54	MG	1a	1690	1/1	0.86	0.39	69,69,69,69	0
54	MG	1A	3956	1/1	0.86	0.12	55,55,55,55	0
54	MG	1y	202	1/1	0.86	0.15	68,68,68,68	0
54	MG	2a	3060	1/1	0.86	0.32	80,80,80,80	0
54	MG	1A	4023	1/1	0.86	0.15	60,60,60,60	0
54	MG	1A	3817	1/1	0.86	0.18	77,77,77,77	0
54	MG	2A	3016	1/1	0.86	0.32	74,74,74,74	0
54	MG	1A	3131	1/1	0.86	0.18	45,45,45,45	0
54	MG	2A	3551	1/1	0.86	0.13	51,51,51,51	0
54	MG	2a	3074	1/1	0.86	0.25	75,75,75,75	0
54	MG	2a	3078	1/1	0.86	0.39	71,71,71,71	0
54	MG	2A	3552	1/1	0.86	0.14	44,44,44,44	0
54	MG	2A	3025	1/1	0.86	0.13	62,62,62,62	0
54	MG	2A	3034	1/1	0.86	0.23	77,77,77,77	0
54	MG	2a	3092	1/1	0.86	0.12	89,89,89,89	0
54	MG	2a	3096	1/1	0.86	0.10	63,63,63,63	0
54	MG	1A	3719	1/1	0.86	0.14	60,60,60,60	0
54	MG	1a	1801	1/1	0.86	0.32	85,85,85,85	0
54	MG	2a	3102	1/1	0.86	0.10	67,67,67,67	0
54	MG	1a	1803	1/1	0.86	0.16	80,80,80,80	0
54	MG	1a	1631	1/1	0.86	0.20	54,54,54,54	0
54	MG	1a	1635	1/1	0.86	0.20	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3059	1/1	0.86	0.28	58,58,58,58	0
54	MG	1A	3461	1/1	0.86	0.23	74,74,74,74	0
54	MG	2A	3076	1/1	0.86	0.14	63,63,63,63	0
54	MG	2a	3118	1/1	0.86	0.20	61,61,61,61	0
54	MG	2A	3340	1/1	0.86	0.17	50,50,50,50	0
54	MG	1a	1716	1/1	0.86	0.26	65,65,65,65	0
54	MG	1A	3087	1/1	0.86	0.17	59,59,59,59	0
54	MG	1B	225	1/1	0.86	0.12	72,72,72,72	0
54	MG	1a	1721	1/1	0.86	0.11	75,75,75,75	0
54	MG	2A	3100	1/1	0.86	0.17	71,71,71,71	0
54	MG	2a	3171	1/1	0.86	0.13	83,83,83,83	0
54	MG	2A	3101	1/1	0.86	0.27	61,61,61,61	0
54	MG	2B	201	1/1	0.86	0.14	82,82,82,82	0
54	MG	1a	1644	1/1	0.86	0.27	68,68,68,68	0
54	MG	1A	3543	1/1	0.86	0.08	26,26,26,26	0
54	MG	2A	3112	1/1	0.86	0.35	73,73,73,73	0
54	MG	2A	3113	1/1	0.86	0.19	67,67,67,67	0
54	MG	1A	3148	1/1	0.86	0.11	58,58,58,58	0
54	MG	1a	1728	1/1	0.86	0.29	65,65,65,65	0
57	MPD	2A	3714	8/8	0.86	0.28	49,56,62,62	0
54	MG	1a	1653	1/1	0.86	0.28	70,70,70,70	0
54	MG	2B	214	1/1	0.86	0.11	76,76,76,76	0
54	MG	2B	212	1/1	0.87	0.09	97,97,97,97	0
54	MG	2A	3375	1/1	0.87	0.12	60,60,60,60	0
54	MG	2A	3082	1/1	0.87	0.16	50,50,50,50	0
54	MG	1a	1805	1/1	0.87	0.17	79,79,79,79	0
54	MG	1a	1806	1/1	0.87	0.18	70,70,70,70	0
54	MG	2A	3404	1/1	0.87	0.15	60,60,60,60	0
54	MG	2A	3088	1/1	0.87	0.21	77,77,77,77	0
54	MG	1A	3822	1/1	0.87	0.11	45,45,45,45	0
54	MG	1a	1810	1/1	0.87	0.21	71,71,71,71	0
54	MG	1a	1811	1/1	0.87	0.16	63,63,63,63	0
54	MG	1a	1812	1/1	0.87	0.19	77,77,77,77	0
54	MG	2A	3423	1/1	0.87	0.15	69,69,69,69	0
54	MG	15	108	1/1	0.87	0.18	76,76,76,76	0
54	MG	1A	3982	1/1	0.87	0.15	68,68,68,68	0
54	MG	1a	1705	1/1	0.87	0.22	75,75,75,75	0
54	MG	1a	1819	1/1	0.87	0.23	68,68,68,68	0
54	MG	2A	3441	1/1	0.87	0.13	68,68,68,68	0
54	MG	1A	3180	1/1	0.87	0.43	67,67,67,67	0
54	MG	2A	3446	1/1	0.87	0.18	69,69,69,69	0
54	MG	2a	3027	1/1	0.87	0.20	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3121	1/1	0.87	0.17	70,70,70,70	0
54	MG	1a	1602	1/1	0.87	0.13	81,81,81,81	0
54	MG	2A	3131	1/1	0.87	0.14	71,71,71,71	0
54	MG	2A	3152	1/1	0.87	0.19	66,66,66,66	0
54	MG	1A	3837	1/1	0.87	0.10	54,54,54,54	0
54	MG	2A	3154	1/1	0.87	0.21	62,62,62,62	0
54	MG	2a	3039	1/1	0.87	0.20	80,80,80,80	0
54	MG	1a	1610	1/1	0.87	0.32	60,60,60,60	0
54	MG	1A	3647	1/1	0.87	0.21	69,69,69,69	0
54	MG	1a	1840	1/1	0.87	0.19	51,51,51,51	0
54	MG	1A	3408	1/1	0.87	0.27	68,68,68,68	0
54	MG	1a	1848	1/1	0.87	0.15	65,65,65,65	0
54	MG	2A	3489	1/1	0.87	0.12	83,83,83,83	0
54	MG	1A	3503	1/1	0.87	0.09	33,33,33,33	0
54	MG	1A	3652	1/1	0.87	0.12	59,59,59,59	0
54	MG	1A	3437	1/1	0.87	0.16	76,76,76,76	0
54	MG	1a	1722	1/1	0.87	0.17	64,64,64,64	0
54	MG	1A	4007	1/1	0.87	0.16	53,53,53,53	0
54	MG	1A	3098	1/1	0.87	0.09	63,63,63,63	0
54	MG	1A	3525	1/1	0.87	0.15	66,66,66,66	0
54	MG	1A	3737	1/1	0.87	0.17	45,45,45,45	0
54	MG	1A	3528	1/1	0.87	0.10	51,51,51,51	0
54	MG	1A	3596	1/1	0.87	0.10	31,31,31,31	0
54	MG	1A	3155	1/1	0.87	0.14	47,47,47,47	0
54	MG	1A	3763	1/1	0.87	0.17	43,43,43,43	0
54	MG	2a	3084	1/1	0.87	0.22	69,69,69,69	0
54	MG	1A	3764	1/1	0.87	0.23	56,56,56,56	0
54	MG	1a	1656	1/1	0.87	0.33	61,61,61,61	0
54	MG	1A	3783	1/1	0.87	0.10	45,45,45,45	0
54	MG	1B	221	1/1	0.87	0.11	59,59,59,59	0
54	MG	2A	3558	1/1	0.87	0.10	78,78,78,78	0
54	MG	1A	3933	1/1	0.87	0.13	61,61,61,61	0
54	MG	1A	3066	1/1	0.87	0.19	57,57,57,57	0
54	MG	1a	1663	1/1	0.87	0.20	75,75,75,75	0
54	MG	1A	3790	1/1	0.87	0.10	30,30,30,30	0
54	MG	2A	3260	1/1	0.87	0.22	68,68,68,68	0
54	MG	1A	3792	1/1	0.87	0.11	45,45,45,45	0
54	MG	1A	3284	1/1	0.87	0.32	74,74,74,74	0
54	MG	2A	3613	1/1	0.87	0.22	81,81,81,81	0
54	MG	2A	3631	1/1	0.87	0.13	53,53,53,53	0
54	MG	1a	1779	1/1	0.87	0.16	72,72,72,72	0
54	MG	2a	3134	1/1	0.87	0.09	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3656	1/1	0.87	0.10	78,78,78,78	0
54	MG	2A	3006	1/1	0.87	0.21	71,71,71,71	0
54	MG	1a	1780	1/1	0.87	0.20	78,78,78,78	0
54	MG	1a	1670	1/1	0.87	0.30	61,61,61,61	0
54	MG	1G	203	1/1	0.87	0.12	63,63,63,63	0
54	MG	1a	1789	1/1	0.87	0.17	83,83,83,83	0
54	MG	1A	3297	1/1	0.87	0.13	53,53,53,53	0
54	MG	2a	3175	1/1	0.87	0.09	79,79,79,79	0
54	MG	2A	3330	1/1	0.87	0.13	39,39,39,39	0
54	MG	1A	3803	1/1	0.87	0.23	69,69,69,69	0
54	MG	2e	201	1/1	0.87	0.20	75,75,75,75	0
54	MG	1A	3400	1/1	0.87	0.18	56,56,56,56	0
54	MG	1A	3810	1/1	0.87	0.16	65,65,65,65	0
54	MG	1T	204	1/1	0.87	0.18	67,67,67,67	0
54	MG	1A	3298	1/1	0.87	0.16	74,74,74,74	0
54	MG	2B	205	1/1	0.87	0.20	64,64,64,64	0
54	MG	1a	1799	1/1	0.87	0.11	73,73,73,73	0
54	MG	1a	1689	1/1	0.87	0.27	70,70,70,70	0
54	MG	1A	3631	1/1	0.87	0.20	53,53,53,53	0
54	MG	2A	3031	1/1	0.88	0.14	68,68,68,68	0
54	MG	1a	1674	1/1	0.88	0.32	66,66,66,66	0
54	MG	2A	3692	1/1	0.88	0.10	89,89,89,89	0
54	MG	2A	3300	1/1	0.88	0.15	63,63,63,63	0
54	MG	2A	3307	1/1	0.88	0.12	54,54,54,54	0
54	MG	2A	3319	1/1	0.88	0.10	48,48,48,48	0
54	MG	2A	3324	1/1	0.88	0.18	65,65,65,65	0
54	MG	1a	1676	1/1	0.88	0.13	75,75,75,75	0
54	MG	2A	3041	1/1	0.88	0.13	50,50,50,50	0
54	MG	1R	205	1/1	0.88	0.19	49,49,49,49	0
54	MG	2A	3046	1/1	0.88	0.11	65,65,65,65	0
54	MG	1A	3974	1/1	0.88	0.19	59,59,59,59	0
54	MG	1a	1681	1/1	0.88	0.15	62,62,62,62	0
54	MG	1A	3430	1/1	0.88	0.15	54,54,54,54	0
54	MG	2A	3357	1/1	0.88	0.09	35,35,35,35	0
54	MG	1A	3198	1/1	0.88	0.14	61,61,61,61	0
54	MG	2A	3361	1/1	0.88	0.20	69,69,69,69	0
54	MG	2D	309	1/1	0.88	0.21	55,55,55,55	0
54	MG	2A	3367	1/1	0.88	0.14	42,42,42,42	0
54	MG	2A	3070	1/1	0.88	0.20	65,65,65,65	0
54	MG	10	103	1/1	0.88	0.13	60,60,60,60	0
54	MG	1A	3616	1/1	0.88	0.12	45,45,45,45	0
54	MG	2A	3388	1/1	0.88	0.09	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3536	1/1	0.88	0.11	28,28,28,28	0
54	MG	2P	201	1/1	0.88	0.25	72,72,72,72	0
54	MG	1a	1808	1/1	0.88	0.28	70,70,70,70	0
54	MG	2I	101	1/1	0.88	0.09	88,88,88,88	0
54	MG	1a	1692	1/1	0.88	0.19	62,62,62,62	0
54	MG	1A	3344	1/1	0.88	0.28	51,51,51,51	0
54	MG	1A	3843	1/1	0.88	0.11	54,54,54,54	0
54	MG	1a	1703	1/1	0.88	0.38	78,78,78,78	0
54	MG	1A	3351	1/1	0.88	0.14	70,70,70,70	0
54	MG	1A	3204	1/1	0.88	0.23	64,64,64,64	0
54	MG	1A	3008	1/1	0.88	0.15	50,50,50,50	0
54	MG	1A	3859	1/1	0.88	0.17	54,54,54,54	0
54	MG	2A	3429	1/1	0.88	0.15	62,62,62,62	0
54	MG	1a	1604	1/1	0.88	0.38	78,78,78,78	0
54	MG	2a	3029	1/1	0.88	0.29	64,64,64,64	0
54	MG	2A	3431	1/1	0.88	0.12	66,66,66,66	0
54	MG	1A	3116	1/1	0.88	0.23	47,47,47,47	0
54	MG	2A	3116	1/1	0.88	0.16	76,76,76,76	0
54	MG	1a	1712	1/1	0.88	0.33	80,80,80,80	0
54	MG	1a	1611	1/1	0.88	0.28	71,71,71,71	0
54	MG	1a	1834	1/1	0.88	0.10	84,84,84,84	0
54	MG	2a	3041	1/1	0.88	0.22	65,65,65,65	0
54	MG	2a	3043	1/1	0.88	0.32	70,70,70,70	0
54	MG	2A	3127	1/1	0.88	0.21	58,58,58,58	0
54	MG	1A	3392	1/1	0.88	0.10	40,40,40,40	0
54	MG	1A	4001	1/1	0.88	0.30	45,45,45,45	0
54	MG	1a	1719	1/1	0.88	0.47	75,75,75,75	0
54	MG	2a	3054	1/1	0.88	0.21	72,72,72,72	0
54	MG	1a	1843	1/1	0.88	0.21	85,85,85,85	0
54	MG	1a	1844	1/1	0.88	0.14	61,61,61,61	0
54	MG	1a	1616	1/1	0.88	0.20	80,80,80,80	0
54	MG	1A	3557	1/1	0.88	0.12	59,59,59,59	0
54	MG	2A	3474	1/1	0.88	0.16	67,67,67,67	0
54	MG	2A	3167	1/1	0.88	0.26	61,61,61,61	0
54	MG	2A	3170	1/1	0.88	0.17	62,62,62,62	0
54	MG	2A	3485	1/1	0.88	0.10	63,63,63,63	0
54	MG	1A	3756	1/1	0.88	0.24	61,61,61,61	0
54	MG	1a	1851	1/1	0.88	0.17	71,71,71,71	0
54	MG	1a	1861	1/1	0.88	0.33	73,73,73,73	0
54	MG	2A	3492	1/1	0.88	0.12	71,71,71,71	0
54	MG	2A	3182	1/1	0.88	0.18	73,73,73,73	0
54	MG	2A	3494	1/1	0.88	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3495	1/1	0.88	0.09	65,65,65,65	0
54	MG	1A	3471	1/1	0.88	0.14	59,59,59,59	0
54	MG	1A	3570	1/1	0.88	0.09	44,44,44,44	0
54	MG	2a	3087	1/1	0.88	0.13	73,73,73,73	0
54	MG	1a	1632	1/1	0.88	0.32	79,79,79,79	0
54	MG	2a	3094	1/1	0.88	0.21	74,74,74,74	0
54	MG	1A	3896	1/1	0.88	0.15	64,64,64,64	0
54	MG	1A	3310	1/1	0.88	0.48	49,49,49,49	0
54	MG	2A	3199	1/1	0.88	0.25	71,71,71,71	0
54	MG	1A	3766	1/1	0.88	0.19	62,62,62,62	0
54	MG	1A	3911	1/1	0.88	0.23	41,41,41,41	0
54	MG	2A	3520	1/1	0.88	0.10	34,34,34,34	0
54	MG	1A	3579	1/1	0.88	0.13	64,64,64,64	0
54	MG	1a	1646	1/1	0.88	0.29	61,61,61,61	0
54	MG	1A	3260	1/1	0.88	0.13	66,66,66,66	0
54	MG	2A	3549	1/1	0.88	0.13	41,41,41,41	0
54	MG	1A	3489	1/1	0.88	0.13	64,64,64,64	0
54	MG	1A	3679	1/1	0.88	0.12	56,56,56,56	0
54	MG	2a	3121	1/1	0.88	0.10	76,76,76,76	0
54	MG	2a	3125	1/1	0.88	0.11	81,81,81,81	0
54	MG	2A	3215	1/1	0.88	0.11	58,58,58,58	0
54	MG	2a	3142	1/1	0.88	0.10	83,83,83,83	0
54	MG	1a	1759	1/1	0.88	0.18	68,68,68,68	0
54	MG	1a	1763	1/1	0.88	0.21	64,64,64,64	0
54	MG	2a	3155	1/1	0.88	0.10	72,72,72,72	0
54	MG	2A	3584	1/1	0.88	0.13	53,53,53,53	0
54	MG	2A	3588	1/1	0.88	0.09	70,70,70,70	0
54	MG	1A	3184	1/1	0.88	0.15	52,52,52,52	0
54	MG	1A	3954	1/1	0.88	0.09	30,30,30,30	0
54	MG	1l	202	1/1	0.88	0.23	79,79,79,79	0
54	MG	1A	3401	1/1	0.88	0.08	75,75,75,75	0
54	MG	2a	3177	1/1	0.88	0.24	80,80,80,80	0
54	MG	1D	311	1/1	0.88	0.21	64,64,64,64	0
54	MG	1D	315	1/1	0.88	0.16	74,74,74,74	0
54	MG	1A	3153	1/1	0.88	0.35	72,72,72,72	0
54	MG	1E	306	1/1	0.88	0.18	53,53,53,53	0
54	MG	1F	315	1/1	0.88	0.60	55,55,55,55	0
54	MG	2A	3639	1/1	0.88	0.12	37,37,37,37	0
54	MG	1A	3597	1/1	0.88	0.20	55,55,55,55	0
54	MG	1A	3128	1/1	0.88	0.22	66,66,66,66	0
57	MPD	1a	1882	8/8	0.88	0.11	54,70,76,81	0
54	MG	2A	3286	1/1	0.88	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3191	1/1	0.88	0.33	65,65,65,65	0
54	MG	1O	201	1/1	0.88	0.14	63,63,63,63	0
54	MG	1A	3833	1/1	0.89	0.08	20,20,20,20	0
54	MG	1A	3642	1/1	0.89	0.21	68,68,68,68	0
54	MG	1O	102	1/1	0.89	0.18	47,47,47,47	0
54	MG	2A	3174	1/1	0.89	0.13	63,63,63,63	0
54	MG	2A	3178	1/1	0.89	0.18	75,75,75,75	0
54	MG	1e	202	1/1	0.89	0.28	63,63,63,63	0
54	MG	1f	201	1/1	0.89	0.25	74,74,74,74	0
54	MG	1f	202	1/1	0.89	0.11	49,49,49,49	0
54	MG	2A	3184	1/1	0.89	0.18	66,66,66,66	0
54	MG	1A	3168	1/1	0.89	0.26	63,63,63,63	0
54	MG	1g	203	1/1	0.89	0.18	69,69,69,69	0
54	MG	1a	1783	1/1	0.89	0.24	77,77,77,77	0
54	MG	1A	3838	1/1	0.89	0.16	68,68,68,68	0
54	MG	1A	3839	1/1	0.89	0.12	59,59,59,59	0
54	MG	1A	3586	1/1	0.89	0.18	61,61,61,61	0
54	MG	1A	3332	1/1	0.89	0.14	61,61,61,61	0
54	MG	1o	101	1/1	0.89	0.25	58,58,58,58	0
54	MG	17	106	1/1	0.89	0.19	61,61,61,61	0
54	MG	2A	3479	1/1	0.89	0.09	71,71,71,71	0
54	MG	1A	3243	1/1	0.89	0.09	47,47,47,47	0
54	MG	2A	3484	1/1	0.89	0.24	60,60,60,60	0
54	MG	1A	3848	1/1	0.89	0.13	50,50,50,50	0
54	MG	2A	3005	1/1	0.89	0.15	65,65,65,65	0
54	MG	1A	3137	1/1	0.89	0.10	53,53,53,53	0
54	MG	1A	3302	1/1	0.89	0.16	42,42,42,42	0
54	MG	1A	3406	1/1	0.89	0.14	47,47,47,47	0
54	MG	2a	3037	1/1	0.89	0.24	73,73,73,73	0
54	MG	2A	3223	1/1	0.89	0.36	56,56,56,56	0
54	MG	2A	3226	1/1	0.89	0.37	65,65,65,65	0
54	MG	1A	3210	1/1	0.89	0.38	77,77,77,77	0
54	MG	2A	3496	1/1	0.89	0.25	66,66,66,66	0
54	MG	2a	3046	1/1	0.89	0.36	75,75,75,75	0
54	MG	1A	3660	1/1	0.89	0.17	70,70,70,70	0
54	MG	2A	3027	1/1	0.89	0.14	59,59,59,59	0
54	MG	2A	3500	1/1	0.89	0.15	74,74,74,74	0
54	MG	2A	3239	1/1	0.89	0.29	61,61,61,61	0
54	MG	2A	3505	1/1	0.89	0.15	69,69,69,69	0
54	MG	1A	3215	1/1	0.89	0.18	78,78,78,78	0
54	MG	1A	3873	1/1	0.89	0.10	48,48,48,48	0
54	MG	2A	3511	1/1	0.89	0.13	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3674	1/1	0.89	0.16	69,69,69,69	0
54	MG	1a	1709	1/1	0.89	0.38	75,75,75,75	0
54	MG	1A	3603	1/1	0.89	0.15	67,67,67,67	0
54	MG	2a	3062	1/1	0.89	0.15	75,75,75,75	0
54	MG	1a	1621	1/1	0.89	0.21	65,65,65,65	0
54	MG	1a	1624	1/1	0.89	0.23	60,60,60,60	0
54	MG	1A	3890	1/1	0.89	0.10	68,68,68,68	0
54	MG	2A	3543	1/1	0.89	0.15	80,80,80,80	0
54	MG	1A	3894	1/1	0.89	0.13	53,53,53,53	0
54	MG	2a	3076	1/1	0.89	0.31	74,74,74,74	0
54	MG	1A	3607	1/1	0.89	0.14	52,52,52,52	0
54	MG	1A	4025	1/1	0.89	0.22	82,82,82,82	0
54	MG	1a	1825	1/1	0.89	0.15	72,72,72,72	0
54	MG	1A	3677	1/1	0.89	0.11	29,29,29,29	0
54	MG	1A	3435	1/1	0.89	0.24	54,54,54,54	0
54	MG	2A	3298	1/1	0.89	0.24	64,64,64,64	0
54	MG	1A	3903	1/1	0.89	0.11	59,59,59,59	0
54	MG	1B	215	1/1	0.89	0.11	50,50,50,50	0
54	MG	1A	3680	1/1	0.89	0.32	37,37,37,37	0
54	MG	2a	3098	1/1	0.89	0.12	66,66,66,66	0
54	MG	1A	3313	1/1	0.89	0.12	62,62,62,62	0
54	MG	1A	3920	1/1	0.89	0.09	45,45,45,45	0
54	MG	2A	3091	1/1	0.89	0.19	58,58,58,58	0
54	MG	2A	3604	1/1	0.89	0.15	41,41,41,41	0
54	MG	2A	3605	1/1	0.89	0.17	48,48,48,48	0
54	MG	2A	3098	1/1	0.89	0.25	62,62,62,62	0
54	MG	1a	1732	1/1	0.89	0.14	61,61,61,61	0
54	MG	2a	3115	1/1	0.89	0.15	71,71,71,71	0
54	MG	2A	3342	1/1	0.89	0.36	71,71,71,71	0
54	MG	1A	3687	1/1	0.89	0.14	60,60,60,60	0
54	MG	1A	3793	1/1	0.89	0.14	43,43,43,43	0
54	MG	1A	3565	1/1	0.89	0.13	47,47,47,47	0
54	MG	2A	3641	1/1	0.89	0.12	49,49,49,49	0
54	MG	2A	3644	1/1	0.89	0.11	79,79,79,79	0
54	MG	1A	3279	1/1	0.89	0.18	65,65,65,65	0
54	MG	2a	3140	1/1	0.89	0.15	77,77,77,77	0
54	MG	1A	3942	1/1	0.89	0.17	63,63,63,63	0
54	MG	2A	3114	1/1	0.89	0.11	54,54,54,54	0
54	MG	2A	3677	1/1	0.89	0.08	57,57,57,57	0
54	MG	2a	3149	1/1	0.89	0.11	54,54,54,54	0
54	MG	1a	1753	1/1	0.89	0.08	53,53,53,53	0
54	MG	2A	3682	1/1	0.89	0.11	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3161	1/1	0.89	0.09	68,68,68,68	0
54	MG	2A	3118	1/1	0.89	0.24	47,47,47,47	0
54	MG	1A	3625	1/1	0.89	0.32	39,39,39,39	0
54	MG	1a	1866	1/1	0.89	0.11	57,57,57,57	0
54	MG	2A	3378	1/1	0.89	0.11	65,65,65,65	0
54	MG	2A	3382	1/1	0.89	0.15	73,73,73,73	0
54	MG	1A	3805	1/1	0.89	0.21	63,63,63,63	0
54	MG	1F	317	1/1	0.89	0.16	52,52,52,52	0
54	MG	1a	1760	1/1	0.89	0.16	81,81,81,81	0
54	MG	2A	3402	1/1	0.89	0.14	71,71,71,71	0
54	MG	2A	3135	1/1	0.89	0.17	68,68,68,68	0
54	MG	2A	3138	1/1	0.89	0.11	49,49,49,49	0
54	MG	1A	3697	1/1	0.89	0.10	78,78,78,78	0
54	MG	2t	201	1/1	0.89	0.20	58,58,58,58	0
54	MG	1A	3961	1/1	0.89	0.11	57,57,57,57	0
54	MG	1A	3217	1/1	0.89	0.18	46,46,46,46	0
54	MG	1A	3039	1/1	0.89	0.35	69,69,69,69	0
54	MG	2A	3419	1/1	0.89	0.14	64,64,64,64	0
57	MPD	2A	3715	8/8	0.89	0.17	68,71,77,78	0
54	MG	1A	3639	1/1	0.89	0.12	66,66,66,66	0
54	MG	1A	3708	1/1	0.89	0.11	53,53,53,53	0
54	MG	2A	3352	1/1	0.90	0.17	57,57,57,57	0
54	MG	1A	3851	1/1	0.90	0.13	53,53,53,53	0
54	MG	1A	3448	1/1	0.90	0.13	44,44,44,44	0
54	MG	1A	3527	1/1	0.90	0.14	58,58,58,58	0
54	MG	1a	1823	1/1	0.90	0.24	74,74,74,74	0
54	MG	2A	3362	1/1	0.90	0.09	69,69,69,69	0
54	MG	1A	3858	1/1	0.90	0.13	42,42,42,42	0
54	MG	2A	3099	1/1	0.90	0.24	55,55,55,55	0
54	MG	2A	3372	1/1	0.90	0.10	57,57,57,57	0
54	MG	18	102	1/1	0.90	0.25	47,47,47,47	0
54	MG	1A	3289	1/1	0.90	0.14	57,57,57,57	0
54	MG	1a	1830	1/1	0.90	0.12	75,75,75,75	0
54	MG	2B	211	1/1	0.90	0.16	74,74,74,74	0
54	MG	1A	3635	1/1	0.90	0.10	24,24,24,24	0
54	MG	2A	3110	1/1	0.90	0.29	67,67,67,67	0
54	MG	1A	3991	1/1	0.90	0.15	46,46,46,46	0
54	MG	2A	3396	1/1	0.90	0.24	73,73,73,73	0
54	MG	2A	3397	1/1	0.90	0.13	51,51,51,51	0
54	MG	1A	3638	1/1	0.90	0.12	42,42,42,42	0
54	MG	2A	3399	1/1	0.90	0.18	67,67,67,67	0
54	MG	2A	3401	1/1	0.90	0.26	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1713	1/1	0.90	0.23	72,72,72,72	0
54	MG	1A	3995	1/1	0.90	0.08	89,89,89,89	0
54	MG	1a	1605	1/1	0.90	0.16	63,63,63,63	0
54	MG	1A	3369	1/1	0.90	0.11	47,47,47,47	0
54	MG	1A	3767	1/1	0.90	0.13	44,44,44,44	0
54	MG	2A	3413	1/1	0.90	0.22	86,86,86,86	0
54	MG	25	101	1/1	0.90	0.59	49,49,49,49	0
54	MG	28	102	1/1	0.90	0.25	68,68,68,68	0
54	MG	1A	3773	1/1	0.90	0.17	49,49,49,49	0
54	MG	2a	3003	1/1	0.90	0.42	77,77,77,77	0
54	MG	1A	3881	1/1	0.90	0.18	31,31,31,31	0
54	MG	2A	3128	1/1	0.90	0.18	77,77,77,77	0
54	MG	1A	3190	1/1	0.90	0.12	61,61,61,61	0
54	MG	1A	3889	1/1	0.90	0.08	25,25,25,25	0
54	MG	1A	4014	1/1	0.90	0.13	38,38,38,38	0
54	MG	2A	3144	1/1	0.90	0.23	58,58,58,58	0
54	MG	2A	3148	1/1	0.90	0.28	57,57,57,57	0
54	MG	2A	3433	1/1	0.90	0.16	64,64,64,64	0
54	MG	1A	3200	1/1	0.90	0.27	53,53,53,53	0
54	MG	1A	3892	1/1	0.90	0.14	53,53,53,53	0
54	MG	1a	1628	1/1	0.90	0.34	70,70,70,70	0
54	MG	2A	3443	1/1	0.90	0.23	60,60,60,60	0
54	MG	1A	3539	1/1	0.90	0.10	26,26,26,26	0
54	MG	1a	1740	1/1	0.90	0.19	58,58,58,58	0
54	MG	1A	3299	1/1	0.90	0.20	50,50,50,50	0
54	MG	2A	3164	1/1	0.90	0.29	56,56,56,56	0
54	MG	1A	3649	1/1	0.90	0.22	59,59,59,59	0
54	MG	2a	3040	1/1	0.90	0.11	84,84,84,84	0
54	MG	1A	3702	1/1	0.90	0.09	71,71,71,71	0
54	MG	2a	3042	1/1	0.90	0.13	66,66,66,66	0
54	MG	2A	3458	1/1	0.90	0.20	75,75,75,75	0
54	MG	2a	3044	1/1	0.90	0.29	80,80,80,80	0
54	MG	2A	3460	1/1	0.90	0.24	74,74,74,74	0
54	MG	2A	3461	1/1	0.90	0.09	71,71,71,71	0
54	MG	1a	1876	1/1	0.90	0.14	76,76,76,76	0
54	MG	1A	4027	1/1	0.90	0.15	69,69,69,69	0
54	MG	1A	3798	1/1	0.90	0.20	63,63,63,63	0
54	MG	1A	3283	1/1	0.90	0.12	41,41,41,41	0
54	MG	1A	3478	1/1	0.90	0.13	44,44,44,44	0
54	MG	1B	220	1/1	0.90	0.25	78,78,78,78	0
54	MG	1A	3912	1/1	0.90	0.09	20,20,20,20	0
54	MG	1a	1651	1/1	0.90	0.29	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1761	1/1	0.90	0.27	51,51,51,51	0
54	MG	1A	3916	1/1	0.90	0.10	35,35,35,35	0
54	MG	2A	3189	1/1	0.90	0.32	72,72,72,72	0
54	MG	1a	1764	1/1	0.90	0.28	77,77,77,77	0
54	MG	1A	3709	1/1	0.90	0.29	44,44,44,44	0
54	MG	1A	3711	1/1	0.90	0.11	55,55,55,55	0
54	MG	1A	3928	1/1	0.90	0.08	73,73,73,73	0
54	MG	1a	1772	1/1	0.90	0.17	62,62,62,62	0
54	MG	1n	102	1/1	0.90	0.29	71,71,71,71	0
54	MG	1A	3346	1/1	0.90	0.48	76,76,76,76	0
54	MG	1A	3716	1/1	0.90	0.27	45,45,45,45	0
54	MG	1A	3815	1/1	0.90	0.08	59,59,59,59	0
54	MG	1y	201	1/1	0.90	0.08	72,72,72,72	0
54	MG	2A	3210	1/1	0.90	0.13	59,59,59,59	0
54	MG	2A	3504	1/1	0.90	0.15	59,59,59,59	0
54	MG	1A	3440	1/1	0.90	0.09	28,28,28,28	0
54	MG	2a	3088	1/1	0.90	0.15	76,76,76,76	0
54	MG	1A	3818	1/1	0.90	0.14	33,33,33,33	0
54	MG	2A	3221	1/1	0.90	0.25	48,48,48,48	0
54	MG	1A	3441	1/1	0.90	0.11	28,28,28,28	0
54	MG	1F	318	1/1	0.90	0.12	67,67,67,67	0
54	MG	1a	1785	1/1	0.90	0.18	52,52,52,52	0
54	MG	1a	1669	1/1	0.90	0.41	68,68,68,68	0
54	MG	2A	3229	1/1	0.90	0.17	63,63,63,63	0
54	MG	2A	3527	1/1	0.90	0.08	65,65,65,65	0
54	MG	2A	3017	1/1	0.90	0.17	60,60,60,60	0
54	MG	2A	3023	1/1	0.90	0.17	62,62,62,62	0
54	MG	1G	201	1/1	0.90	0.07	79,79,79,79	0
54	MG	2A	3248	1/1	0.90	0.30	48,48,48,48	0
54	MG	1A	3832	1/1	0.90	0.15	66,66,66,66	0
54	MG	1A	3558	1/1	0.90	0.22	58,58,58,58	0
54	MG	2A	3028	1/1	0.90	0.14	44,44,44,44	0
54	MG	1A	3729	1/1	0.90	0.27	41,41,41,41	0
54	MG	1A	3663	1/1	0.90	0.08	49,49,49,49	0
54	MG	2A	3560	1/1	0.90	0.12	54,54,54,54	0
54	MG	1P	203	1/1	0.90	0.24	40,40,40,40	0
54	MG	2A	3037	1/1	0.90	0.25	74,74,74,74	0
54	MG	2A	3279	1/1	0.90	0.12	73,73,73,73	0
54	MG	1P	206	1/1	0.90	0.14	71,71,71,71	0
54	MG	1A	3060	1/1	0.90	0.11	49,49,49,49	0
54	MG	2A	3044	1/1	0.90	0.14	53,53,53,53	0
54	MG	2a	3153	1/1	0.90	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3599	1/1	0.90	0.14	39,39,39,39	0
54	MG	2a	3156	1/1	0.90	0.08	84,84,84,84	0
54	MG	2a	3157	1/1	0.90	0.21	69,69,69,69	0
54	MG	1A	3362	1/1	0.90	0.12	38,38,38,38	0
54	MG	1a	1683	1/1	0.90	0.22	67,67,67,67	0
54	MG	1A	3973	1/1	0.90	0.07	61,61,61,61	0
54	MG	2A	3606	1/1	0.90	0.12	60,60,60,60	0
54	MG	1A	3617	1/1	0.90	0.09	62,62,62,62	0
54	MG	2A	3056	1/1	0.90	0.23	60,60,60,60	0
54	MG	2A	3302	1/1	0.90	0.16	68,68,68,68	0
54	MG	2A	3304	1/1	0.90	0.32	69,69,69,69	0
54	MG	1a	1688	1/1	0.90	0.14	64,64,64,64	0
54	MG	2A	3637	1/1	0.90	0.09	82,82,82,82	0
54	MG	2a	3181	1/1	0.90	0.10	96,96,96,96	0
54	MG	2A	3062	1/1	0.90	0.15	60,60,60,60	0
54	MG	2A	3065	1/1	0.90	0.25	65,65,65,65	0
54	MG	1T	205	1/1	0.90	0.14	73,73,73,73	0
54	MG	1A	3740	1/1	0.90	0.13	70,70,70,70	0
54	MG	1A	3747	1/1	0.90	0.20	45,45,45,45	0
54	MG	2A	3335	1/1	0.90	0.08	39,39,39,39	0
54	MG	2A	3336	1/1	0.90	0.21	72,72,72,72	0
54	MG	2A	3077	1/1	0.90	0.10	59,59,59,59	0
54	MG	1A	3447	1/1	0.90	0.10	31,31,31,31	0
54	MG	2A	3684	1/1	0.90	0.10	67,67,67,67	0
54	MG	1l	104	1/1	0.90	0.13	55,55,55,55	0
54	MG	1a	1700	1/1	0.90	0.29	78,78,78,78	0
54	MG	1A	3311	1/1	0.91	0.15	59,59,59,59	0
54	MG	1A	3673	1/1	0.91	0.06	29,29,29,29	0
54	MG	1A	3442	1/1	0.91	0.14	27,27,27,27	0
54	MG	2A	3354	1/1	0.91	0.10	71,71,71,71	0
54	MG	1A	3602	1/1	0.91	0.24	58,58,58,58	0
54	MG	2A	3356	1/1	0.91	0.15	64,64,64,64	0
54	MG	1A	3758	1/1	0.91	0.16	63,63,63,63	0
54	MG	1a	1820	1/1	0.91	0.16	71,71,71,71	0
54	MG	2A	3693	1/1	0.91	0.13	80,80,80,80	0
54	MG	2A	3695	1/1	0.91	0.09	74,74,74,74	0
54	MG	2A	3704	1/1	0.91	0.08	49,49,49,49	0
54	MG	1a	1697	1/1	0.91	0.17	67,67,67,67	0
54	MG	1W	203	1/1	0.91	0.09	57,57,57,57	0
54	MG	1A	3053	1/1	0.91	0.24	44,44,44,44	0
54	MG	2A	3368	1/1	0.91	0.13	64,64,64,64	0
54	MG	1a	1701	1/1	0.91	0.22	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3860	1/1	0.91	0.10	66,66,66,66	0
54	MG	2A	3374	1/1	0.91	0.14	46,46,46,46	0
54	MG	1A	3125	1/1	0.91	0.23	55,55,55,55	0
54	MG	2A	3111	1/1	0.91	0.15	45,45,45,45	0
54	MG	1A	3987	1/1	0.91	0.11	50,50,50,50	0
54	MG	1a	1833	1/1	0.91	0.20	77,77,77,77	0
54	MG	2A	3386	1/1	0.91	0.09	57,57,57,57	0
54	MG	1A	3678	1/1	0.91	0.12	48,48,48,48	0
54	MG	15	105	1/1	0.91	0.22	36,36,36,36	0
54	MG	2B	216	1/1	0.91	0.07	84,84,84,84	0
54	MG	2B	217	1/1	0.91	0.06	75,75,75,75	0
54	MG	1a	1837	1/1	0.91	0.11	82,82,82,82	0
54	MG	1a	1838	1/1	0.91	0.19	72,72,72,72	0
54	MG	2E	303	1/1	0.91	0.10	32,32,32,32	0
54	MG	1a	1839	1/1	0.91	0.18	52,52,52,52	0
54	MG	1A	3990	1/1	0.91	0.07	22,22,22,22	0
54	MG	1A	3765	1/1	0.91	0.12	60,60,60,60	0
54	MG	1A	3192	1/1	0.91	0.09	67,67,67,67	0
54	MG	1a	1711	1/1	0.91	0.35	71,71,71,71	0
54	MG	1a	1847	1/1	0.91	0.31	57,57,57,57	0
54	MG	17	107	1/1	0.91	0.12	59,59,59,59	0
54	MG	2T	201	1/1	0.91	0.26	72,72,72,72	0
54	MG	2T	203	1/1	0.91	0.16	61,61,61,61	0
54	MG	1A	3994	1/1	0.91	0.25	43,43,43,43	0
54	MG	19	101	1/1	0.91	0.24	57,57,57,57	0
54	MG	1A	3386	1/1	0.91	0.10	42,42,42,42	0
54	MG	1a	1858	1/1	0.91	0.13	57,57,57,57	0
54	MG	2a	3001	1/1	0.91	0.12	46,46,46,46	0
54	MG	1A	3876	1/1	0.91	0.12	46,46,46,46	0
54	MG	1A	3681	1/1	0.91	0.16	71,71,71,71	0
54	MG	1A	3883	1/1	0.91	0.09	60,60,60,60	0
54	MG	1A	3774	1/1	0.91	0.14	54,54,54,54	0
54	MG	1A	3391	1/1	0.91	0.19	75,75,75,75	0
54	MG	1a	1607	1/1	0.91	0.08	73,73,73,73	0
54	MG	2A	3169	1/1	0.91	0.08	51,51,51,51	0
54	MG	1A	3285	1/1	0.91	0.18	66,66,66,66	0
54	MG	1A	4011	1/1	0.91	0.21	50,50,50,50	0
54	MG	2a	3023	1/1	0.91	0.16	74,74,74,74	0
54	MG	2A	3173	1/1	0.91	0.28	62,62,62,62	0
54	MG	1A	3620	1/1	0.91	0.07	39,39,39,39	0
54	MG	1a	1613	1/1	0.91	0.17	30,30,30,30	0
54	MG	1a	1730	1/1	0.91	0.24	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3329	1/1	0.91	0.06	40,40,40,40	0
54	MG	1A	3195	1/1	0.91	0.25	47,47,47,47	0
54	MG	2A	3183	1/1	0.91	0.20	60,60,60,60	0
54	MG	1b	301	1/1	0.91	0.13	84,84,84,84	0
54	MG	2a	3036	1/1	0.91	0.24	67,67,67,67	0
54	MG	2A	3456	1/1	0.91	0.12	74,74,74,74	0
54	MG	2a	3038	1/1	0.91	0.31	67,67,67,67	0
54	MG	1a	1741	1/1	0.91	0.12	77,77,77,77	0
54	MG	1a	1742	1/1	0.91	0.21	65,65,65,65	0
54	MG	1a	1743	1/1	0.91	0.11	63,63,63,63	0
54	MG	1A	4022	1/1	0.91	0.21	66,66,66,66	0
54	MG	1a	1745	1/1	0.91	0.11	68,68,68,68	0
54	MG	2A	3468	1/1	0.91	0.22	65,65,65,65	0
54	MG	1A	3469	1/1	0.91	0.12	64,64,64,64	0
54	MG	1A	3034	1/1	0.91	0.09	52,52,52,52	0
54	MG	1A	3254	1/1	0.91	0.09	72,72,72,72	0
54	MG	1A	3800	1/1	0.91	0.12	63,63,63,63	0
54	MG	1a	1629	1/1	0.91	0.29	72,72,72,72	0
54	MG	2A	3481	1/1	0.91	0.10	60,60,60,60	0
54	MG	1A	3337	1/1	0.91	0.40	68,68,68,68	0
54	MG	2A	3483	1/1	0.91	0.09	61,61,61,61	0
54	MG	1B	202	1/1	0.91	0.19	77,77,77,77	0
54	MG	2A	3207	1/1	0.91	0.33	65,65,65,65	0
54	MG	1A	3568	1/1	0.91	0.17	48,48,48,48	0
54	MG	1B	205	1/1	0.91	0.10	53,53,53,53	0
54	MG	1B	206	1/1	0.91	0.22	67,67,67,67	0
54	MG	1B	208	1/1	0.91	0.09	55,55,55,55	0
54	MG	2A	3216	1/1	0.91	0.20	71,71,71,71	0
54	MG	1u	101	1/1	0.91	0.13	76,76,76,76	0
54	MG	2A	3220	1/1	0.91	0.19	60,60,60,60	0
54	MG	2a	3068	1/1	0.91	0.33	68,68,68,68	0
54	MG	1B	209	1/1	0.91	0.13	61,61,61,61	0
54	MG	1A	3403	1/1	0.91	0.07	37,37,37,37	0
54	MG	2A	3224	1/1	0.91	0.13	74,74,74,74	0
54	MG	1B	211	1/1	0.91	0.09	64,64,64,64	0
54	MG	2a	3079	1/1	0.91	0.35	59,59,59,59	0
54	MG	1B	214	1/1	0.91	0.09	69,69,69,69	0
54	MG	2a	3082	1/1	0.91	0.17	70,70,70,70	0
54	MG	1A	3645	1/1	0.91	0.09	40,40,40,40	0
54	MG	1A	3340	1/1	0.91	0.08	48,48,48,48	0
54	MG	1A	3577	1/1	0.91	0.10	55,55,55,55	0
54	MG	2A	3236	1/1	0.91	0.09	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3257	1/1	0.91	0.31	45,45,45,45	0
54	MG	1A	3718	1/1	0.91	0.20	63,63,63,63	0
54	MG	2A	3241	1/1	0.91	0.17	70,70,70,70	0
54	MG	1A	3110	1/1	0.91	0.10	70,70,70,70	0
54	MG	2A	3518	1/1	0.91	0.14	67,67,67,67	0
54	MG	2A	3253	1/1	0.91	0.24	50,50,50,50	0
54	MG	2a	3100	1/1	0.91	0.13	83,83,83,83	0
54	MG	1A	3827	1/1	0.91	0.13	73,73,73,73	0
54	MG	2A	3255	1/1	0.91	0.29	61,61,61,61	0
54	MG	1B	228	1/1	0.91	0.19	71,71,71,71	0
54	MG	2A	3534	1/1	0.91	0.19	58,58,58,58	0
54	MG	2a	3109	1/1	0.91	0.29	75,75,75,75	0
54	MG	2A	3536	1/1	0.91	0.11	60,60,60,60	0
54	MG	1A	3943	1/1	0.91	0.09	51,51,51,51	0
54	MG	2a	3114	1/1	0.91	0.20	75,75,75,75	0
54	MG	2A	3546	1/1	0.91	0.09	73,73,73,73	0
54	MG	2A	3261	1/1	0.91	0.36	74,74,74,74	0
54	MG	1D	314	1/1	0.91	0.08	63,63,63,63	0
54	MG	1A	3201	1/1	0.91	0.29	62,62,62,62	0
54	MG	1A	3517	1/1	0.91	0.14	35,35,35,35	0
54	MG	1E	304	1/1	0.91	0.10	27,27,27,27	0
54	MG	2a	3123	1/1	0.91	0.11	79,79,79,79	0
54	MG	2A	3040	1/1	0.91	0.24	61,61,61,61	0
54	MG	1A	3955	1/1	0.91	0.10	62,62,62,62	0
54	MG	2A	3562	1/1	0.91	0.13	74,74,74,74	0
54	MG	2A	3563	1/1	0.91	0.09	52,52,52,52	0
54	MG	1F	314	1/1	0.91	0.38	51,51,51,51	0
54	MG	2A	3577	1/1	0.91	0.17	74,74,74,74	0
54	MG	1A	3523	1/1	0.91	0.11	42,42,42,42	0
54	MG	2A	3045	1/1	0.91	0.14	67,67,67,67	0
54	MG	1a	1797	1/1	0.91	0.26	68,68,68,68	0
54	MG	2A	3296	1/1	0.91	0.15	62,62,62,62	0
54	MG	2A	3047	1/1	0.91	0.12	68,68,68,68	0
54	MG	1A	3960	1/1	0.91	0.09	76,76,76,76	0
54	MG	1A	3133	1/1	0.91	0.24	37,37,37,37	0
54	MG	2A	3602	1/1	0.91	0.23	64,64,64,64	0
54	MG	1a	1800	1/1	0.91	0.23	66,66,66,66	0
54	MG	1a	1678	1/1	0.91	0.26	54,54,54,54	0
54	MG	1A	3962	1/1	0.91	0.13	65,65,65,65	0
54	MG	2A	3317	1/1	0.91	0.12	59,59,59,59	0
54	MG	2A	3318	1/1	0.91	0.14	42,42,42,42	0
54	MG	1a	1804	1/1	0.91	0.11	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3618	1/1	0.91	0.12	64,64,64,64	0
54	MG	1A	3595	1/1	0.91	0.15	66,66,66,66	0
54	MG	1A	3353	1/1	0.91	0.11	57,57,57,57	0
54	MG	2A	3331	1/1	0.91	0.16	76,76,76,76	0
54	MG	2A	3072	1/1	0.91	0.16	62,62,62,62	0
54	MG	1a	1807	1/1	0.91	0.08	73,73,73,73	0
54	MG	1A	3113	1/1	0.91	0.13	52,52,52,52	0
56	ZIT	2A	3713	52/52	0.91	0.19	43,67,78,85	0
54	MG	1A	3842	1/1	0.91	0.12	53,53,53,53	0
54	MG	2A	3658	1/1	0.91	0.10	52,52,52,52	0
54	MG	2A	3666	1/1	0.91	0.12	44,44,44,44	0
54	MG	2A	3668	1/1	0.91	0.16	69,69,69,69	0
54	MG	2A	3670	1/1	0.91	0.20	73,73,73,73	0
54	MG	1A	3739	1/1	0.91	0.17	46,46,46,46	0
54	MG	1A	3665	1/1	0.91	0.07	42,42,42,42	0
54	MG	1A	3753	1/1	0.92	0.11	58,58,58,58	0
54	MG	2A	3676	1/1	0.92	0.17	70,70,70,70	0
54	MG	1A	3643	1/1	0.92	0.13	62,62,62,62	0
54	MG	2A	3107	1/1	0.92	0.12	62,62,62,62	0
54	MG	1A	3266	1/1	0.92	0.36	71,71,71,71	0
54	MG	2A	3365	1/1	0.92	0.08	65,65,65,65	0
54	MG	1A	3270	1/1	0.92	0.16	63,63,63,63	0
54	MG	1A	3161	1/1	0.92	0.27	64,64,64,64	0
54	MG	1A	3277	1/1	0.92	0.26	35,35,35,35	0
54	MG	1A	3927	1/1	0.92	0.09	47,47,47,47	0
54	MG	1A	3545	1/1	0.92	0.13	64,64,64,64	0
54	MG	1F	310	1/1	0.92	0.23	59,59,59,59	0
54	MG	2A	3699	1/1	0.92	0.08	49,49,49,49	0
54	MG	2A	3701	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3930	1/1	0.92	0.13	48,48,48,48	0
54	MG	2A	3706	1/1	0.92	0.11	40,40,40,40	0
54	MG	1a	1832	1/1	0.92	0.11	68,68,68,68	0
54	MG	2A	3379	1/1	0.92	0.19	78,78,78,78	0
54	MG	2A	3710	1/1	0.92	0.24	64,64,64,64	0
54	MG	1A	3550	1/1	0.92	0.40	37,37,37,37	0
54	MG	1A	3199	1/1	0.92	0.31	51,51,51,51	0
54	MG	2A	3125	1/1	0.92	0.19	51,51,51,51	0
54	MG	1A	3552	1/1	0.92	0.19	63,63,63,63	0
54	MG	2A	3393	1/1	0.92	0.12	56,56,56,56	0
54	MG	2A	3394	1/1	0.92	0.09	51,51,51,51	0
54	MG	1A	3281	1/1	0.92	0.05	78,78,78,78	0
54	MG	2A	3129	1/1	0.92	0.36	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2B	210	1/1	0.92	0.11	71,71,71,71	0
54	MG	1G	202	1/1	0.92	0.07	69,69,69,69	0
54	MG	2A	3133	1/1	0.92	0.20	62,62,62,62	0
54	MG	1A	3780	1/1	0.92	0.19	61,61,61,61	0
54	MG	1A	3134	1/1	0.92	0.06	57,57,57,57	0
54	MG	2A	3140	1/1	0.92	0.33	61,61,61,61	0
54	MG	2A	3405	1/1	0.92	0.24	57,57,57,57	0
54	MG	2D	304	1/1	0.92	0.34	43,43,43,43	0
54	MG	1N	201	1/1	0.92	0.20	49,49,49,49	0
54	MG	2A	3407	1/1	0.92	0.12	50,50,50,50	0
54	MG	2E	301	1/1	0.92	0.22	49,49,49,49	0
54	MG	1A	3046	1/1	0.92	0.17	33,33,33,33	0
54	MG	1A	3173	1/1	0.92	0.14	52,52,52,52	0
54	MG	2A	3411	1/1	0.92	0.10	40,40,40,40	0
54	MG	1A	3791	1/1	0.92	0.15	48,48,48,48	0
54	MG	1A	3959	1/1	0.92	0.10	66,66,66,66	0
54	MG	2A	3158	1/1	0.92	0.14	46,46,46,46	0
54	MG	2A	3416	1/1	0.92	0.28	74,74,74,74	0
54	MG	1A	3175	1/1	0.92	0.14	63,63,63,63	0
54	MG	2R	201	1/1	0.92	0.12	53,53,53,53	0
54	MG	1A	3666	1/1	0.92	0.13	54,54,54,54	0
54	MG	1A	3178	1/1	0.92	0.17	42,42,42,42	0
54	MG	2Y	201	1/1	0.92	0.20	69,69,69,69	0
54	MG	1A	3670	1/1	0.92	0.40	55,55,55,55	0
54	MG	1A	3569	1/1	0.92	0.08	34,34,34,34	0
54	MG	1A	3965	1/1	0.92	0.14	57,57,57,57	0
54	MG	1Z	301	1/1	0.92	0.12	68,68,68,68	0
54	MG	2A	3437	1/1	0.92	0.10	56,56,56,56	0
54	MG	1A	3967	1/1	0.92	0.11	76,76,76,76	0
54	MG	1a	1868	1/1	0.92	0.24	68,68,68,68	0
54	MG	2a	3006	1/1	0.92	0.08	79,79,79,79	0
54	MG	2a	3007	1/1	0.92	0.47	72,72,72,72	0
54	MG	1A	3290	1/1	0.92	0.13	52,52,52,52	0
54	MG	2A	3442	1/1	0.92	0.10	58,58,58,58	0
54	MG	10	104	1/1	0.92	0.08	58,58,58,58	0
54	MG	1A	3291	1/1	0.92	0.14	43,43,43,43	0
54	MG	1A	3216	1/1	0.92	0.18	62,62,62,62	0
54	MG	1A	3370	1/1	0.92	0.10	51,51,51,51	0
54	MG	15	103	1/1	0.92	0.34	46,46,46,46	0
54	MG	1A	3582	1/1	0.92	0.18	62,62,62,62	0
54	MG	2a	3024	1/1	0.92	0.18	66,66,66,66	0
54	MG	2a	3025	1/1	0.92	0.26	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3811	1/1	0.92	0.09	39,39,39,39	0
54	MG	1A	3812	1/1	0.92	0.35	40,40,40,40	0
54	MG	1a	1880	1/1	0.92	0.16	67,67,67,67	0
54	MG	2A	3459	1/1	0.92	0.09	63,63,63,63	0
54	MG	2a	3031	1/1	0.92	0.12	46,46,46,46	0
54	MG	2A	3188	1/1	0.92	0.18	48,48,48,48	0
54	MG	17	102	1/1	0.92	0.17	55,55,55,55	0
54	MG	2A	3190	1/1	0.92	0.20	67,67,67,67	0
54	MG	2A	3192	1/1	0.92	0.08	60,60,60,60	0
54	MG	1A	3813	1/1	0.92	0.11	71,71,71,71	0
54	MG	1a	1731	1/1	0.92	0.19	60,60,60,60	0
54	MG	1A	3470	1/1	0.92	0.20	74,74,74,74	0
54	MG	1a	1733	1/1	0.92	0.14	56,56,56,56	0
54	MG	1a	1737	1/1	0.92	0.09	55,55,55,55	0
54	MG	1A	3139	1/1	0.92	0.27	51,51,51,51	0
54	MG	1A	3472	1/1	0.92	0.11	50,50,50,50	0
54	MG	1A	3985	1/1	0.92	0.11	54,54,54,54	0
54	MG	1A	3683	1/1	0.92	0.17	64,64,64,64	0
54	MG	1A	3588	1/1	0.92	0.22	51,51,51,51	0
54	MG	1A	3686	1/1	0.92	0.10	50,50,50,50	0
54	MG	1a	1746	1/1	0.92	0.18	43,43,43,43	0
54	MG	1A	3589	1/1	0.92	0.09	23,23,23,23	0
54	MG	2a	3050	1/1	0.92	0.28	64,64,64,64	0
54	MG	2A	3490	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3691	1/1	0.92	0.06	55,55,55,55	0
54	MG	2A	3218	1/1	0.92	0.12	65,65,65,65	0
54	MG	1a	1606	1/1	0.92	0.20	58,58,58,58	0
54	MG	1A	3692	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3014	1/1	0.92	0.28	68,68,68,68	0
54	MG	1A	3123	1/1	0.92	0.12	38,38,38,38	0
54	MG	1A	3695	1/1	0.92	0.11	65,65,65,65	0
54	MG	2A	3225	1/1	0.92	0.19	66,66,66,66	0
54	MG	1A	3999	1/1	0.92	0.10	58,58,58,58	0
54	MG	2A	3002	1/1	0.92	0.08	58,58,58,58	0
54	MG	2A	3503	1/1	0.92	0.27	49,49,49,49	0
54	MG	2A	3003	1/1	0.92	0.10	65,65,65,65	0
54	MG	1A	3594	1/1	0.92	0.17	70,70,70,70	0
54	MG	1A	3388	1/1	0.92	0.09	47,47,47,47	0
54	MG	2a	3073	1/1	0.92	0.10	68,68,68,68	0
54	MG	2A	3507	1/1	0.92	0.24	68,68,68,68	0
54	MG	2A	3508	1/1	0.92	0.17	66,66,66,66	0
54	MG	1A	4006	1/1	0.92	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
54	MG	1a	1620	1/1	0.92	0.09	65,65,65,65	0
54	MG	1A	3487	1/1	0.92	0.10	49,49,49,49	0
54	MG	2a	3081	1/1	0.92	0.30	63,63,63,63	0
54	MG	2A	3019	1/1	0.92	0.23	52,52,52,52	0
54	MG	1A	3488	1/1	0.92	0.13	57,57,57,57	0
54	MG	1A	3241	1/1	0.92	0.22	63,63,63,63	0
54	MG	1A	3100	1/1	0.92	0.19	57,57,57,57	0
54	MG	2A	3525	1/1	0.92	0.09	53,53,53,53	0
54	MG	1A	4013	1/1	0.92	0.07	36,36,36,36	0
54	MG	2A	3257	1/1	0.92	0.18	55,55,55,55	0
54	MG	1A	3496	1/1	0.92	0.13	55,55,55,55	0
54	MG	2A	3533	1/1	0.92	0.07	88,88,88,88	0
54	MG	1a	1776	1/1	0.92	0.13	73,73,73,73	0
54	MG	1A	4015	1/1	0.92	0.08	28,28,28,28	0
54	MG	2A	3538	1/1	0.92	0.12	44,44,44,44	0
54	MG	1A	4017	1/1	0.92	0.17	71,71,71,71	0
54	MG	1A	4018	1/1	0.92	0.21	63,63,63,63	0
54	MG	1a	1637	1/1	0.92	0.10	48,48,48,48	0
54	MG	1A	3251	1/1	0.92	0.16	51,51,51,51	0
54	MG	1A	3710	1/1	0.92	0.21	39,39,39,39	0
54	MG	1a	1786	1/1	0.92	0.23	63,63,63,63	0
54	MG	1A	3504	1/1	0.92	0.11	33,33,33,33	0
54	MG	1A	3712	1/1	0.92	0.22	58,58,58,58	0
54	MG	1a	1790	1/1	0.92	0.07	76,76,76,76	0
54	MG	2A	3048	1/1	0.92	0.43	76,76,76,76	0
54	MG	2A	3295	1/1	0.92	0.10	34,34,34,34	0
54	MG	1A	3506	1/1	0.92	0.12	40,40,40,40	0
54	MG	1A	3075	1/1	0.92	0.07	38,38,38,38	0
54	MG	1A	3510	1/1	0.92	0.11	50,50,50,50	0
54	MG	1A	3108	1/1	0.92	0.10	47,47,47,47	0
54	MG	2A	3057	1/1	0.92	0.23	70,70,70,70	0
54	MG	2a	3128	1/1	0.92	0.12	79,79,79,79	0
54	MG	2a	3133	1/1	0.92	0.06	80,80,80,80	0
54	MG	2A	3303	1/1	0.92	0.13	69,69,69,69	0
54	MG	2A	3596	1/1	0.92	0.09	37,37,37,37	0
54	MG	1A	3720	1/1	0.92	0.08	50,50,50,50	0
54	MG	1A	3521	1/1	0.92	0.08	69,69,69,69	0
54	MG	2A	3312	1/1	0.92	0.10	46,46,46,46	0
54	MG	1A	3879	1/1	0.92	0.07	31,31,31,31	0
54	MG	1a	1658	1/1	0.92	0.10	81,81,81,81	0
54	MG	1A	3314	1/1	0.92	0.12	47,47,47,47	0
54	MG	2A	3323	1/1	0.92	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
54	MG	1A	3622	1/1	0.92	0.10	52,52,52,52	0
54	MG	2A	3608	1/1	0.92	0.11	65,65,65,65	0
54	MG	2A	3611	1/1	0.92	0.16	64,64,64,64	0
54	MG	1A	3624	1/1	0.92	0.16	38,38,38,38	0
54	MG	1A	3012	1/1	0.92	0.17	40,40,40,40	0
54	MG	2A	3081	1/1	0.92	0.62	52,52,52,52	0
54	MG	1A	3160	1/1	0.92	0.32	62,62,62,62	0
54	MG	1A	3321	1/1	0.92	0.12	66,66,66,66	0
54	MG	1a	1667	1/1	0.92	0.07	78,78,78,78	0
54	MG	2A	3638	1/1	0.92	0.10	49,49,49,49	0
54	MG	2a	3179	1/1	0.92	0.14	81,81,81,81	0
54	MG	2A	3337	1/1	0.92	0.11	37,37,37,37	0
54	MG	1A	3633	1/1	0.92	0.17	65,65,65,65	0
54	MG	2A	3643	1/1	0.92	0.07	31,31,31,31	0
54	MG	1B	217	1/1	0.92	0.07	47,47,47,47	0
54	MG	2f	201	1/1	0.92	0.17	57,57,57,57	0
54	MG	2A	3646	1/1	0.92	0.09	78,78,78,78	0
54	MG	1A	3324	1/1	0.92	0.10	58,58,58,58	0
54	MG	2A	3657	1/1	0.92	0.09	62,62,62,62	0
54	MG	1A	3262	1/1	0.92	0.30	55,55,55,55	0
54	MG	2A	3092	1/1	0.92	0.12	74,74,74,74	0
54	MG	1A	3409	1/1	0.92	0.15	42,42,42,42	0
54	MG	2A	3669	1/1	0.92	0.22	74,74,74,74	0
54	MG	1A	3427	1/1	0.92	0.08	33,33,33,33	0
54	MG	1A	3908	1/1	0.92	0.21	73,73,73,73	0
54	MG	2A	3672	1/1	0.92	0.11	59,59,59,59	0
54	MG	2A	3674	1/1	0.92	0.13	46,46,46,46	0
54	MG	1A	3700	1/1	0.93	0.09	46,46,46,46	0
54	MG	2A	3122	1/1	0.93	0.34	49,49,49,49	0
54	MG	2A	3385	1/1	0.93	0.20	64,64,64,64	0
54	MG	1A	3820	1/1	0.93	0.13	41,41,41,41	0
54	MG	2A	3694	1/1	0.93	0.11	63,63,63,63	0
54	MG	1P	207	1/1	0.93	0.11	64,64,64,64	0
54	MG	2A	3126	1/1	0.93	0.22	67,67,67,67	0
54	MG	1a	1835	1/1	0.93	0.15	63,63,63,63	0
54	MG	1a	1694	1/1	0.93	0.22	75,75,75,75	0
54	MG	1a	1695	1/1	0.93	0.07	82,82,82,82	0
54	MG	1R	203	1/1	0.93	0.21	66,66,66,66	0
54	MG	1A	3238	1/1	0.93	0.27	64,64,64,64	0
54	MG	2A	3134	1/1	0.93	0.09	55,55,55,55	0
54	MG	1A	3091	1/1	0.93	0.09	48,48,48,48	0
54	MG	1T	201	1/1	0.93	0.06	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3403	1/1	0.93	0.19	56,56,56,56	0
54	MG	1A	3619	1/1	0.93	0.09	41,41,41,41	0
54	MG	1A	3117	1/1	0.93	0.26	40,40,40,40	0
54	MG	1a	1845	1/1	0.93	0.24	66,66,66,66	0
54	MG	1a	1846	1/1	0.93	0.19	67,67,67,67	0
54	MG	1A	3312	1/1	0.93	0.21	40,40,40,40	0
54	MG	1U	201	1/1	0.93	0.20	44,44,44,44	0
54	MG	2A	3155	1/1	0.93	0.10	73,73,73,73	0
54	MG	2A	3156	1/1	0.93	0.27	48,48,48,48	0
54	MG	1V	203	1/1	0.93	0.12	61,61,61,61	0
54	MG	2A	3159	1/1	0.93	0.16	71,71,71,71	0
54	MG	1A	3247	1/1	0.93	0.12	47,47,47,47	0
54	MG	1W	204	1/1	0.93	0.12	49,49,49,49	0
54	MG	1a	1854	1/1	0.93	0.10	58,58,58,58	0
54	MG	2D	306	1/1	0.93	0.17	55,55,55,55	0
54	MG	1Y	201	1/1	0.93	0.16	68,68,68,68	0
54	MG	2A	3427	1/1	0.93	0.09	66,66,66,66	0
54	MG	2A	3428	1/1	0.93	0.08	61,61,61,61	0
54	MG	1A	3249	1/1	0.93	0.08	62,62,62,62	0
54	MG	1A	3097	1/1	0.93	0.09	54,54,54,54	0
54	MG	1A	3253	1/1	0.93	0.07	52,52,52,52	0
54	MG	2A	3432	1/1	0.93	0.07	69,69,69,69	0
54	MG	1A	3841	1/1	0.93	0.08	51,51,51,51	0
54	MG	2A	3435	1/1	0.93	0.21	66,66,66,66	0
54	MG	1A	3412	1/1	0.93	0.07	34,34,34,34	0
54	MG	1A	3632	1/1	0.93	0.12	33,33,33,33	0
54	MG	1A	3844	1/1	0.93	0.13	36,36,36,36	0
54	MG	15	101	1/1	0.93	0.17	41,41,41,41	0
54	MG	15	102	1/1	0.93	0.29	33,33,33,33	0
54	MG	2W	202	1/1	0.93	0.28	55,55,55,55	0
54	MG	1A	3532	1/1	0.93	0.12	55,55,55,55	0
54	MG	1A	3413	1/1	0.93	0.08	37,37,37,37	0
54	MG	1A	3850	1/1	0.93	0.19	54,54,54,54	0
54	MG	2A	3447	1/1	0.93	0.10	57,57,57,57	0
54	MG	15	107	1/1	0.93	0.08	51,51,51,51	0
54	MG	1A	3721	1/1	0.93	0.09	61,61,61,61	0
54	MG	1A	3853	1/1	0.93	0.26	50,50,50,50	0
54	MG	1a	1881	1/1	0.93	0.08	60,60,60,60	0
54	MG	2a	3004	1/1	0.93	0.09	59,59,59,59	0
54	MG	2A	3454	1/1	0.93	0.14	77,77,77,77	0
54	MG	2A	3455	1/1	0.93	0.08	35,35,35,35	0
54	MG	1A	3997	1/1	0.93	0.17	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3009	1/1	0.93	0.14	59,59,59,59	0
54	MG	1A	3124	1/1	0.93	0.15	39,39,39,39	0
54	MG	2a	3012	1/1	0.93	0.25	67,67,67,67	0
54	MG	2a	3013	1/1	0.93	0.18	61,61,61,61	0
54	MG	2a	3015	1/1	0.93	0.36	64,64,64,64	0
54	MG	2A	3191	1/1	0.93	0.40	74,74,74,74	0
54	MG	1A	3429	1/1	0.93	0.17	54,54,54,54	0
54	MG	1A	3857	1/1	0.93	0.16	40,40,40,40	0
54	MG	1A	3323	1/1	0.93	0.17	67,67,67,67	0
54	MG	1e	203	1/1	0.93	0.09	66,66,66,66	0
54	MG	2A	3467	1/1	0.93	0.11	43,43,43,43	0
54	MG	2A	3201	1/1	0.93	0.29	74,74,74,74	0
54	MG	1A	4004	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	3067	1/1	0.93	0.22	41,41,41,41	0
54	MG	2A	3472	1/1	0.93	0.11	65,65,65,65	0
54	MG	1A	3157	1/1	0.93	0.36	37,37,37,37	0
54	MG	1A	3439	1/1	0.93	0.10	49,49,49,49	0
54	MG	1A	3865	1/1	0.93	0.13	52,52,52,52	0
54	MG	1h	202	1/1	0.93	0.19	64,64,64,64	0
54	MG	1A	4010	1/1	0.93	0.13	66,66,66,66	0
54	MG	1A	3044	1/1	0.93	0.12	22,22,22,22	0
54	MG	1A	3867	1/1	0.93	0.10	47,47,47,47	0
54	MG	2A	3212	1/1	0.93	0.13	53,53,53,53	0
54	MG	2A	3213	1/1	0.93	0.21	72,72,72,72	0
54	MG	1A	3106	1/1	0.93	0.17	41,41,41,41	0
54	MG	1A	3164	1/1	0.93	0.07	38,38,38,38	0
54	MG	1A	4016	1/1	0.93	0.07	48,48,48,48	0
54	MG	1A	3741	1/1	0.93	0.12	36,36,36,36	0
54	MG	1a	1754	1/1	0.93	0.13	65,65,65,65	0
54	MG	1A	3334	1/1	0.93	0.08	33,33,33,33	0
54	MG	1A	3748	1/1	0.93	0.10	55,55,55,55	0
54	MG	1A	3065	1/1	0.93	0.10	69,69,69,69	0
54	MG	1A	3653	1/1	0.93	0.28	33,33,33,33	0
54	MG	1A	3271	1/1	0.93	0.10	60,60,60,60	0
54	MG	2a	3048	1/1	0.93	0.23	56,56,56,56	0
54	MG	1a	1762	1/1	0.93	0.07	63,63,63,63	0
54	MG	1a	1625	1/1	0.93	0.26	56,56,56,56	0
54	MG	1A	3085	1/1	0.93	0.39	47,47,47,47	0
54	MG	2A	3231	1/1	0.93	0.11	67,67,67,67	0
54	MG	1a	1627	1/1	0.93	0.10	56,56,56,56	0
54	MG	1A	3453	1/1	0.93	0.07	36,36,36,36	0
54	MG	2A	3238	1/1	0.93	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3018	1/1	0.93	0.30	52,52,52,52	0
54	MG	1A	3206	1/1	0.93	0.25	54,54,54,54	0
54	MG	1a	1771	1/1	0.93	0.15	82,82,82,82	0
54	MG	2A	3243	1/1	0.93	0.13	63,63,63,63	0
54	MG	2A	3513	1/1	0.93	0.12	67,67,67,67	0
54	MG	1A	3278	1/1	0.93	0.38	47,47,47,47	0
54	MG	2A	3516	1/1	0.93	0.14	75,75,75,75	0
54	MG	2A	3249	1/1	0.93	0.15	48,48,48,48	0
54	MG	1A	3086	1/1	0.93	0.50	49,49,49,49	0
54	MG	1A	3211	1/1	0.93	0.38	46,46,46,46	0
54	MG	1B	204	1/1	0.93	0.08	51,51,51,51	0
54	MG	2A	3256	1/1	0.93	0.29	66,66,66,66	0
54	MG	1a	1636	1/1	0.93	0.33	67,67,67,67	0
54	MG	2A	3033	1/1	0.93	0.29	57,57,57,57	0
54	MG	1a	1778	1/1	0.93	0.12	72,72,72,72	0
54	MG	1A	3465	1/1	0.93	0.09	52,52,52,52	0
54	MG	1A	3899	1/1	0.93	0.10	58,58,58,58	0
54	MG	2A	3265	1/1	0.93	0.16	60,60,60,60	0
54	MG	2a	3083	1/1	0.93	0.10	71,71,71,71	0
54	MG	1a	1781	1/1	0.93	0.33	63,63,63,63	0
54	MG	1a	1639	1/1	0.93	0.30	82,82,82,82	0
54	MG	1A	3578	1/1	0.93	0.10	39,39,39,39	0
54	MG	2A	3278	1/1	0.93	0.09	56,56,56,56	0
54	MG	1A	3672	1/1	0.93	0.06	45,45,45,45	0
54	MG	1A	3213	1/1	0.93	0.14	32,32,32,32	0
54	MG	1a	1787	1/1	0.93	0.08	71,71,71,71	0
54	MG	2A	3289	1/1	0.93	0.09	42,42,42,42	0
54	MG	1a	1645	1/1	0.93	0.19	53,53,53,53	0
54	MG	1A	3777	1/1	0.93	0.07	53,53,53,53	0
54	MG	1A	3354	1/1	0.93	0.08	27,27,27,27	0
54	MG	1A	3913	1/1	0.93	0.11	26,26,26,26	0
54	MG	1A	3111	1/1	0.93	0.37	33,33,33,33	0
54	MG	2A	3582	1/1	0.93	0.10	64,64,64,64	0
54	MG	1B	219	1/1	0.93	0.20	43,43,43,43	0
54	MG	2A	3586	1/1	0.93	0.08	79,79,79,79	0
54	MG	1A	3584	1/1	0.93	0.21	62,62,62,62	0
54	MG	1A	3144	1/1	0.93	0.09	40,40,40,40	0
54	MG	1A	3042	1/1	0.93	0.12	60,60,60,60	0
54	MG	2A	3064	1/1	0.93	0.19	62,62,62,62	0
54	MG	1A	3219	1/1	0.93	0.37	44,44,44,44	0
54	MG	2A	3067	1/1	0.93	0.12	51,51,51,51	0
54	MG	2A	3069	1/1	0.93	0.20	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3373	1/1	0.93	0.13	54,54,54,54	0
54	MG	2a	3120	1/1	0.93	0.10	77,77,77,77	0
54	MG	2A	3071	1/1	0.93	0.24	53,53,53,53	0
54	MG	1A	3483	1/1	0.93	0.11	27,27,27,27	0
54	MG	1A	3484	1/1	0.93	0.15	58,58,58,58	0
54	MG	1a	1802	1/1	0.93	0.12	58,58,58,58	0
54	MG	2a	3132	1/1	0.93	0.11	75,75,75,75	0
54	MG	1B	229	1/1	0.93	0.16	60,60,60,60	0
54	MG	2A	3079	1/1	0.93	0.41	67,67,67,67	0
54	MG	2a	3137	1/1	0.93	0.07	46,46,46,46	0
54	MG	1A	3934	1/1	0.93	0.11	42,42,42,42	0
54	MG	1A	3936	1/1	0.93	0.13	64,64,64,64	0
54	MG	2A	3616	1/1	0.93	0.08	59,59,59,59	0
54	MG	2a	3144	1/1	0.93	0.10	64,64,64,64	0
54	MG	1A	3374	1/1	0.93	0.09	56,56,56,56	0
54	MG	2A	3627	1/1	0.93	0.10	88,88,88,88	0
54	MG	2a	3152	1/1	0.93	0.09	79,79,79,79	0
54	MG	1A	3221	1/1	0.93	0.27	52,52,52,52	0
54	MG	1A	3223	1/1	0.93	0.56	44,44,44,44	0
54	MG	2A	3339	1/1	0.93	0.08	36,36,36,36	0
54	MG	1A	3804	1/1	0.93	0.17	60,60,60,60	0
54	MG	2A	3341	1/1	0.93	0.12	77,77,77,77	0
54	MG	1a	1672	1/1	0.93	0.10	62,62,62,62	0
54	MG	1E	308	1/1	0.93	0.12	63,63,63,63	0
54	MG	1A	3950	1/1	0.93	0.06	45,45,45,45	0
54	MG	1A	3688	1/1	0.93	0.25	41,41,41,41	0
54	MG	2A	3648	1/1	0.93	0.07	71,71,71,71	0
54	MG	2A	3651	1/1	0.93	0.08	59,59,59,59	0
54	MG	1a	1677	1/1	0.93	0.17	58,58,58,58	0
54	MG	1A	3806	1/1	0.93	0.06	77,77,77,77	0
54	MG	1A	3293	1/1	0.93	0.22	50,50,50,50	0
54	MG	2A	3659	1/1	0.93	0.13	74,74,74,74	0
54	MG	2A	3105	1/1	0.93	0.12	58,58,58,58	0
54	MG	2a	3182	1/1	0.93	0.08	75,75,75,75	0
54	MG	1A	3227	1/1	0.93	0.17	61,61,61,61	0
54	MG	1A	3500	1/1	0.93	0.08	24,24,24,24	0
54	MG	1A	3501	1/1	0.93	0.08	36,36,36,36	0
54	MG	2A	3109	1/1	0.93	0.22	67,67,67,67	0
54	MG	1a	1824	1/1	0.93	0.20	63,63,63,63	0
54	MG	1A	3232	1/1	0.93	0.42	47,47,47,47	0
56	ZIT	1A	4033	52/52	0.93	0.13	35,56,72,82	0
54	MG	1a	1826	1/1	0.93	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3234	1/1	0.93	0.15	39,39,39,39	0
54	MG	2A	3373	1/1	0.93	0.07	49,49,49,49	0
54	MG	2A	3678	1/1	0.93	0.08	65,65,65,65	0
54	MG	1a	1828	1/1	0.93	0.10	71,71,71,71	0
54	MG	1A	3182	1/1	0.93	0.20	42,42,42,42	0
54	MG	1A	3816	1/1	0.93	0.26	49,49,49,49	0
54	MG	1A	3146	1/1	0.93	0.08	34,34,34,34	0
59	ZN	24	501	1/1	0.93	0.16	146,146,146,146	0
54	MG	1A	3885	1/1	0.94	0.14	43,43,43,43	0
54	MG	1B	207	1/1	0.94	0.34	65,65,65,65	0
54	MG	1a	1648	1/1	0.94	0.26	61,61,61,61	0
54	MG	1a	1649	1/1	0.94	0.19	48,48,48,48	0
54	MG	1A	3529	1/1	0.94	0.08	30,30,30,30	0
54	MG	1A	3421	1/1	0.94	0.16	43,43,43,43	0
54	MG	2A	3363	1/1	0.94	0.12	66,66,66,66	0
54	MG	1A	3228	1/1	0.94	0.21	36,36,36,36	0
54	MG	2A	3366	1/1	0.94	0.10	38,38,38,38	0
54	MG	2A	3683	1/1	0.94	0.15	61,61,61,61	0
54	MG	1A	3891	1/1	0.94	0.07	38,38,38,38	0
54	MG	2A	3685	1/1	0.94	0.14	57,57,57,57	0
54	MG	1A	3333	1/1	0.94	0.12	48,48,48,48	0
54	MG	2A	3687	1/1	0.94	0.09	62,62,62,62	0
54	MG	2A	3370	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	3114	1/1	0.94	0.28	45,45,45,45	0
54	MG	1A	3432	1/1	0.94	0.18	71,71,71,71	0
54	MG	1a	1815	1/1	0.94	0.19	70,70,70,70	0
54	MG	1A	3233	1/1	0.94	0.24	42,42,42,42	0
54	MG	1a	1817	1/1	0.94	0.10	61,61,61,61	0
54	MG	1a	1818	1/1	0.94	0.12	72,72,72,72	0
54	MG	1a	1661	1/1	0.94	0.30	68,68,68,68	0
54	MG	2A	3702	1/1	0.94	0.14	69,69,69,69	0
54	MG	1A	3196	1/1	0.94	0.10	57,57,57,57	0
54	MG	2A	3115	1/1	0.94	0.31	57,57,57,57	0
54	MG	2A	3383	1/1	0.94	0.18	55,55,55,55	0
54	MG	2A	3384	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3339	1/1	0.94	0.11	53,53,53,53	0
54	MG	1a	1664	1/1	0.94	0.11	67,67,67,67	0
54	MG	1A	3197	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3391	1/1	0.94	0.10	41,41,41,41	0
54	MG	1A	3547	1/1	0.94	0.09	62,62,62,62	0
54	MG	1A	3288	1/1	0.94	0.25	49,49,49,49	0
54	MG	1A	3655	1/1	0.94	0.19	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3769	1/1	0.94	0.08	50,50,50,50	0
54	MG	1A	3343	1/1	0.94	0.13	33,33,33,33	0
54	MG	1A	3056	1/1	0.94	0.09	51,51,51,51	0
54	MG	1D	312	1/1	0.94	0.16	30,30,30,30	0
54	MG	1A	3918	1/1	0.94	0.11	25,25,25,25	0
54	MG	1A	3919	1/1	0.94	0.12	26,26,26,26	0
54	MG	1A	3775	1/1	0.94	0.12	50,50,50,50	0
54	MG	1A	3923	1/1	0.94	0.34	46,46,46,46	0
54	MG	1A	3776	1/1	0.94	0.13	65,65,65,65	0
54	MG	2D	303	1/1	0.94	0.42	48,48,48,48	0
54	MG	1A	3658	1/1	0.94	0.12	58,58,58,58	0
54	MG	1E	309	1/1	0.94	0.10	32,32,32,32	0
54	MG	1F	305	1/1	0.94	0.12	43,43,43,43	0
54	MG	2A	3145	1/1	0.94	0.09	48,48,48,48	0
54	MG	1A	3555	1/1	0.94	0.09	61,61,61,61	0
54	MG	1A	3781	1/1	0.94	0.07	32,32,32,32	0
54	MG	1A	3084	1/1	0.94	0.34	44,44,44,44	0
54	MG	2F	301	1/1	0.94	0.26	50,50,50,50	0
54	MG	1F	316	1/1	0.94	0.13	63,63,63,63	0
54	MG	1a	1686	1/1	0.94	0.17	65,65,65,65	0
54	MG	1A	3349	1/1	0.94	0.12	40,40,40,40	0
54	MG	1A	3789	1/1	0.94	0.15	44,44,44,44	0
54	MG	1A	3170	1/1	0.94	0.15	39,39,39,39	0
54	MG	1a	1691	1/1	0.94	0.16	45,45,45,45	0
54	MG	2Q	202	1/1	0.94	0.08	65,65,65,65	0
54	MG	1A	3938	1/1	0.94	0.09	47,47,47,47	0
54	MG	1A	3940	1/1	0.94	0.07	63,63,63,63	0
54	MG	1A	3171	1/1	0.94	0.18	51,51,51,51	0
54	MG	2V	203	1/1	0.94	0.10	71,71,71,71	0
54	MG	1A	3244	1/1	0.94	0.16	46,46,46,46	0
54	MG	1A	3669	1/1	0.94	0.14	56,56,56,56	0
54	MG	1a	1863	1/1	0.94	0.09	64,64,64,64	0
54	MG	1A	3795	1/1	0.94	0.12	54,54,54,54	0
54	MG	23	101	1/1	0.94	0.14	57,57,57,57	0
54	MG	1a	1699	1/1	0.94	0.25	70,70,70,70	0
54	MG	1A	3948	1/1	0.94	0.12	56,56,56,56	0
54	MG	1P	205	1/1	0.94	0.13	54,54,54,54	0
54	MG	2A	3440	1/1	0.94	0.10	39,39,39,39	0
54	MG	1A	3355	1/1	0.94	0.14	27,27,27,27	0
54	MG	1A	3952	1/1	0.94	0.07	31,31,31,31	0
54	MG	1Q	205	1/1	0.94	0.08	56,56,56,56	0
54	MG	1A	3356	1/1	0.94	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3246	1/1	0.94	0.13	45,45,45,45	0
54	MG	1A	3571	1/1	0.94	0.13	40,40,40,40	0
54	MG	1A	3573	1/1	0.94	0.25	60,60,60,60	0
54	MG	1A	3120	1/1	0.94	0.31	35,35,35,35	0
54	MG	1a	1878	1/1	0.94	0.25	68,68,68,68	0
54	MG	1A	3468	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3103	1/1	0.94	0.08	57,57,57,57	0
54	MG	1T	206	1/1	0.94	0.17	57,57,57,57	0
54	MG	2a	3019	1/1	0.94	0.07	54,54,54,54	0
54	MG	1A	3807	1/1	0.94	0.07	48,48,48,48	0
54	MG	2A	3457	1/1	0.94	0.09	63,63,63,63	0
54	MG	1V	201	1/1	0.94	0.34	34,34,34,34	0
54	MG	1A	3301	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3198	1/1	0.94	0.22	52,52,52,52	0
54	MG	1V	204	1/1	0.94	0.15	59,59,59,59	0
54	MG	2A	3200	1/1	0.94	0.34	64,64,64,64	0
54	MG	1W	201	1/1	0.94	0.14	51,51,51,51	0
54	MG	1A	3207	1/1	0.94	0.13	42,42,42,42	0
54	MG	1A	3303	1/1	0.94	0.27	38,38,38,38	0
54	MG	1A	3968	1/1	0.94	0.17	58,58,58,58	0
54	MG	1g	201	1/1	0.94	0.32	69,69,69,69	0
54	MG	1A	3473	1/1	0.94	0.10	54,54,54,54	0
54	MG	2A	3473	1/1	0.94	0.07	42,42,42,42	0
54	MG	1A	3971	1/1	0.94	0.06	32,32,32,32	0
54	MG	1A	3376	1/1	0.94	0.09	43,43,43,43	0
54	MG	1A	3209	1/1	0.94	0.38	48,48,48,48	0
54	MG	10	105	1/1	0.94	0.12	55,55,55,55	0
54	MG	2A	3211	1/1	0.94	0.32	70,70,70,70	0
54	MG	11	101	1/1	0.94	0.14	48,48,48,48	0
54	MG	1A	3378	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3480	1/1	0.94	0.08	63,63,63,63	0
54	MG	1a	1736	1/1	0.94	0.16	74,74,74,74	0
54	MG	2A	3488	1/1	0.94	0.09	64,64,64,64	0
54	MG	1A	3689	1/1	0.94	0.08	68,68,68,68	0
54	MG	1A	3380	1/1	0.94	0.08	36,36,36,36	0
54	MG	1A	3819	1/1	0.94	0.14	50,50,50,50	0
54	MG	1A	3383	1/1	0.94	0.07	26,26,26,26	0
54	MG	1A	3384	1/1	0.94	0.08	48,48,48,48	0
54	MG	1A	3826	1/1	0.94	0.12	51,51,51,51	0
54	MG	2A	3001	1/1	0.94	0.28	61,61,61,61	0
54	MG	1A	3058	1/1	0.94	0.20	59,59,59,59	0
54	MG	1A	3828	1/1	0.94	0.15	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3051	1/1	0.94	0.24	51,51,51,51	0
54	MG	1A	3212	1/1	0.94	0.11	55,55,55,55	0
54	MG	2A	3501	1/1	0.94	0.07	43,43,43,43	0
54	MG	2A	3007	1/1	0.94	0.06	45,45,45,45	0
54	MG	2A	3233	1/1	0.94	0.30	44,44,44,44	0
54	MG	2A	3009	1/1	0.94	0.12	40,40,40,40	0
54	MG	1A	3126	1/1	0.94	0.28	53,53,53,53	0
54	MG	2a	3063	1/1	0.94	0.24	70,70,70,70	0
54	MG	2a	3064	1/1	0.94	0.09	69,69,69,69	0
54	MG	2A	3237	1/1	0.94	0.11	56,56,56,56	0
54	MG	18	101	1/1	0.94	0.19	58,58,58,58	0
54	MG	1A	3835	1/1	0.94	0.08	32,32,32,32	0
54	MG	2A	3509	1/1	0.94	0.06	60,60,60,60	0
54	MG	2a	3070	1/1	0.94	0.22	61,61,61,61	0
54	MG	2a	3071	1/1	0.94	0.14	65,65,65,65	0
54	MG	1A	3836	1/1	0.94	0.07	26,26,26,26	0
54	MG	19	102	1/1	0.94	0.10	65,65,65,65	0
54	MG	2A	3242	1/1	0.94	0.23	71,71,71,71	0
54	MG	2a	3075	1/1	0.94	0.11	57,57,57,57	0
54	MG	2A	3020	1/1	0.94	0.18	47,47,47,47	0
54	MG	2a	3077	1/1	0.94	0.38	61,61,61,61	0
54	MG	2A	3022	1/1	0.94	0.18	57,57,57,57	0
54	MG	1A	3498	1/1	0.94	0.09	23,23,23,23	0
54	MG	2A	3250	1/1	0.94	0.14	37,37,37,37	0
54	MG	2A	3251	1/1	0.94	0.12	58,58,58,58	0
54	MG	1A	3068	1/1	0.94	0.17	45,45,45,45	0
54	MG	2A	3524	1/1	0.94	0.10	58,58,58,58	0
54	MG	1A	3316	1/1	0.94	0.16	61,61,61,61	0
54	MG	1A	3605	1/1	0.94	0.09	49,49,49,49	0
54	MG	1A	3703	1/1	0.94	0.15	50,50,50,50	0
54	MG	2A	3030	1/1	0.94	0.18	36,36,36,36	0
54	MG	1A	3704	1/1	0.94	0.12	57,57,57,57	0
54	MG	2a	3090	1/1	0.94	0.14	82,82,82,82	0
54	MG	2A	3032	1/1	0.94	0.22	60,60,60,60	0
54	MG	1A	3606	1/1	0.94	0.10	54,54,54,54	0
54	MG	2A	3262	1/1	0.94	0.08	63,63,63,63	0
54	MG	1A	4002	1/1	0.94	0.13	18,18,18,18	0
54	MG	2A	3544	1/1	0.94	0.08	64,64,64,64	0
54	MG	2A	3035	1/1	0.94	0.23	65,65,65,65	0
54	MG	2A	3266	1/1	0.94	0.10	49,49,49,49	0
54	MG	1a	1608	1/1	0.94	0.09	72,72,72,72	0
54	MG	1A	3020	1/1	0.94	0.26	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3038	1/1	0.94	0.17	56,56,56,56	0
54	MG	2a	3106	1/1	0.94	0.12	67,67,67,67	0
54	MG	2A	3555	1/1	0.94	0.06	58,58,58,58	0
54	MG	2A	3270	1/1	0.94	0.15	60,60,60,60	0
54	MG	2A	3275	1/1	0.94	0.15	49,49,49,49	0
54	MG	1A	3609	1/1	0.94	0.11	58,58,58,58	0
54	MG	1A	3267	1/1	0.94	0.22	55,55,55,55	0
54	MG	2A	3280	1/1	0.94	0.09	43,43,43,43	0
54	MG	2A	3281	1/1	0.94	0.21	52,52,52,52	0
54	MG	2A	3573	1/1	0.94	0.07	46,46,46,46	0
54	MG	2A	3575	1/1	0.94	0.08	63,63,63,63	0
54	MG	1A	3611	1/1	0.94	0.19	60,60,60,60	0
54	MG	2A	3578	1/1	0.94	0.09	61,61,61,61	0
54	MG	2A	3283	1/1	0.94	0.12	57,57,57,57	0
54	MG	1A	3188	1/1	0.94	0.31	53,53,53,53	0
54	MG	1A	3507	1/1	0.94	0.09	32,32,32,32	0
54	MG	2A	3290	1/1	0.94	0.14	64,64,64,64	0
54	MG	2A	3590	1/1	0.94	0.07	37,37,37,37	0
54	MG	1a	1617	1/1	0.94	0.09	75,75,75,75	0
54	MG	1A	3322	1/1	0.94	0.20	60,60,60,60	0
54	MG	1a	1619	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3294	1/1	0.94	0.13	47,47,47,47	0
54	MG	2A	3598	1/1	0.94	0.11	61,61,61,61	0
54	MG	2A	3050	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3618	1/1	0.94	0.09	49,49,49,49	0
54	MG	1A	3132	1/1	0.94	0.15	45,45,45,45	0
54	MG	2a	3151	1/1	0.94	0.07	84,84,84,84	0
54	MG	1a	1623	1/1	0.94	0.07	56,56,56,56	0
54	MG	2A	3054	1/1	0.94	0.26	64,64,64,64	0
54	MG	1A	3511	1/1	0.94	0.10	27,27,27,27	0
54	MG	1a	1784	1/1	0.94	0.10	61,61,61,61	0
54	MG	1A	3513	1/1	0.94	0.08	44,44,44,44	0
54	MG	2A	3609	1/1	0.94	0.07	55,55,55,55	0
54	MG	2A	3610	1/1	0.94	0.06	78,78,78,78	0
54	MG	2a	3163	1/1	0.94	0.08	83,83,83,83	0
54	MG	2A	3061	1/1	0.94	0.07	46,46,46,46	0
54	MG	2a	3165	1/1	0.94	0.08	68,68,68,68	0
54	MG	1A	3404	1/1	0.94	0.11	55,55,55,55	0
54	MG	2A	3063	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	3519	1/1	0.94	0.12	53,53,53,53	0
54	MG	1A	3728	1/1	0.94	0.09	67,67,67,67	0
54	MG	2A	3626	1/1	0.94	0.07	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3158	1/1	0.94	0.22	42,42,42,42	0
54	MG	1A	3093	1/1	0.94	0.32	39,39,39,39	0
54	MG	2A	3327	1/1	0.94	0.07	57,57,57,57	0
54	MG	1A	3627	1/1	0.94	0.20	42,42,42,42	0
54	MG	1a	1792	1/1	0.94	0.13	73,73,73,73	0
54	MG	1A	3630	1/1	0.94	0.19	38,38,38,38	0
54	MG	1A	3327	1/1	0.94	0.13	51,51,51,51	0
54	MG	2A	3075	1/1	0.94	0.13	63,63,63,63	0
54	MG	1A	3328	1/1	0.94	0.23	49,49,49,49	0
54	MG	1A	3878	1/1	0.94	0.11	74,74,74,74	0
54	MG	2A	3338	1/1	0.94	0.06	45,45,45,45	0
54	MG	1A	4030	1/1	0.94	0.13	64,64,64,64	0
54	MG	2A	3652	1/1	0.94	0.08	72,72,72,72	0
54	MG	1B	201	1/1	0.94	0.14	54,54,54,54	0
54	MG	1a	1640	1/1	0.94	0.17	74,74,74,74	0
54	MG	1A	3224	1/1	0.94	0.53	42,42,42,42	0
54	MG	1A	3880	1/1	0.94	0.12	50,50,50,50	0
54	MG	2A	3086	1/1	0.94	0.13	50,50,50,50	0
54	MG	1A	3076	1/1	0.94	0.23	47,47,47,47	0
58	ARG	1B	230	12/12	0.94	0.10	33,49,59,61	0
54	MG	2A	3353	1/1	0.94	0.12	66,66,66,66	0
54	MG	1A	3745	1/1	0.94	0.12	63,63,63,63	0
54	MG	1A	3010	1/1	0.95	0.14	62,62,62,62	0
54	MG	2A	3010	1/1	0.95	0.11	73,73,73,73	0
54	MG	1A	3537	1/1	0.95	0.06	38,38,38,38	0
54	MG	2A	3015	1/1	0.95	0.21	41,41,41,41	0
54	MG	1A	3229	1/1	0.95	0.21	39,39,39,39	0
54	MG	1A	3154	1/1	0.95	0.20	47,47,47,47	0
54	MG	1A	3348	1/1	0.95	0.07	39,39,39,39	0
54	MG	1a	1768	1/1	0.95	0.12	67,67,67,67	0
54	MG	2B	215	1/1	0.95	0.10	66,66,66,66	0
54	MG	1A	3893	1/1	0.95	0.06	49,49,49,49	0
54	MG	1A	3760	1/1	0.95	0.15	56,56,56,56	0
54	MG	2A	3450	1/1	0.95	0.12	69,69,69,69	0
54	MG	1a	1622	1/1	0.95	0.06	55,55,55,55	0
54	MG	2D	305	1/1	0.95	0.12	49,49,49,49	0
54	MG	1A	3069	1/1	0.95	0.24	41,41,41,41	0
54	MG	1A	3127	1/1	0.95	0.09	52,52,52,52	0
54	MG	1A	3544	1/1	0.95	0.16	43,43,43,43	0
54	MG	1a	1775	1/1	0.95	0.11	68,68,68,68	0
54	MG	1A	3650	1/1	0.95	0.14	50,50,50,50	0
54	MG	1A	3444	1/1	0.95	0.09	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3193	1/1	0.95	0.21	55,55,55,55	0
54	MG	2F	303	1/1	0.95	0.16	52,52,52,52	0
54	MG	1A	3072	1/1	0.95	0.06	45,45,45,45	0
54	MG	1A	3654	1/1	0.95	0.21	52,52,52,52	0
54	MG	1A	3296	1/1	0.95	0.14	40,40,40,40	0
54	MG	1A	3449	1/1	0.95	0.11	29,29,29,29	0
54	MG	2A	3466	1/1	0.95	0.12	33,33,33,33	0
54	MG	1B	216	1/1	0.95	0.06	61,61,61,61	0
54	MG	1A	3452	1/1	0.95	0.10	19,19,19,19	0
54	MG	2A	3039	1/1	0.95	0.19	64,64,64,64	0
54	MG	1A	3129	1/1	0.95	0.10	67,67,67,67	0
54	MG	2T	202	1/1	0.95	0.11	70,70,70,70	0
54	MG	1A	3360	1/1	0.95	0.09	15,15,15,15	0
54	MG	2V	201	1/1	0.95	0.12	70,70,70,70	0
54	MG	1A	3782	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3922	1/1	0.95	0.06	45,45,45,45	0
54	MG	1A	3054	1/1	0.95	0.17	38,38,38,38	0
54	MG	1A	3661	1/1	0.95	0.15	42,42,42,42	0
54	MG	1a	1643	1/1	0.95	0.07	62,62,62,62	0
54	MG	1A	3662	1/1	0.95	0.09	39,39,39,39	0
54	MG	1A	3559	1/1	0.95	0.08	58,58,58,58	0
54	MG	28	101	1/1	0.95	0.10	63,63,63,63	0
54	MG	1A	3561	1/1	0.95	0.14	59,59,59,59	0
54	MG	2A	3252	1/1	0.95	0.29	54,54,54,54	0
54	MG	1D	301	1/1	0.95	0.18	57,57,57,57	0
54	MG	1D	305	1/1	0.95	0.08	44,44,44,44	0
54	MG	1D	310	1/1	0.95	0.16	44,44,44,44	0
54	MG	2a	3005	1/1	0.95	0.31	61,61,61,61	0
54	MG	2A	3055	1/1	0.95	0.09	41,41,41,41	0
54	MG	1A	3163	1/1	0.95	0.11	50,50,50,50	0
54	MG	1A	3459	1/1	0.95	0.11	53,53,53,53	0
54	MG	1D	313	1/1	0.95	0.21	49,49,49,49	0
54	MG	2A	3060	1/1	0.95	0.07	52,52,52,52	0
54	MG	1a	1655	1/1	0.95	0.18	58,58,58,58	0
54	MG	1A	3460	1/1	0.95	0.06	61,61,61,61	0
54	MG	1A	3935	1/1	0.95	0.07	50,50,50,50	0
54	MG	1A	3365	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3462	1/1	0.95	0.06	19,19,19,19	0
54	MG	2A	3066	1/1	0.95	0.29	46,46,46,46	0
54	MG	1A	3939	1/1	0.95	0.10	57,57,57,57	0
54	MG	2A	3068	1/1	0.95	0.14	33,33,33,33	0
54	MG	2A	3272	1/1	0.95	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
54	MG	1A	3464	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3055	1/1	0.95	0.46	36,36,36,36	0
54	MG	1F	303	1/1	0.95	0.25	38,38,38,38	0
54	MG	1A	3801	1/1	0.95	0.07	40,40,40,40	0
54	MG	1A	3245	1/1	0.95	0.36	49,49,49,49	0
54	MG	2A	3074	1/1	0.95	0.06	47,47,47,47	0
54	MG	1F	312	1/1	0.95	0.14	50,50,50,50	0
54	MG	2A	3284	1/1	0.95	0.07	58,58,58,58	0
54	MG	1F	313	1/1	0.95	0.09	33,33,33,33	0
54	MG	2A	3514	1/1	0.95	0.18	63,63,63,63	0
54	MG	1A	3944	1/1	0.95	0.07	68,68,68,68	0
54	MG	1A	3946	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3109	1/1	0.95	0.09	43,43,43,43	0
54	MG	1A	3166	1/1	0.95	0.26	36,36,36,36	0
54	MG	1A	3203	1/1	0.95	0.28	47,47,47,47	0
54	MG	1A	3951	1/1	0.95	0.08	74,74,74,74	0
54	MG	1A	3580	1/1	0.95	0.07	50,50,50,50	0
54	MG	1A	3309	1/1	0.95	0.33	51,51,51,51	0
54	MG	1A	3250	1/1	0.95	0.30	68,68,68,68	0
54	MG	2A	3530	1/1	0.95	0.06	68,68,68,68	0
54	MG	1A	3167	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3957	1/1	0.95	0.11	50,50,50,50	0
54	MG	1N	204	1/1	0.95	0.23	60,60,60,60	0
54	MG	2A	3535	1/1	0.95	0.07	63,63,63,63	0
54	MG	2A	3093	1/1	0.95	0.10	64,64,64,64	0
54	MG	2A	3096	1/1	0.95	0.12	56,56,56,56	0
54	MG	1A	3585	1/1	0.95	0.09	68,68,68,68	0
54	MG	2A	3309	1/1	0.95	0.10	38,38,38,38	0
54	MG	1A	3477	1/1	0.95	0.06	65,65,65,65	0
54	MG	2A	3547	1/1	0.95	0.08	59,59,59,59	0
54	MG	2A	3313	1/1	0.95	0.12	47,47,47,47	0
54	MG	1A	3038	1/1	0.95	0.14	51,51,51,51	0
54	MG	2A	3550	1/1	0.95	0.07	64,64,64,64	0
54	MG	1A	3169	1/1	0.95	0.07	41,41,41,41	0
54	MG	1A	3255	1/1	0.95	0.10	54,54,54,54	0
54	MG	2A	3321	1/1	0.95	0.10	35,35,35,35	0
54	MG	1A	3690	1/1	0.95	0.07	59,59,59,59	0
54	MG	1A	3482	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3208	1/1	0.95	0.09	48,48,48,48	0
54	MG	2A	3328	1/1	0.95	0.16	69,69,69,69	0
54	MG	2A	3329	1/1	0.95	0.08	44,44,44,44	0
54	MG	2A	3564	1/1	0.95	0.09	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3570	1/1	0.95	0.10	47,47,47,47	0
54	MG	1A	3593	1/1	0.95	0.10	61,61,61,61	0
54	MG	1A	3969	1/1	0.95	0.11	57,57,57,57	0
54	MG	2A	3332	1/1	0.95	0.11	53,53,53,53	0
54	MG	1A	3387	1/1	0.95	0.06	15,15,15,15	0
54	MG	1T	203	1/1	0.95	0.06	57,57,57,57	0
54	MG	1A	3317	1/1	0.95	0.21	47,47,47,47	0
54	MG	1A	3057	1/1	0.95	0.14	56,56,56,56	0
54	MG	1a	1696	1/1	0.95	0.20	55,55,55,55	0
54	MG	1a	1842	1/1	0.95	0.20	78,78,78,78	0
54	MG	2A	3117	1/1	0.95	0.19	57,57,57,57	0
54	MG	1A	3138	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	3829	1/1	0.95	0.24	43,43,43,43	0
54	MG	1U	202	1/1	0.95	0.13	36,36,36,36	0
54	MG	2A	3343	1/1	0.95	0.09	59,59,59,59	0
54	MG	1U	204	1/1	0.95	0.10	48,48,48,48	0
54	MG	1U	207	1/1	0.95	0.21	45,45,45,45	0
54	MG	2A	3600	1/1	0.95	0.08	50,50,50,50	0
54	MG	2A	3351	1/1	0.95	0.21	52,52,52,52	0
54	MG	1a	1702	1/1	0.95	0.35	71,71,71,71	0
54	MG	2A	3603	1/1	0.95	0.07	89,89,89,89	0
54	MG	2a	3091	1/1	0.95	0.07	41,41,41,41	0
54	MG	1A	3598	1/1	0.95	0.09	32,32,32,32	0
54	MG	2a	3093	1/1	0.95	0.12	70,70,70,70	0
54	MG	1A	3599	1/1	0.95	0.16	47,47,47,47	0
54	MG	1A	3393	1/1	0.95	0.08	35,35,35,35	0
54	MG	1A	3495	1/1	0.95	0.12	61,61,61,61	0
54	MG	1a	1855	1/1	0.95	0.20	74,74,74,74	0
54	MG	2A	3132	1/1	0.95	0.12	69,69,69,69	0
54	MG	1A	3320	1/1	0.95	0.09	45,45,45,45	0
54	MG	1a	1859	1/1	0.95	0.12	57,57,57,57	0
54	MG	1A	3002	1/1	0.95	0.09	55,55,55,55	0
54	MG	2A	3136	1/1	0.95	0.13	47,47,47,47	0
54	MG	1A	3265	1/1	0.95	0.19	67,67,67,67	0
54	MG	1A	3028	1/1	0.95	0.29	38,38,38,38	0
54	MG	1A	3176	1/1	0.95	0.24	41,41,41,41	0
54	MG	2A	3369	1/1	0.95	0.16	70,70,70,70	0
54	MG	1A	3608	1/1	0.95	0.09	55,55,55,55	0
54	MG	2A	3147	1/1	0.95	0.26	55,55,55,55	0
54	MG	2A	3635	1/1	0.95	0.06	55,55,55,55	0
54	MG	2A	3636	1/1	0.95	0.10	59,59,59,59	0
54	MG	1A	3269	1/1	0.95	0.09	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3151	1/1	0.95	0.16	64,64,64,64	0
54	MG	1A	3029	1/1	0.95	0.17	40,40,40,40	0
54	MG	2A	3640	1/1	0.95	0.09	33,33,33,33	0
54	MG	10	106	1/1	0.95	0.10	65,65,65,65	0
54	MG	1A	3064	1/1	0.95	0.12	34,34,34,34	0
54	MG	2a	3127	1/1	0.95	0.10	74,74,74,74	0
54	MG	1a	1718	1/1	0.95	0.08	72,72,72,72	0
54	MG	1A	3613	1/1	0.95	0.14	51,51,51,51	0
54	MG	2A	3157	1/1	0.95	0.27	57,57,57,57	0
54	MG	1A	3508	1/1	0.95	0.08	33,33,33,33	0
54	MG	2a	3136	1/1	0.95	0.07	73,73,73,73	0
54	MG	1A	3181	1/1	0.95	0.31	50,50,50,50	0
54	MG	2A	3655	1/1	0.95	0.07	37,37,37,37	0
54	MG	1A	3996	1/1	0.95	0.07	55,55,55,55	0
54	MG	1A	3273	1/1	0.95	0.28	39,39,39,39	0
54	MG	1A	3275	1/1	0.95	0.14	59,59,59,59	0
54	MG	2A	3163	1/1	0.95	0.19	62,62,62,62	0
54	MG	2a	3148	1/1	0.95	0.09	68,68,68,68	0
54	MG	2A	3663	1/1	0.95	0.09	75,75,75,75	0
54	MG	2A	3665	1/1	0.95	0.08	83,83,83,83	0
54	MG	1a	1725	1/1	0.95	0.17	71,71,71,71	0
54	MG	1a	1726	1/1	0.95	0.18	73,73,73,73	0
54	MG	2a	3154	1/1	0.95	0.11	71,71,71,71	0
54	MG	1A	3722	1/1	0.95	0.08	52,52,52,52	0
54	MG	1A	3724	1/1	0.95	0.13	39,39,39,39	0
54	MG	1A	3147	1/1	0.95	0.38	42,42,42,42	0
54	MG	2A	3172	1/1	0.95	0.08	49,49,49,49	0
54	MG	1A	3220	1/1	0.95	0.08	48,48,48,48	0
54	MG	2a	3162	1/1	0.95	0.14	56,56,56,56	0
54	MG	17	101	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	4003	1/1	0.95	0.06	58,58,58,58	0
54	MG	1A	3518	1/1	0.95	0.07	54,54,54,54	0
54	MG	1a	1734	1/1	0.95	0.08	34,34,34,34	0
54	MG	2a	3168	1/1	0.95	0.13	69,69,69,69	0
54	MG	1a	1735	1/1	0.95	0.15	49,49,49,49	0
54	MG	2a	3172	1/1	0.95	0.10	79,79,79,79	0
54	MG	1A	3417	1/1	0.95	0.08	28,28,28,28	0
54	MG	1A	3045	1/1	0.95	0.18	34,34,34,34	0
54	MG	1a	1739	1/1	0.95	0.09	74,74,74,74	0
54	MG	1A	3732	1/1	0.95	0.07	32,32,32,32	0
54	MG	1A	3425	1/1	0.95	0.12	30,30,30,30	0
54	MG	1A	3734	1/1	0.95	0.07	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3426	1/1	0.95	0.06	24,24,24,24	0
54	MG	1A	3871	1/1	0.95	0.07	60,60,60,60	0
54	MG	1A	3280	1/1	0.95	0.18	52,52,52,52	0
54	MG	2A	3418	1/1	0.95	0.08	67,67,67,67	0
54	MG	1A	3874	1/1	0.95	0.10	39,39,39,39	0
54	MG	1A	3526	1/1	0.95	0.13	54,54,54,54	0
54	MG	2I	201	1/1	0.95	0.13	68,68,68,68	0
54	MG	1A	3001	1/1	0.95	0.05	41,41,41,41	0
54	MG	2A	3425	1/1	0.95	0.06	58,58,58,58	0
55	HGR	2A	3712	36/36	0.95	0.12	38,43,49,51	0
54	MG	2A	3197	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3186	1/1	0.95	0.27	41,41,41,41	0
54	MG	1A	3016	1/1	0.95	0.34	40,40,40,40	0
54	MG	1A	3433	1/1	0.95	0.07	25,25,25,25	0
54	MG	1A	4021	1/1	0.95	0.09	60,60,60,60	0
54	MG	1a	1755	1/1	0.95	0.12	61,61,61,61	0
54	MG	1A	3636	1/1	0.95	0.07	29,29,29,29	0
54	MG	2A	3434	1/1	0.95	0.09	73,73,73,73	0
54	MG	1A	3342	1/1	0.95	0.09	56,56,56,56	0
54	MG	1A	3750	1/1	0.95	0.07	39,39,39,39	0
59	ZN	14	501	1/1	0.95	0.16	140,140,140,140	0
54	MG	1a	1614	1/1	0.95	0.07	60,60,60,60	0
54	MG	1A	3494	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3415	1/1	0.96	0.06	33,33,33,33	0
54	MG	1A	3258	1/1	0.96	0.26	40,40,40,40	0
54	MG	2A	3008	1/1	0.96	0.08	43,43,43,43	0
54	MG	1A	3671	1/1	0.96	0.12	41,41,41,41	0
54	MG	2V	202	1/1	0.96	0.14	56,56,56,56	0
54	MG	1A	3877	1/1	0.96	0.05	38,38,38,38	0
54	MG	2W	201	1/1	0.96	0.42	51,51,51,51	0
54	MG	2A	3011	1/1	0.96	0.06	40,40,40,40	0
54	MG	1A	3768	1/1	0.96	0.07	55,55,55,55	0
54	MG	2A	3522	1/1	0.96	0.11	37,37,37,37	0
54	MG	2A	3013	1/1	0.96	0.05	26,26,26,26	0
54	MG	1A	3497	1/1	0.96	0.12	59,59,59,59	0
54	MG	2A	3526	1/1	0.96	0.05	83,83,83,83	0
54	MG	2A	3166	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3770	1/1	0.96	0.08	58,58,58,58	0
54	MG	1A	3771	1/1	0.96	0.09	46,46,46,46	0
54	MG	1a	1675	1/1	0.96	0.25	53,53,53,53	0
54	MG	2A	3532	1/1	0.96	0.09	67,67,67,67	0
54	MG	1A	3772	1/1	0.96	0.20	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1U	205	1/1	0.96	0.30	36,36,36,36	0
54	MG	1U	206	1/1	0.96	0.23	42,42,42,42	0
54	MG	1A	4005	1/1	0.96	0.04	41,41,41,41	0
54	MG	2A	3175	1/1	0.96	0.10	52,52,52,52	0
54	MG	2A	3541	1/1	0.96	0.07	61,61,61,61	0
54	MG	2A	3177	1/1	0.96	0.30	70,70,70,70	0
54	MG	1A	3418	1/1	0.96	0.07	25,25,25,25	0
54	MG	2A	3545	1/1	0.96	0.07	65,65,65,65	0
54	MG	1A	3886	1/1	0.96	0.10	28,28,28,28	0
54	MG	2A	3026	1/1	0.96	0.08	55,55,55,55	0
54	MG	2a	3017	1/1	0.96	0.09	57,57,57,57	0
54	MG	2A	3181	1/1	0.96	0.08	54,54,54,54	0
54	MG	1A	3092	1/1	0.96	0.26	36,36,36,36	0
54	MG	1A	3424	1/1	0.96	0.07	21,21,21,21	0
54	MG	1A	3306	1/1	0.96	0.16	40,40,40,40	0
54	MG	1A	3307	1/1	0.96	0.33	43,43,43,43	0
54	MG	2A	3554	1/1	0.96	0.09	35,35,35,35	0
54	MG	1A	3778	1/1	0.96	0.08	37,37,37,37	0
54	MG	1a	1687	1/1	0.96	0.09	55,55,55,55	0
54	MG	2a	3026	1/1	0.96	0.22	60,60,60,60	0
54	MG	1A	3779	1/1	0.96	0.19	64,64,64,64	0
54	MG	1A	3308	1/1	0.96	0.20	49,49,49,49	0
54	MG	1A	3183	1/1	0.96	0.06	62,62,62,62	0
54	MG	1A	3218	1/1	0.96	0.11	51,51,51,51	0
54	MG	1A	3358	1/1	0.96	0.08	24,24,24,24	0
54	MG	2A	3565	1/1	0.96	0.16	49,49,49,49	0
54	MG	2A	3567	1/1	0.96	0.08	48,48,48,48	0
54	MG	1A	3784	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3901	1/1	0.96	0.07	55,55,55,55	0
54	MG	1A	3682	1/1	0.96	0.06	50,50,50,50	0
54	MG	2A	3042	1/1	0.96	0.08	29,29,29,29	0
54	MG	2A	3576	1/1	0.96	0.09	73,73,73,73	0
54	MG	1A	3904	1/1	0.96	0.10	48,48,48,48	0
54	MG	11	105	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3788	1/1	0.96	0.07	54,54,54,54	0
54	MG	2A	3380	1/1	0.96	0.06	43,43,43,43	0
54	MG	2A	3381	1/1	0.96	0.06	35,35,35,35	0
54	MG	13	103	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3018	1/1	0.96	0.23	32,32,32,32	0
54	MG	1A	3040	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3512	1/1	0.96	0.07	27,27,27,27	0
54	MG	1a	1822	1/1	0.96	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3071	1/1	0.96	0.20	38,38,38,38	0
54	MG	2A	3389	1/1	0.96	0.09	60,60,60,60	0
54	MG	2a	3051	1/1	0.96	0.09	83,83,83,83	0
54	MG	2A	3390	1/1	0.96	0.13	74,74,74,74	0
54	MG	1A	4029	1/1	0.96	0.09	61,61,61,61	0
54	MG	1A	3156	1/1	0.96	0.24	38,38,38,38	0
54	MG	1A	3367	1/1	0.96	0.09	33,33,33,33	0
54	MG	1A	3315	1/1	0.96	0.17	62,62,62,62	0
54	MG	2A	3395	1/1	0.96	0.05	37,37,37,37	0
54	MG	1A	3099	1/1	0.96	0.14	38,38,38,38	0
54	MG	17	103	1/1	0.96	0.07	41,41,41,41	0
54	MG	17	104	1/1	0.96	0.26	45,45,45,45	0
54	MG	1A	3225	1/1	0.96	0.14	34,34,34,34	0
54	MG	2A	3217	1/1	0.96	0.08	52,52,52,52	0
54	MG	1A	3226	1/1	0.96	0.33	37,37,37,37	0
54	MG	1A	3011	1/1	0.96	0.25	64,64,64,64	0
54	MG	1A	3802	1/1	0.96	0.08	73,73,73,73	0
54	MG	1a	1715	1/1	0.96	0.11	52,52,52,52	0
54	MG	1A	3101	1/1	0.96	0.21	47,47,47,47	0
54	MG	2a	3069	1/1	0.96	0.31	50,50,50,50	0
54	MG	1A	3130	1/1	0.96	0.06	37,37,37,37	0
54	MG	1A	3162	1/1	0.96	0.09	38,38,38,38	0
54	MG	1A	3698	1/1	0.96	0.08	58,58,58,58	0
54	MG	2A	3629	1/1	0.96	0.06	57,57,57,57	0
54	MG	2A	3410	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3451	1/1	0.96	0.08	29,29,29,29	0
54	MG	1A	3808	1/1	0.96	0.08	33,33,33,33	0
54	MG	1A	3381	1/1	0.96	0.05	20,20,20,20	0
54	MG	1A	3033	1/1	0.96	0.20	58,58,58,58	0
54	MG	2A	3232	1/1	0.96	0.50	47,47,47,47	0
54	MG	1A	3535	1/1	0.96	0.08	24,24,24,24	0
54	MG	1A	3022	1/1	0.96	0.05	45,45,45,45	0
54	MG	2A	3421	1/1	0.96	0.06	63,63,63,63	0
54	MG	1A	3077	1/1	0.96	0.29	37,37,37,37	0
54	MG	1B	223	1/1	0.96	0.08	68,68,68,68	0
54	MG	2A	3078	1/1	0.96	0.15	56,56,56,56	0
54	MG	2A	3647	1/1	0.96	0.07	69,69,69,69	0
54	MG	2A	3426	1/1	0.96	0.04	55,55,55,55	0
54	MG	1A	3326	1/1	0.96	0.27	38,38,38,38	0
54	MG	2A	3080	1/1	0.96	0.11	47,47,47,47	0
54	MG	2A	3654	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3458	1/1	0.96	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3623	1/1	0.96	0.11	58,58,58,58	0
54	MG	1A	3023	1/1	0.96	0.15	36,36,36,36	0
54	MG	2A	3244	1/1	0.96	0.22	46,46,46,46	0
54	MG	2a	3097	1/1	0.96	0.11	58,58,58,58	0
54	MG	2A	3245	1/1	0.96	0.12	46,46,46,46	0
54	MG	2A	3660	1/1	0.96	0.06	68,68,68,68	0
54	MG	2A	3661	1/1	0.96	0.06	59,59,59,59	0
54	MG	2A	3246	1/1	0.96	0.15	60,60,60,60	0
54	MG	2A	3664	1/1	0.96	0.06	82,82,82,82	0
54	MG	1A	3541	1/1	0.96	0.06	53,53,53,53	0
54	MG	2A	3436	1/1	0.96	0.12	44,44,44,44	0
54	MG	2a	3105	1/1	0.96	0.09	71,71,71,71	0
54	MG	2A	3667	1/1	0.96	0.06	46,46,46,46	0
54	MG	1A	3080	1/1	0.96	0.24	45,45,45,45	0
54	MG	1A	3389	1/1	0.96	0.09	21,21,21,21	0
54	MG	1A	3081	1/1	0.96	0.12	49,49,49,49	0
54	MG	1a	1860	1/1	0.96	0.15	56,56,56,56	0
54	MG	1A	3463	1/1	0.96	0.19	62,62,62,62	0
54	MG	1a	1862	1/1	0.96	0.12	44,44,44,44	0
54	MG	1A	3063	1/1	0.96	0.05	40,40,40,40	0
54	MG	1A	3140	1/1	0.96	0.08	36,36,36,36	0
54	MG	2A	3097	1/1	0.96	0.31	63,63,63,63	0
54	MG	2A	3258	1/1	0.96	0.28	51,51,51,51	0
54	MG	1A	3394	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3395	1/1	0.96	0.12	40,40,40,40	0
54	MG	1A	3048	1/1	0.96	0.22	56,56,56,56	0
54	MG	2a	3126	1/1	0.96	0.05	71,71,71,71	0
54	MG	1A	3397	1/1	0.96	0.12	53,53,53,53	0
54	MG	2A	3104	1/1	0.96	0.09	56,56,56,56	0
54	MG	2a	3129	1/1	0.96	0.05	61,61,61,61	0
54	MG	2a	3131	1/1	0.96	0.08	83,83,83,83	0
54	MG	2A	3453	1/1	0.96	0.07	65,65,65,65	0
54	MG	1E	301	1/1	0.96	0.17	38,38,38,38	0
54	MG	1A	3172	1/1	0.96	0.22	38,38,38,38	0
54	MG	1E	305	1/1	0.96	0.05	39,39,39,39	0
54	MG	1A	3335	1/1	0.96	0.14	50,50,50,50	0
54	MG	1A	3026	1/1	0.96	0.28	37,37,37,37	0
54	MG	2a	3141	1/1	0.96	0.08	72,72,72,72	0
54	MG	1A	3730	1/1	0.96	0.19	41,41,41,41	0
54	MG	2A	3271	1/1	0.96	0.05	39,39,39,39	0
54	MG	2A	3698	1/1	0.96	0.15	73,73,73,73	0
54	MG	1A	3560	1/1	0.96	0.14	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3146	1/1	0.96	0.12	78,78,78,78	0
54	MG	2A	3700	1/1	0.96	0.06	63,63,63,63	0
54	MG	1A	3174	1/1	0.96	0.15	34,34,34,34	0
54	MG	2A	3277	1/1	0.96	0.10	51,51,51,51	0
54	MG	1F	307	1/1	0.96	0.07	43,43,43,43	0
54	MG	2A	3705	1/1	0.96	0.12	46,46,46,46	0
54	MG	1A	3115	1/1	0.96	0.13	36,36,36,36	0
54	MG	1A	3037	1/1	0.96	0.08	40,40,40,40	0
54	MG	1A	3567	1/1	0.96	0.09	38,38,38,38	0
54	MG	1a	1758	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3252	1/1	0.96	0.28	33,33,33,33	0
54	MG	2a	3160	1/1	0.96	0.08	78,78,78,78	0
54	MG	2A	3119	1/1	0.96	0.05	42,42,42,42	0
54	MG	1A	3481	1/1	0.96	0.10	50,50,50,50	0
54	MG	2A	3288	1/1	0.96	0.09	37,37,37,37	0
54	MG	1A	3089	1/1	0.96	0.05	41,41,41,41	0
54	MG	1A	3407	1/1	0.96	0.21	57,57,57,57	0
54	MG	2B	207	1/1	0.96	0.09	73,73,73,73	0
54	MG	1A	3572	1/1	0.96	0.07	56,56,56,56	0
54	MG	1A	3179	1/1	0.96	0.39	42,42,42,42	0
54	MG	1A	3485	1/1	0.96	0.09	63,63,63,63	0
54	MG	1a	1766	1/1	0.96	0.12	57,57,57,57	0
54	MG	1A	3980	1/1	0.96	0.12	53,53,53,53	0
54	MG	1A	3575	1/1	0.96	0.09	36,36,36,36	0
54	MG	1A	3486	1/1	0.96	0.07	58,58,58,58	0
54	MG	1A	3004	1/1	0.96	0.10	44,44,44,44	0
54	MG	1A	3752	1/1	0.96	0.11	26,26,26,26	0
54	MG	1m	201	1/1	0.96	0.04	81,81,81,81	0
54	MG	1A	3411	1/1	0.96	0.08	34,34,34,34	0
54	MG	1A	3754	1/1	0.96	0.10	53,53,53,53	0
54	MG	2A	3137	1/1	0.96	0.10	58,58,58,58	0
54	MG	1A	3345	1/1	0.96	0.17	43,43,43,43	0
54	MG	2D	307	1/1	0.96	0.10	63,63,63,63	0
54	MG	2A	3310	1/1	0.96	0.10	52,52,52,52	0
54	MG	1A	3581	1/1	0.96	0.08	48,48,48,48	0
54	MG	1A	3664	1/1	0.96	0.09	60,60,60,60	0
54	MG	2A	3314	1/1	0.96	0.12	37,37,37,37	0
54	MG	1Q	201	1/1	0.96	0.10	43,43,43,43	0
54	MG	1Q	204	1/1	0.96	0.20	56,56,56,56	0
54	MG	1A	3869	1/1	0.96	0.10	45,45,45,45	0
54	MG	2A	3320	1/1	0.96	0.10	50,50,50,50	0
57	MPD	18	103	8/8	0.96	0.11	32,41,48,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3150	1/1	0.96	0.17	61,61,61,61	0
54	MG	2A	3322	1/1	0.96	0.07	39,39,39,39	0
54	MG	1R	202	1/1	0.96	0.11	45,45,45,45	0
54	MG	2O	201	1/1	0.96	0.16	68,68,68,68	0
54	MG	1A	3151	1/1	0.96	0.10	58,58,58,58	0
54	MG	1R	204	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3492	1/1	0.96	0.05	56,56,56,56	0
54	MG	2Q	203	1/1	0.96	0.06	75,75,75,75	0
54	MG	1A	3862	1/1	0.97	0.10	26,26,26,26	0
54	MG	2A	3350	1/1	0.97	0.06	62,62,62,62	0
54	MG	1a	1654	1/1	0.97	0.07	47,47,47,47	0
54	MG	2W	203	1/1	0.97	0.12	73,73,73,73	0
54	MG	2A	3537	1/1	0.97	0.07	79,79,79,79	0
54	MG	2A	3021	1/1	0.97	0.05	44,44,44,44	0
54	MG	2A	3540	1/1	0.97	0.05	27,27,27,27	0
54	MG	1G	204	1/1	0.97	0.11	56,56,56,56	0
54	MG	2A	3542	1/1	0.97	0.08	65,65,65,65	0
54	MG	27	101	1/1	0.97	0.19	46,46,46,46	0
54	MG	1A	3159	1/1	0.97	0.12	40,40,40,40	0
54	MG	1A	3009	1/1	0.97	0.07	39,39,39,39	0
54	MG	1N	202	1/1	0.97	0.14	49,49,49,49	0
54	MG	1A	3450	1/1	0.97	0.06	30,30,30,30	0
54	MG	2A	3358	1/1	0.97	0.07	65,65,65,65	0
54	MG	1A	3520	1/1	0.97	0.13	30,30,30,30	0
54	MG	1A	3231	1/1	0.97	0.19	35,35,35,35	0
54	MG	2A	3029	1/1	0.97	0.08	47,47,47,47	0
54	MG	1P	202	1/1	0.97	0.28	36,36,36,36	0
54	MG	1A	3522	1/1	0.97	0.08	43,43,43,43	0
54	MG	1P	204	1/1	0.97	0.10	67,67,67,67	0
54	MG	1A	3019	1/1	0.97	0.14	36,36,36,36	0
54	MG	1A	3989	1/1	0.97	0.04	57,57,57,57	0
54	MG	1A	3015	1/1	0.97	0.11	38,38,38,38	0
54	MG	1A	3390	1/1	0.97	0.07	19,19,19,19	0
54	MG	2A	3561	1/1	0.97	0.06	50,50,50,50	0
54	MG	2A	3193	1/1	0.97	0.06	49,49,49,49	0
54	MG	1Q	202	1/1	0.97	0.09	45,45,45,45	0
54	MG	1Q	203	1/1	0.97	0.06	41,41,41,41	0
54	MG	2A	3196	1/1	0.97	0.09	51,51,51,51	0
54	MG	1A	3021	1/1	0.97	0.21	45,45,45,45	0
54	MG	1A	3456	1/1	0.97	0.05	32,32,32,32	0
54	MG	1R	201	1/1	0.97	0.14	46,46,46,46	0
54	MG	1A	3235	1/1	0.97	0.12	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3102	1/1	0.97	0.26	38,38,38,38	0
54	MG	1A	3041	1/1	0.97	0.17	47,47,47,47	0
54	MG	1A	3531	1/1	0.97	0.09	50,50,50,50	0
54	MG	1A	3104	1/1	0.97	0.20	26,26,26,26	0
54	MG	2A	3581	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3105	1/1	0.97	0.25	35,35,35,35	0
54	MG	2A	3583	1/1	0.97	0.06	38,38,38,38	0
54	MG	1A	3136	1/1	0.97	0.36	33,33,33,33	0
54	MG	1A	3202	1/1	0.97	0.19	39,39,39,39	0
54	MG	2A	3587	1/1	0.97	0.06	71,71,71,71	0
54	MG	1A	3292	1/1	0.97	0.08	49,49,49,49	0
54	MG	1A	3785	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3059	1/1	0.97	0.12	21,21,21,21	0
54	MG	1A	3615	1/1	0.97	0.04	37,37,37,37	0
54	MG	2A	3595	1/1	0.97	0.08	57,57,57,57	0
54	MG	1A	3294	1/1	0.97	0.14	47,47,47,47	0
54	MG	1A	3030	1/1	0.97	0.05	39,39,39,39	0
54	MG	1A	3205	1/1	0.97	0.23	41,41,41,41	0
54	MG	2A	3058	1/1	0.97	0.09	50,50,50,50	0
54	MG	1A	3248	1/1	0.97	0.10	54,54,54,54	0
54	MG	1A	3043	1/1	0.97	0.09	36,36,36,36	0
54	MG	1A	3897	1/1	0.97	0.18	39,39,39,39	0
54	MG	1V	202	1/1	0.97	0.21	38,38,38,38	0
54	MG	1A	3794	1/1	0.97	0.07	49,49,49,49	0
54	MG	2A	3222	1/1	0.97	0.14	53,53,53,53	0
54	MG	1A	3083	1/1	0.97	0.28	38,38,38,38	0
54	MG	1A	3546	1/1	0.97	0.12	26,26,26,26	0
54	MG	1W	202	1/1	0.97	0.15	39,39,39,39	0
54	MG	1A	3902	1/1	0.97	0.13	49,49,49,49	0
54	MG	1A	3143	1/1	0.97	0.07	31,31,31,31	0
54	MG	1A	3062	1/1	0.97	0.18	34,34,34,34	0
54	MG	1A	3907	1/1	0.97	0.08	65,65,65,65	0
54	MG	2A	3230	1/1	0.97	0.11	43,43,43,43	0
54	MG	2A	3614	1/1	0.97	0.09	73,73,73,73	0
54	MG	1A	3031	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3706	1/1	0.97	0.22	55,55,55,55	0
54	MG	1A	3112	1/1	0.97	0.32	37,37,37,37	0
54	MG	1A	3553	1/1	0.97	0.08	32,32,32,32	0
54	MG	2A	3235	1/1	0.97	0.21	47,47,47,47	0
54	MG	1A	3628	1/1	0.97	0.22	40,40,40,40	0
54	MG	1A	3914	1/1	0.97	0.05	39,39,39,39	0
54	MG	2A	3634	1/1	0.97	0.06	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3420	1/1	0.97	0.11	44,44,44,44	0
54	MG	1A	3629	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	4028	1/1	0.97	0.20	63,63,63,63	0
54	MG	1A	3917	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3554	1/1	0.97	0.09	57,57,57,57	0
54	MG	1A	4031	1/1	0.97	0.05	57,57,57,57	0
54	MG	1A	3177	1/1	0.97	0.12	32,32,32,32	0
54	MG	2A	3083	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3414	1/1	0.97	0.08	44,44,44,44	0
54	MG	1A	3714	1/1	0.97	0.20	46,46,46,46	0
54	MG	1A	3715	1/1	0.97	0.08	57,57,57,57	0
54	MG	2A	3087	1/1	0.97	0.17	55,55,55,55	0
54	MG	1A	3925	1/1	0.97	0.09	51,51,51,51	0
54	MG	1A	3032	1/1	0.97	0.05	24,24,24,24	0
54	MG	1A	3634	1/1	0.97	0.05	44,44,44,44	0
54	MG	1A	3416	1/1	0.97	0.05	30,30,30,30	0
54	MG	1A	3214	1/1	0.97	0.24	34,34,34,34	0
54	MG	1a	1856	1/1	0.97	0.06	61,61,61,61	0
54	MG	2A	3094	1/1	0.97	0.12	55,55,55,55	0
54	MG	1A	3259	1/1	0.97	0.07	34,34,34,34	0
54	MG	1A	3419	1/1	0.97	0.13	34,34,34,34	0
54	MG	1A	3640	1/1	0.97	0.12	55,55,55,55	0
54	MG	2A	3662	1/1	0.97	0.09	46,46,46,46	0
54	MG	1A	3641	1/1	0.97	0.09	25,25,25,25	0
54	MG	2A	3444	1/1	0.97	0.07	69,69,69,69	0
54	MG	1A	3420	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3563	1/1	0.97	0.09	26,26,26,26	0
54	MG	2A	3263	1/1	0.97	0.06	72,72,72,72	0
54	MG	1a	1864	1/1	0.97	0.07	59,59,59,59	0
54	MG	1B	218	1/1	0.97	0.10	35,35,35,35	0
54	MG	1A	3564	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3824	1/1	0.97	0.07	51,51,51,51	0
54	MG	1A	3825	1/1	0.97	0.11	53,53,53,53	0
54	MG	1A	3005	1/1	0.97	0.09	22,22,22,22	0
54	MG	1A	3149	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3364	1/1	0.97	0.10	29,29,29,29	0
54	MG	1A	3945	1/1	0.97	0.05	75,75,75,75	0
54	MG	2a	3107	1/1	0.97	0.06	74,74,74,74	0
54	MG	2A	3273	1/1	0.97	0.12	20,20,20,20	0
54	MG	2A	3679	1/1	0.97	0.07	69,69,69,69	0
54	MG	2a	3112	1/1	0.97	0.07	71,71,71,71	0
54	MG	1a	1873	1/1	0.97	0.06	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3681	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3088	1/1	0.97	0.10	52,52,52,52	0
54	MG	1A	3831	1/1	0.97	0.21	42,42,42,42	0
54	MG	1A	3264	1/1	0.97	0.34	37,37,37,37	0
54	MG	1a	1738	1/1	0.97	0.12	47,47,47,47	0
54	MG	1a	1609	1/1	0.97	0.05	64,64,64,64	0
54	MG	1A	3017	1/1	0.97	0.31	39,39,39,39	0
54	MG	1D	302	1/1	0.97	0.09	60,60,60,60	0
54	MG	2a	3122	1/1	0.97	0.14	56,56,56,56	0
54	MG	1D	304	1/1	0.97	0.12	40,40,40,40	0
54	MG	1A	3090	1/1	0.97	0.08	43,43,43,43	0
54	MG	1D	306	1/1	0.97	0.16	44,44,44,44	0
54	MG	1D	308	1/1	0.97	0.06	46,46,46,46	0
54	MG	1A	3738	1/1	0.97	0.08	52,52,52,52	0
54	MG	2A	3696	1/1	0.97	0.06	55,55,55,55	0
54	MG	2a	3130	1/1	0.97	0.05	80,80,80,80	0
54	MG	2A	3697	1/1	0.97	0.09	35,35,35,35	0
54	MG	1A	3953	1/1	0.97	0.06	31,31,31,31	0
54	MG	2A	3475	1/1	0.97	0.12	57,57,57,57	0
54	MG	2A	3476	1/1	0.97	0.06	74,74,74,74	0
54	MG	2a	3135	1/1	0.97	0.05	72,72,72,72	0
54	MG	1A	3431	1/1	0.97	0.10	31,31,31,31	0
54	MG	2A	3478	1/1	0.97	0.05	30,30,30,30	0
54	MG	2a	3139	1/1	0.97	0.06	78,78,78,78	0
54	MG	2A	3703	1/1	0.97	0.10	52,52,52,52	0
54	MG	1A	3372	1/1	0.97	0.07	31,31,31,31	0
54	MG	2A	3130	1/1	0.97	0.05	36,36,36,36	0
54	MG	1a	1751	1/1	0.97	0.11	59,59,59,59	0
54	MG	1A	3118	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3743	1/1	0.97	0.05	35,35,35,35	0
54	MG	2A	3709	1/1	0.97	0.11	64,64,64,64	0
54	MG	2a	3147	1/1	0.97	0.06	76,76,76,76	0
54	MG	1D	316	1/1	0.97	0.09	63,63,63,63	0
54	MG	2A	3711	1/1	0.97	0.05	55,55,55,55	0
54	MG	2A	3299	1/1	0.97	0.14	42,42,42,42	0
54	MG	1D	317	1/1	0.97	0.06	47,47,47,47	0
54	MG	2A	3301	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3958	1/1	0.97	0.05	58,58,58,58	0
54	MG	1A	3576	1/1	0.97	0.09	62,62,62,62	0
54	MG	1l	201	1/1	0.97	0.13	62,62,62,62	0
54	MG	2A	3305	1/1	0.97	0.07	46,46,46,46	0
54	MG	2A	3306	1/1	0.97	0.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1E	302	1/1	0.97	0.20	44,44,44,44	0
54	MG	2A	3142	1/1	0.97	0.17	42,42,42,42	0
54	MG	2A	3143	1/1	0.97	0.10	42,42,42,42	0
54	MG	2A	3311	1/1	0.97	0.08	62,62,62,62	0
54	MG	1A	3268	1/1	0.97	0.13	43,43,43,43	0
54	MG	1A	3375	1/1	0.97	0.06	36,36,36,36	0
54	MG	2A	3146	1/1	0.97	0.18	76,76,76,76	0
54	MG	1A	3050	1/1	0.97	0.18	55,55,55,55	0
54	MG	2a	3169	1/1	0.97	0.08	79,79,79,79	0
54	MG	2a	3170	1/1	0.97	0.06	71,71,71,71	0
54	MG	1E	307	1/1	0.97	0.09	25,25,25,25	0
54	MG	2A	3149	1/1	0.97	0.10	35,35,35,35	0
54	MG	1A	3505	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	3024	1/1	0.97	0.08	24,24,24,24	0
54	MG	2a	3176	1/1	0.97	0.06	67,67,67,67	0
54	MG	1a	1633	1/1	0.97	0.12	41,41,41,41	0
54	MG	1a	1634	1/1	0.97	0.09	48,48,48,48	0
54	MG	1E	310	1/1	0.97	0.09	60,60,60,60	0
54	MG	2A	3325	1/1	0.97	0.09	32,32,32,32	0
54	MG	1A	3846	1/1	0.97	0.12	51,51,51,51	0
54	MG	1F	304	1/1	0.97	0.23	40,40,40,40	0
54	MG	1A	3187	1/1	0.97	0.21	42,42,42,42	0
54	MG	1F	306	1/1	0.97	0.12	35,35,35,35	0
54	MG	2F	302	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3379	1/1	0.97	0.06	24,24,24,24	0
54	MG	2F	304	1/1	0.97	0.23	50,50,50,50	0
54	MG	1A	3025	1/1	0.97	0.26	48,48,48,48	0
54	MG	1F	311	1/1	0.97	0.06	40,40,40,40	0
55	HGR	1A	4032	36/36	0.97	0.08	25,29,35,40	0
54	MG	2A	3519	1/1	0.97	0.07	59,59,59,59	0
54	MG	1A	3095	1/1	0.97	0.17	43,43,43,43	0
54	MG	1A	3757	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3855	1/1	0.97	0.04	51,51,51,51	0
54	MG	1A	3274	1/1	0.97	0.05	44,44,44,44	0
54	MG	2Q	201	1/1	0.97	0.07	63,63,63,63	0
54	MG	1A	3446	1/1	0.97	0.10	31,31,31,31	0
54	MG	2A	3168	1/1	0.97	0.06	55,55,55,55	0
54	MG	2A	3528	1/1	0.97	0.07	66,66,66,66	0
54	MG	1A	3070	1/1	0.97	0.25	37,37,37,37	0
54	MG	1A	3514	1/1	0.97	0.07	72,72,72,72	0
54	MG	1a	1650	1/1	0.97	0.11	55,55,55,55	0
54	MG	1A	3515	1/1	0.97	0.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3861	1/1	0.97	0.11	45,45,45,45	0
59	ZN	2n	3102	1/1	0.97	0.07	103,103,103,103	0
54	MG	2A	3165	1/1	0.98	0.20	46,46,46,46	0
54	MG	1A	3735	1/1	0.98	0.05	46,46,46,46	0
54	MG	2A	3673	1/1	0.98	0.03	53,53,53,53	0
54	MG	1A	3796	1/1	0.98	0.07	40,40,40,40	0
54	MG	1A	3533	1/1	0.98	0.07	25,25,25,25	0
54	MG	1A	3864	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3276	1/1	0.98	0.08	32,32,32,32	0
54	MG	2a	3053	1/1	0.98	0.05	64,64,64,64	0
54	MG	2A	3276	1/1	0.98	0.07	42,42,42,42	0
54	MG	2A	3521	1/1	0.98	0.09	48,48,48,48	0
54	MG	1A	3135	1/1	0.98	0.17	35,35,35,35	0
54	MG	2A	3523	1/1	0.98	0.13	34,34,34,34	0
54	MG	1A	3684	1/1	0.98	0.16	48,48,48,48	0
54	MG	1A	3366	1/1	0.98	0.04	32,32,32,32	0
54	MG	1A	3949	1/1	0.98	0.05	51,51,51,51	0
54	MG	2A	3400	1/1	0.98	0.05	54,54,54,54	0
54	MG	1A	3230	1/1	0.98	0.19	44,44,44,44	0
54	MG	2A	3176	1/1	0.98	0.06	71,71,71,71	0
54	MG	1H	202	1/1	0.98	0.06	58,58,58,58	0
54	MG	2A	3690	1/1	0.98	0.04	85,85,85,85	0
54	MG	1A	3742	1/1	0.98	0.04	56,56,56,56	0
54	MG	2A	3285	1/1	0.98	0.04	42,42,42,42	0
54	MG	1A	3872	1/1	0.98	0.08	32,32,32,32	0
54	MG	2A	3287	1/1	0.98	0.07	38,38,38,38	0
54	MG	1A	3368	1/1	0.98	0.10	46,46,46,46	0
54	MG	1A	3744	1/1	0.98	0.05	41,41,41,41	0
54	MG	1A	3119	1/1	0.98	0.13	34,34,34,34	0
54	MG	1P	201	1/1	0.98	0.30	39,39,39,39	0
54	MG	2A	3539	1/1	0.98	0.05	76,76,76,76	0
54	MG	2A	3412	1/1	0.98	0.06	57,57,57,57	0
54	MG	1A	3746	1/1	0.98	0.04	49,49,49,49	0
54	MG	1A	3082	1/1	0.98	0.17	34,34,34,34	0
54	MG	1A	3371	1/1	0.98	0.09	58,58,58,58	0
54	MG	1A	3256	1/1	0.98	0.06	41,41,41,41	0
54	MG	2A	3417	1/1	0.98	0.05	42,42,42,42	0
54	MG	1A	3121	1/1	0.98	0.10	27,27,27,27	0
54	MG	1A	3410	1/1	0.98	0.05	34,34,34,34	0
54	MG	1A	3338	1/1	0.98	0.09	41,41,41,41	0
54	MG	1A	3644	1/1	0.98	0.07	28,28,28,28	0
54	MG	2A	3422	1/1	0.98	0.05	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3502	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3755	1/1	0.98	0.09	46,46,46,46	0
54	MG	2A	3553	1/1	0.98	0.08	60,60,60,60	0
54	MG	2a	3089	1/1	0.98	0.05	77,77,77,77	0
54	MG	1B	212	1/1	0.98	0.08	47,47,47,47	0
54	MG	1A	3548	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3194	1/1	0.98	0.14	39,39,39,39	0
54	MG	1A	3122	1/1	0.98	0.06	29,29,29,29	0
54	MG	2A	3559	1/1	0.98	0.14	58,58,58,58	0
54	MG	2a	3095	1/1	0.98	0.07	53,53,53,53	0
54	MG	2A	3095	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3094	1/1	0.98	0.06	40,40,40,40	0
54	MG	1A	3821	1/1	0.98	0.09	55,55,55,55	0
54	MG	1A	3287	1/1	0.98	0.10	17,17,17,17	0
54	MG	1A	3823	1/1	0.98	0.05	42,42,42,42	0
54	MG	2A	3004	1/1	0.98	0.06	43,43,43,43	0
54	MG	2A	3566	1/1	0.98	0.04	57,57,57,57	0
54	MG	1A	3761	1/1	0.98	0.07	26,26,26,26	0
54	MG	2A	3568	1/1	0.98	0.04	71,71,71,71	0
54	MG	2A	3102	1/1	0.98	0.06	33,33,33,33	0
54	MG	2B	218	1/1	0.98	0.09	66,66,66,66	0
54	MG	2D	301	1/1	0.98	0.19	49,49,49,49	0
54	MG	2a	3108	1/1	0.98	0.16	61,61,61,61	0
54	MG	2D	302	1/1	0.98	0.08	52,52,52,52	0
54	MG	2a	3110	1/1	0.98	0.06	75,75,75,75	0
54	MG	2A	3315	1/1	0.98	0.07	32,32,32,32	0
54	MG	2A	3316	1/1	0.98	0.11	32,32,32,32	0
54	MG	1B	222	1/1	0.98	0.04	55,55,55,55	0
54	MG	1A	3142	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3013	1/1	0.98	0.08	29,29,29,29	0
54	MG	1A	3239	1/1	0.98	0.28	39,39,39,39	0
54	MG	2A	3579	1/1	0.98	0.05	70,70,70,70	0
54	MG	1A	3705	1/1	0.98	0.05	58,58,58,58	0
54	MG	2E	302	1/1	0.98	0.14	45,45,45,45	0
54	MG	1A	3604	1/1	0.98	0.08	43,43,43,43	0
54	MG	2E	304	1/1	0.98	0.10	30,30,30,30	0
54	MG	1U	203	1/1	0.98	0.38	43,43,43,43	0
54	MG	1A	3830	1/1	0.98	0.25	44,44,44,44	0
54	MG	2A	3214	1/1	0.98	0.06	67,67,67,67	0
54	MG	2A	3326	1/1	0.98	0.05	33,33,33,33	0
54	MG	2A	3014	1/1	0.98	0.06	51,51,51,51	0
54	MG	1A	3382	1/1	0.98	0.13	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3905	1/1	0.98	0.06	29,29,29,29	0
54	MG	2A	3592	1/1	0.98	0.07	65,65,65,65	0
54	MG	1A	3240	1/1	0.98	0.18	36,36,36,36	0
54	MG	2A	3594	1/1	0.98	0.04	48,48,48,48	0
54	MG	1D	303	1/1	0.98	0.09	40,40,40,40	0
54	MG	1A	3096	1/1	0.98	0.09	24,24,24,24	0
54	MG	1A	3909	1/1	0.98	0.03	52,52,52,52	0
54	MG	1A	3423	1/1	0.98	0.07	28,28,28,28	0
54	MG	1A	3466	1/1	0.98	0.11	57,57,57,57	0
54	MG	1D	309	1/1	0.98	0.13	36,36,36,36	0
54	MG	1A	3073	1/1	0.98	0.06	41,41,41,41	0
54	MG	2A	3123	1/1	0.98	0.19	44,44,44,44	0
54	MG	1A	3516	1/1	0.98	0.07	28,28,28,28	0
54	MG	1X	101	1/1	0.98	0.11	43,43,43,43	0
54	MG	2A	3464	1/1	0.98	0.07	66,66,66,66	0
54	MG	1A	3612	1/1	0.98	0.09	27,27,27,27	0
54	MG	1A	3993	1/1	0.98	0.09	63,63,63,63	0
54	MG	10	101	1/1	0.98	0.09	46,46,46,46	0
54	MG	1A	3350	1/1	0.98	0.08	54,54,54,54	0
54	MG	2A	3346	1/1	0.98	0.08	57,57,57,57	0
54	MG	2a	3150	1/1	0.98	0.10	54,54,54,54	0
54	MG	1A	3074	1/1	0.98	0.06	36,36,36,36	0
54	MG	2A	3349	1/1	0.98	0.09	44,44,44,44	0
54	MG	1A	3566	1/1	0.98	0.05	36,36,36,36	0
54	MG	1A	3352	1/1	0.98	0.09	25,25,25,25	0
54	MG	2A	3615	1/1	0.98	0.04	82,82,82,82	0
54	MG	1A	3428	1/1	0.98	0.05	27,27,27,27	0
54	MG	2A	3617	1/1	0.98	0.06	64,64,64,64	0
54	MG	1A	3921	1/1	0.98	0.05	21,21,21,21	0
54	MG	2A	3619	1/1	0.98	0.05	53,53,53,53	0
54	MG	2A	3620	1/1	0.98	0.04	71,71,71,71	0
54	MG	1A	3295	1/1	0.98	0.06	48,48,48,48	0
54	MG	1E	303	1/1	0.98	0.09	43,43,43,43	0
54	MG	2A	3628	1/1	0.98	0.05	48,48,48,48	0
54	MG	1A	3052	1/1	0.98	0.26	44,44,44,44	0
54	MG	2a	3166	1/1	0.98	0.11	55,55,55,55	0
54	MG	2A	3480	1/1	0.98	0.05	42,42,42,42	0
54	MG	13	101	1/1	0.98	0.12	33,33,33,33	0
54	MG	2a	3010	1/1	0.98	0.05	54,54,54,54	0
54	MG	2A	3139	1/1	0.98	0.06	42,42,42,42	0
54	MG	1A	3007	1/1	0.98	0.04	44,44,44,44	0
54	MG	2A	3360	1/1	0.98	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3014	1/1	0.98	0.03	61,61,61,61	0
54	MG	2a	3174	1/1	0.98	0.05	64,64,64,64	0
54	MG	2A	3141	1/1	0.98	0.09	59,59,59,59	0
54	MG	1A	3047	1/1	0.98	0.12	16,16,16,16	0
54	MG	2A	3487	1/1	0.98	0.11	43,43,43,43	0
54	MG	1A	3849	1/1	0.98	0.05	41,41,41,41	0
54	MG	2A	3247	1/1	0.98	0.09	23,23,23,23	0
54	MG	2A	3642	1/1	0.98	0.04	42,42,42,42	0
54	MG	1A	3726	1/1	0.98	0.07	49,49,49,49	0
54	MG	1a	1857	1/1	0.98	0.09	72,72,72,72	0
54	MG	1A	3929	1/1	0.98	0.05	59,59,59,59	0
54	MG	15	104	1/1	0.98	0.17	29,29,29,29	0
54	MG	1A	3786	1/1	0.98	0.05	36,36,36,36	0
54	MG	2A	3649	1/1	0.98	0.04	60,60,60,60	0
54	MG	1a	1767	1/1	0.98	0.07	53,53,53,53	0
54	MG	2A	3049	1/1	0.98	0.16	52,52,52,52	0
54	MG	2A	3497	1/1	0.98	0.06	62,62,62,62	0
54	MG	1F	301	1/1	0.98	0.07	31,31,31,31	0
54	MG	1F	302	1/1	0.98	0.13	40,40,40,40	0
54	MG	1A	3357	1/1	0.98	0.07	25,25,25,25	0
54	MG	1A	3078	1/1	0.98	0.15	45,45,45,45	0
54	MG	2A	3377	1/1	0.98	0.10	39,39,39,39	0
54	MG	1A	3359	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3438	1/1	0.98	0.05	36,36,36,36	0
54	MG	1A	3003	1/1	0.98	0.04	27,27,27,27	0
54	MG	17	105	1/1	0.98	0.17	42,42,42,42	0
54	MG	1F	308	1/1	0.98	0.20	30,30,30,30	0
54	MG	1F	309	1/1	0.98	0.16	35,35,35,35	0
54	MG	1A	3937	1/1	0.98	0.12	47,47,47,47	0
54	MG	1A	3049	1/1	0.98	0.03	27,27,27,27	0
54	MG	1A	3006	1/1	0.98	0.03	29,29,29,29	0
59	ZN	1n	104	1/1	0.98	0.04	74,74,74,74	0
59	ZN	2Y	202	1/1	0.98	0.04	93,93,93,93	0
54	MG	2A	3387	1/1	0.98	0.11	36,36,36,36	0
54	MG	1A	3399	1/1	0.98	0.05	29,29,29,29	0
60	SF4	1d	303	8/8	0.98	0.05	60,65,70,78	0
60	SF4	2d	501	8/8	0.98	0.05	67,82,83,88	0
54	MG	2A	3653	1/1	0.99	0.04	70,70,70,70	0
54	MG	2A	3589	1/1	0.99	0.09	44,44,44,44	0
54	MG	1A	3493	1/1	0.99	0.06	32,32,32,32	0
54	MG	1B	213	1/1	0.99	0.04	42,42,42,42	0
54	MG	2A	3344	1/1	0.99	0.03	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3884	1/1	0.99	0.06	43,43,43,43	0
54	MG	1A	3976	1/1	0.99	0.06	26,26,26,26	0
54	MG	1A	3977	1/1	0.99	0.05	35,35,35,35	0
54	MG	2A	3348	1/1	0.99	0.02	38,38,38,38	0
54	MG	1A	4012	1/1	0.99	0.03	63,63,63,63	0
54	MG	1A	3263	1/1	0.99	0.17	34,34,34,34	0
54	MG	1A	3590	1/1	0.99	0.07	50,50,50,50	0
54	MG	1A	3915	1/1	0.99	0.03	55,55,55,55	0
54	MG	1A	3242	1/1	0.99	0.30	34,34,34,34	0
54	MG	2A	3308	1/1	0.99	0.09	50,50,50,50	0
54	MG	1A	3888	1/1	0.99	0.07	43,43,43,43	0
54	MG	1A	3434	1/1	0.99	0.05	42,42,42,42	0
54	MG	2a	3159	1/1	0.99	0.04	64,64,64,64	0
54	MG	1A	3305	1/1	0.99	0.13	25,25,25,25	0
54	MG	1A	3717	1/1	0.99	0.04	44,44,44,44	0
54	MG	1l	103	1/1	0.99	0.06	53,53,53,53	0
54	MG	1A	3436	1/1	0.99	0.02	30,30,30,30	0
54	MG	2A	3103	1/1	0.99	0.06	68,68,68,68	0
54	MG	1A	3330	1/1	0.99	0.09	21,21,21,21	0
54	MG	1A	3222	1/1	0.99	0.03	41,41,41,41	0
54	MG	2A	3364	1/1	0.99	0.03	62,62,62,62	0
54	MG	2A	3557	1/1	0.99	0.04	49,49,49,49	0
54	MG	2A	3274	1/1	0.99	0.06	51,51,51,51	0
54	MG	1A	3924	1/1	0.99	0.03	42,42,42,42	0
54	MG	1A	3868	1/1	0.99	0.06	54,54,54,54	0
54	MG	1A	3286	1/1	0.99	0.10	22,22,22,22	0
54	MG	2A	3463	1/1	0.99	0.06	37,37,37,37	0
54	MG	1A	3762	1/1	0.99	0.11	38,38,38,38	0
54	MG	1a	1852	1/1	0.99	0.03	47,47,47,47	0
54	MG	2A	3622	1/1	0.99	0.03	66,66,66,66	0
54	MG	2A	3623	1/1	0.99	0.06	35,35,35,35	0
54	MG	2A	3688	1/1	0.99	0.04	52,52,52,52	0
54	MG	2A	3624	1/1	0.99	0.05	40,40,40,40	0
54	MG	2A	3625	1/1	0.99	0.04	60,60,60,60	0
54	MG	1a	1853	1/1	0.99	0.05	61,61,61,61	0
54	MG	1A	3847	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3549	1/1	0.99	0.06	33,33,33,33	0
54	MG	2A	3469	1/1	0.99	0.03	50,50,50,50	0
54	MG	2A	3630	1/1	0.99	0.11	57,57,57,57	0
54	MG	2A	3569	1/1	0.99	0.03	53,53,53,53	0
54	MG	2k	201	1/1	0.99	0.10	57,57,57,57	0
54	MG	1A	3900	1/1	0.99	0.03	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3633	1/1	0.99	0.03	58,58,58,58	0
54	MG	2A	3571	1/1	0.99	0.05	42,42,42,42	0
54	MG	1D	307	1/1	0.99	0.03	19,19,19,19	0
54	MG	1A	3723	1/1	0.99	0.03	36,36,36,36	0
54	MG	2A	3574	1/1	0.99	0.04	41,41,41,41	0
54	MG	2X	101	1/1	0.99	0.07	63,63,63,63	0
54	MG	1A	3932	1/1	0.99	0.06	54,54,54,54	0
54	MG	1A	3668	1/1	0.99	0.04	50,50,50,50	0
54	MG	1A	3474	1/1	0.99	0.04	27,27,27,27	0
54	MG	1A	3966	1/1	0.99	0.03	49,49,49,49	0
54	MG	1A	3852	1/1	0.99	0.06	23,23,23,23	0
54	MG	2A	3580	1/1	0.99	0.06	47,47,47,47	0
54	MG	1A	3475	1/1	0.99	0.06	32,32,32,32	0
54	MG	2A	3645	1/1	0.99	0.03	47,47,47,47	0
54	MG	1A	3906	1/1	0.99	0.05	42,42,42,42	0
59	ZN	1Y	202	1/1	0.99	0.02	62,62,62,62	0
54	MG	1A	3347	1/1	0.99	0.08	30,30,30,30	0
59	ZN	15	109	1/1	0.99	0.02	52,52,52,52	0
59	ZN	16	501	1/1	0.99	0.05	47,47,47,47	0
54	MG	1a	1748	1/1	0.99	0.11	42,42,42,42	0
54	MG	1A	3490	1/1	0.99	0.03	49,49,49,49	0
54	MG	2a	3138	1/1	0.99	0.07	52,52,52,52	0
59	ZN	25	102	1/1	0.99	0.03	68,68,68,68	0
59	ZN	29	501	1/1	0.99	0.03	73,73,73,73	0
54	MG	2A	3650	1/1	0.99	0.04	44,44,44,44	0
54	MG	1A	3141	1/1	0.99	0.13	26,26,26,26	0
54	MG	1A	3422	1/1	0.99	0.08	23,23,23,23	0
54	MG	2A	3621	1/1	1.00	0.02	66,66,66,66	0
59	ZN	19	104	1/1	1.00	0.10	65,65,65,65	0
54	MG	1A	3534	1/1	1.00	0.07	31,31,31,31	0
54	MG	1A	3361	1/1	1.00	0.05	36,36,36,36	0
54	MG	1A	3499	1/1	1.00	0.07	49,49,49,49	0
54	MG	1A	3882	1/1	1.00	0.07	33,33,33,33	0
59	ZN	26	501	1/1	1.00	0.02	65,65,65,65	0
54	MG	1A	3637	1/1	1.00	0.06	32,32,32,32	0
54	MG	1A	3467	1/1	1.00	0.02	27,27,27,27	0
54	MG	2a	3124	1/1	1.00	0.03	60,60,60,60	0
54	MG	2A	3585	1/1	1.00	0.03	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.