



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 12:01 PM EDT

PDB ID : 6XHX / pdb_00006xhx
Title : Crystal structure of the A2058-unmethylated Thermus thermophilus 70S ribosome in complex with erythromycin and protein Y (YfiA) at 2.55Å resolution
Authors : Svetlov, M.S.; Syroegin, E.A.; Aleksandrova, E.V.; Atkinson, G.C.; Gregory, S.T.; Mankin, A.S.; Polikanov, Y.S.
Deposited on : 2020-06-19
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<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

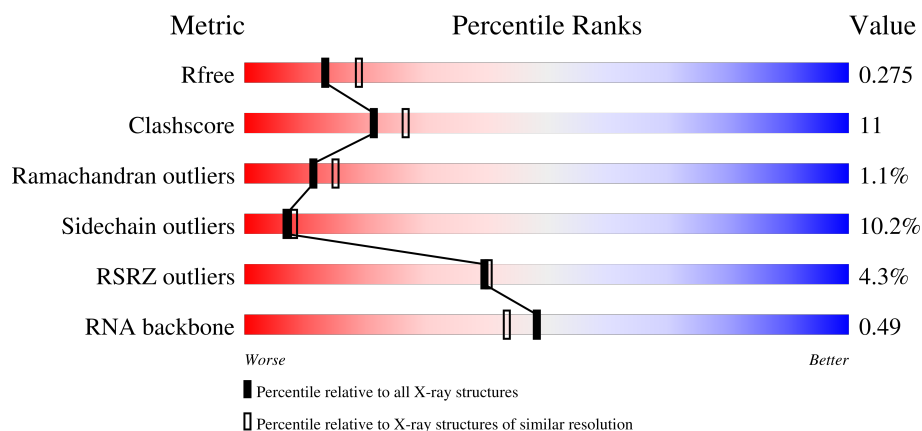
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	2% 61% 31% 7%
1	2A	2915	2% 55% 36% 8%
2	1B	121	63% 31% 5%

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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	

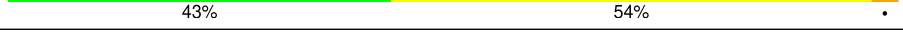
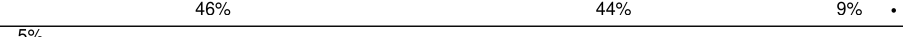
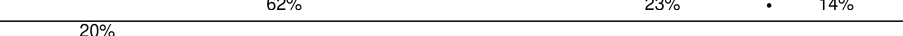
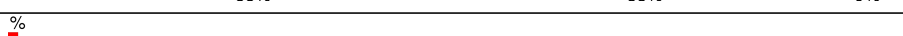
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Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25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

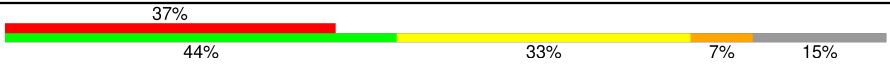
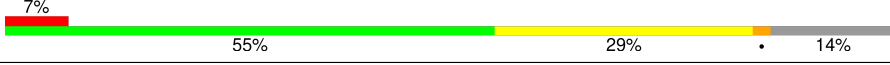
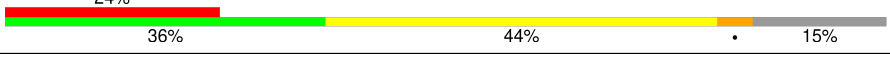
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Mol	Chain	Length	Quality of chain
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	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	2a	3115	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 296819 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
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	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	1020	Total	Mg	0	0
			1020	1020		
54	1B	32	Total	Mg	0	0
			32	32		
54	1D	16	Total	Mg	0	0
			16	16		
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	6	Total	Mg	0	0
			6	6		
54	1Q	4	Total	Mg	0	0
			4	4		
54	1R	5	Total	Mg	0	0
			5	5		
54	1T	3	Total	Mg	0	0
			3	3		
54	1U	8	Total	Mg	0	0
			8	8		
54	1V	7	Total	Mg	0	0
			7	7		
54	1W	4	Total	Mg	0	0
			4	4		
54	1Y	2	Total	Mg	0	0
			2	2		
54	1Z	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	10	7	Total 7	Mg 7	0	0
54	11	4	Total 4	Mg 4	0	0
54	13	4	Total 4	Mg 4	0	0
54	15	6	Total 6	Mg 6	0	0
54	17	5	Total 5	Mg 5	0	0
54	18	2	Total 2	Mg 2	0	0
54	19	1	Total 1	Mg 1	0	0
54	1a	274	Total 274	Mg 274	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	5	Total 5	Mg 5	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
54	1t	2	Total 2	Mg 2	0	0
54	1y	3	Total 3	Mg 3	0	0

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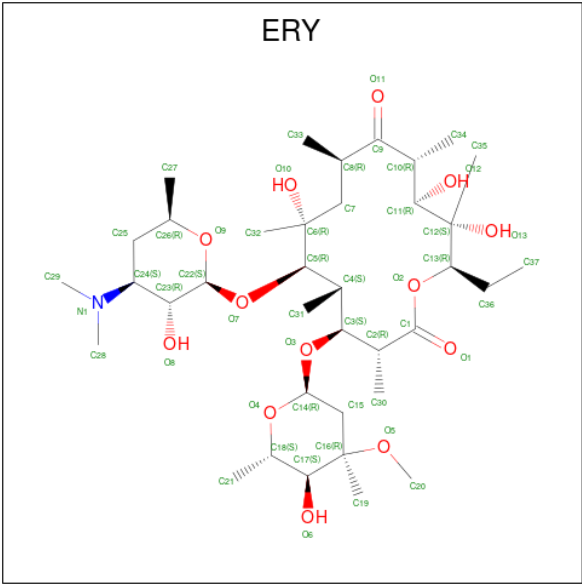
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2A	733	Total 733	Mg 733	0	0
54	2B	18	Total 18	Mg 18	0	0
54	2D	10	Total 10	Mg 10	0	0
54	2E	7	Total 7	Mg 7	0	0
54	2F	4	Total 4	Mg 4	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2I	1	Total 1	Mg 1	0	0
54	2N	1	Total 1	Mg 1	0	0
54	2O	2	Total 2	Mg 2	0	0
54	2P	2	Total 2	Mg 2	0	0
54	2Q	2	Total 2	Mg 2	0	0
54	2R	2	Total 2	Mg 2	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	20	2	Total 2	Mg 2	0	0
54	21	1	Total 1	Mg 1	0	0
54	23	1	Total 1	Mg 1	0	0
54	25	2	Total 2	Mg 2	0	0
54	27	1	Total 1	Mg 1	0	0

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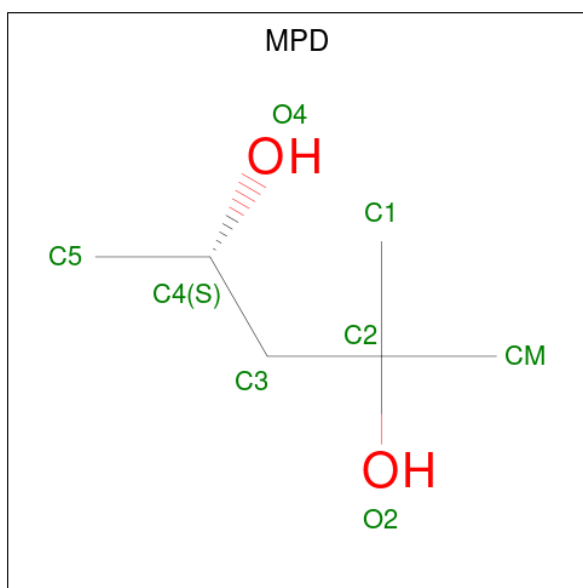
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	28	2	Total	Mg	0	0
			2	2		
54	2a	183	Total	Mg	0	0
			183	183		
54	2e	2	Total	Mg	0	0
			2	2		
54	2f	1	Total	Mg	0	0
			1	1		
54	2j	1	Total	Mg	0	0
			1	1		
54	2l	1	Total	Mg	0	0
			1	1		
54	2n	1	Total	Mg	0	0
			1	1		
54	2o	1	Total	Mg	0	0
			1	1		
54	2t	1	Total	Mg	0	0
			1	1		

- Molecule 55 is ERYTHROMYCIN A (CCD ID: ERY) (formula: C₃₇H₆₇NO₁₃).



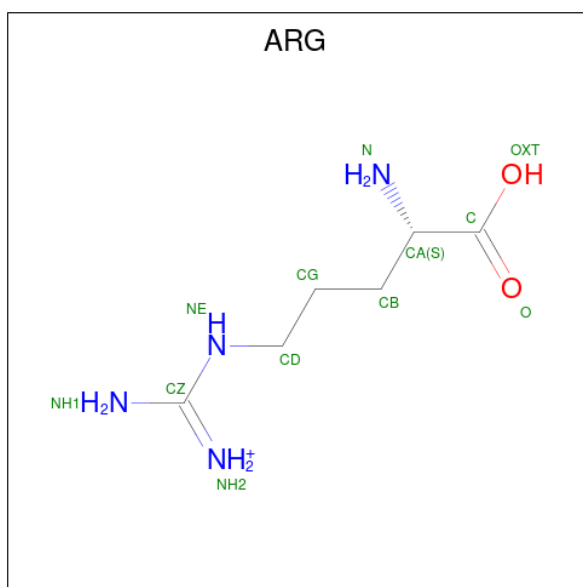
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	1A	1	Total	C	N	O	0	0
			51	37	1	13		
55	2A	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 56 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	1A	1	Total	C	O	0	0
			8	6	2		
56	1T	1	Total	C	O	0	0
			8	6	2		
56	18	1	Total	C	O	0	0
			8	6	2		
56	1a	1	Total	C	O	0	0
			8	6	2		
56	2A	1	Total	C	O	0	0
			8	6	2		
56	2A	1	Total	C	O	0	0
			8	6	2		
56	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 57 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1B	1	Total	C	N	O	0	0
			12	6	4	2		
57	1F	1	Total	C	N	O	0	0
			12	6	4	2		

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

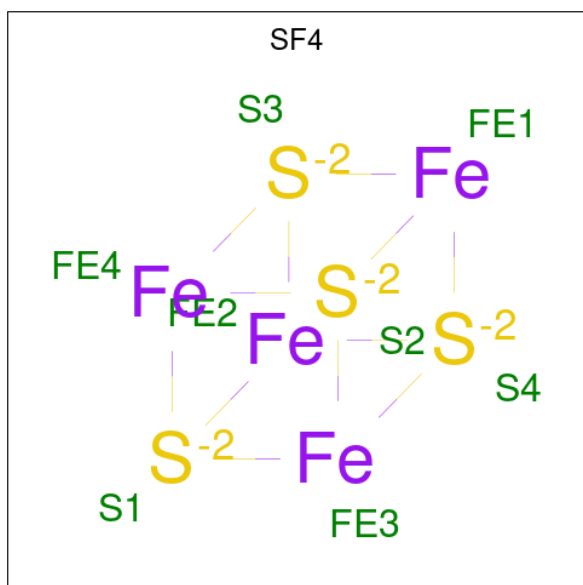
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3765	Total	O	0	0
			3765	3765		
60	1B	106	Total	O	0	0
			106	106		
60	1D	90	Total	O	0	0
			90	90		
60	1E	74	Total	O	0	0
			74	74		
60	1F	67	Total	O	0	0
			67	67		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1G	18	Total	O	0	0
			18	18		
60	1H	14	Total	O	0	0
			14	14		
60	1I	8	Total	O	0	0
			8	8		
60	1N	51	Total	O	0	0
			51	51		
60	1O	26	Total	O	0	0
			26	26		
60	1P	57	Total	O	0	0
			57	57		
60	1Q	41	Total	O	0	0
			41	41		
60	1R	32	Total	O	0	0
			32	32		
60	1S	14	Total	O	0	0
			14	14		
60	1T	33	Total	O	0	0
			33	33		
60	1U	42	Total	O	0	0
			42	42		
60	1V	39	Total	O	0	0
			39	39		
60	1W	27	Total	O	0	0
			27	27		
60	1X	24	Total	O	0	0
			24	24		
60	1Y	18	Total	O	0	0
			18	18		
60	1Z	13	Total	O	0	0
			13	13		
60	10	20	Total	O	0	0
			20	20		
60	11	25	Total	O	0	0
			25	25		
60	12	12	Total	O	0	0
			12	12		
60	13	26	Total	O	0	0
			26	26		
60	14	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	15	28	Total 28	O 28	0	0
60	16	19	Total 19	O 19	0	0
60	17	14	Total 14	O 14	0	0
60	18	28	Total 28	O 28	0	0
60	19	5	Total 5	O 5	0	0
60	1a	465	Total 465	O 465	0	0
60	1d	9	Total 9	O 9	0	0
60	1e	1	Total 1	O 1	0	0
60	1f	2	Total 2	O 2	0	0
60	1h	1	Total 1	O 1	0	0
60	1i	1	Total 1	O 1	0	0
60	1j	1	Total 1	O 1	0	0
60	1k	1	Total 1	O 1	0	0
60	1l	5	Total 5	O 5	0	0
60	1m	3	Total 3	O 3	0	0
60	1o	3	Total 3	O 3	0	0
60	1p	1	Total 1	O 1	0	0
60	1u	1	Total 1	O 1	0	0
60	1y	3	Total 3	O 3	0	0
60	2A	1860	Total 1860	O 1860	0	0
60	2B	53	Total 53	O 53	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2D	40	Total 40	O 40	0	0
60	2E	19	Total 19	O 19	0	0
60	2F	22	Total 22	O 22	0	0
60	2G	7	Total 7	O 7	0	0
60	2H	4	Total 4	O 4	0	0
60	2I	4	Total 4	O 4	0	0
60	2N	3	Total 3	O 3	0	0
60	2O	19	Total 19	O 19	0	0
60	2P	19	Total 19	O 19	0	0
60	2Q	18	Total 18	O 18	0	0
60	2R	17	Total 17	O 17	0	0
60	2S	3	Total 3	O 3	0	0
60	2T	8	Total 8	O 8	0	0
60	2U	16	Total 16	O 16	0	0
60	2V	3	Total 3	O 3	0	0
60	2W	13	Total 13	O 13	0	0
60	2X	6	Total 6	O 6	0	0
60	2Y	5	Total 5	O 5	0	0
60	2Z	7	Total 7	O 7	0	0
60	20	10	Total 10	O 10	0	0
60	21	20	Total 20	O 20	0	0

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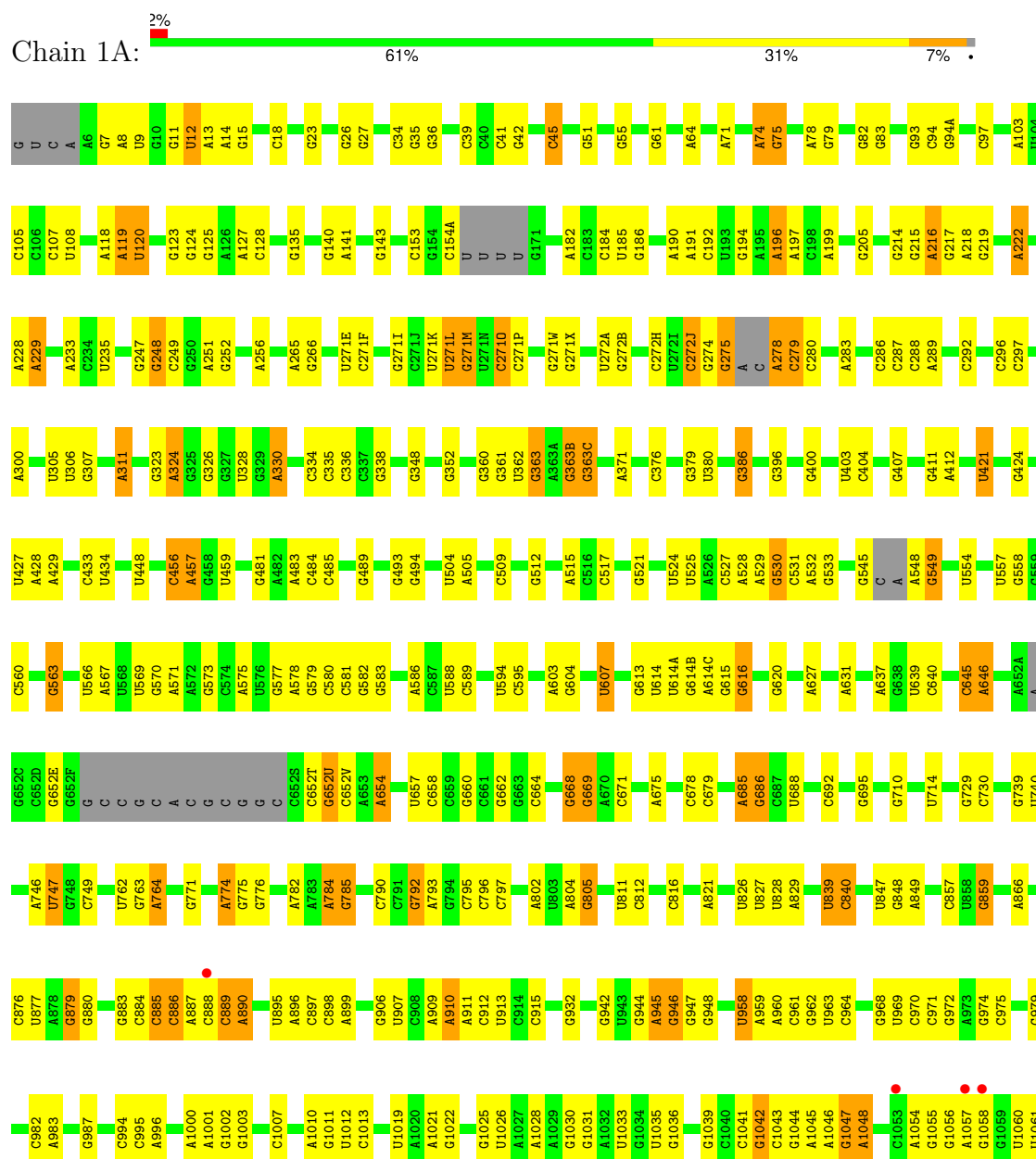
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	22	2	Total 2	O 2	0	0
60	23	3	Total 3	O 3	0	0
60	25	6	Total 6	O 6	0	0
60	26	5	Total 5	O 5	0	0
60	27	9	Total 9	O 9	0	0
60	28	9	Total 9	O 9	0	0
60	29	1	Total 1	O 1	0	0
60	2a	303	Total 303	O 303	0	0
60	2d	2	Total 2	O 2	0	0
60	2e	1	Total 1	O 1	0	0
60	2f	2	Total 2	O 2	0	0
60	2j	2	Total 2	O 2	0	0
60	2l	2	Total 2	O 2	0	0
60	2m	3	Total 3	O 3	0	0
60	2n	1	Total 1	O 1	0	0
60	2o	2	Total 2	O 2	0	0
60	2p	2	Total 2	O 2	0	0
60	2q	1	Total 1	O 1	0	0
60	2r	4	Total 4	O 4	0	0
60	2y	3	Total 3	O 3	0	0

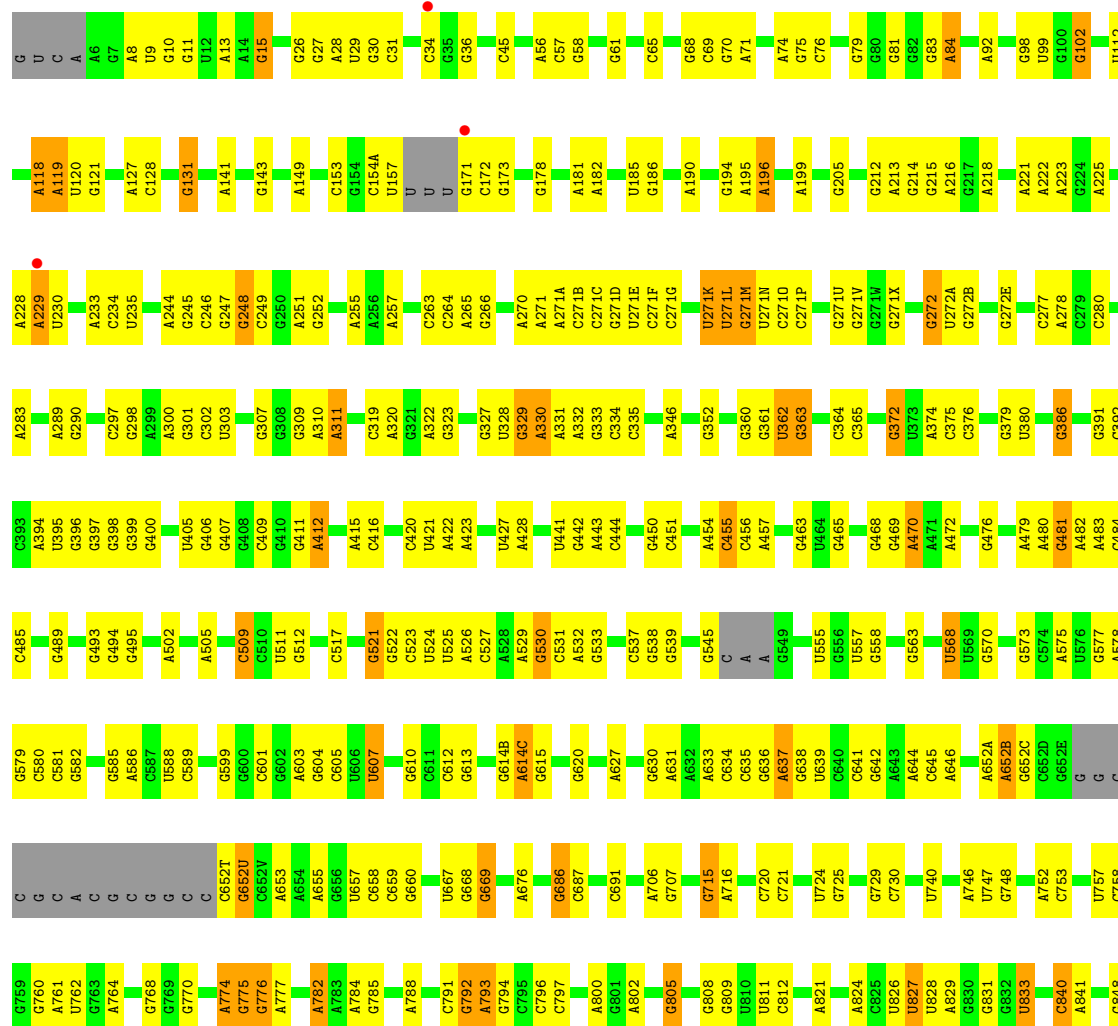
3 Residue-property plots

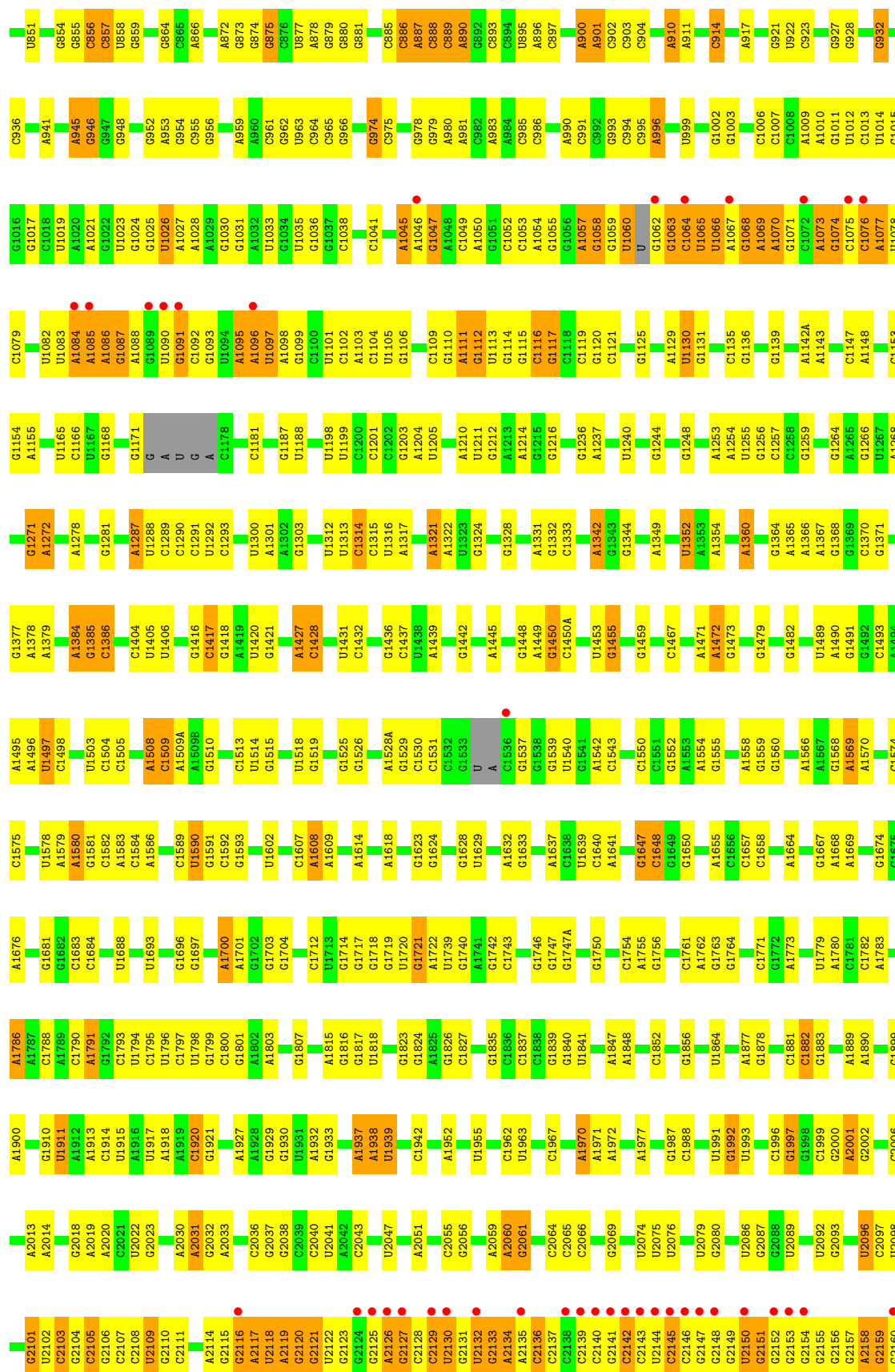
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

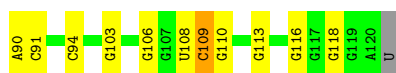


G2421	A2422	U2423	A2424	A2425	A2426	A2427	G2428	G2429	A2430	A2435	U2438	A2439	C2440	C2441	C2442	C2443	C2444	G2445	G2446	G2447	A2448	G2453	C2464	C2465	C2467	G2468	A2469	C2475	A2476	C2477	C2478	A2479	C2480	C2483	G2484	G2485	G2486	G2487	U2491	U2492	C2493	C2498	C2499	G2502	A2503	U2504	G2505	U2506	G2509	C2510		
C2314	G2315	C2316	C2319	A2320	G2325	G2326	A2327	A2328	G2329	G2330	G2331	G2334	A2335	A2336	G2341	G2345	A2346	C2347	U2348	G2349	C2350	G2353	C2354	C2355	C2356	U2357	C2364	G2365	G2372	C2373	C2374	A2375	A2376	A2377	A2378	C2381	G2382	G2383	G2384	C2385	C2386	U2390	A2393	G2396	G2405	U2406	C2313					
G2207	A2208	A2225	G2228	U2232	U2233	G2238	G2239	G2242	U2243	U2244	C2248	U2249	G2250	G2251	C2254	C2258	C2264	A2268	A2273	A2274	C2275	G2276	A2277	A2278	G2279	G2280	C2281	G2282	C2283	A2286	A2287	A2288	G2289	G2290	U2291	C2292	G2303	G2304	A2305	G2308	U2309	A2310	U2311	U2312	U2313	C2202	C2206					
C2137	C2138	C2139	C2140	G2141	G2142	C2143	U2144	C2145	C2146	C2147	G2148	G2149	U2150	G2151	G2153	G2154	G2155	G2156	G2157	A2158	G2159	G2160	G2161	G2162	C2163	C2164	G2165	G2166	U2167	G2168	A2169	A2170	U2171	U2172	A2173	U2180	G2181	G2182	C2183	G2184	C2185	G2186	G2187	C2188	U2189	G2190	G2191	G2192	G2193	A2198	C2202	C2206
A2060	G2061	C2066	G2069	U2074	U2075	U2076	U2079	U2086	G2087	U2092	G2093	G2094	C2095	U2096	U2097	U2098	G2099	G2100	G2101	C2102	C2103	G2104	C2105	G2106	C2107	C2108	U2109	G2110	G2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	G2119	G2120	G2121	U2122	G2123	A2126	G2127	C2128	C2129	U2130	G2131	U2132	G2133	A2134	A2135	C2136
C2137	C2138	C2139	C2140	G2141	G2142	C2143	U2144	C2145	C2146	C2147	G2148	G2149	U2150	G2151	G2153	G2154	G2155	G2156	G2157	A2158	G2159	G2160	G2161	G2162	C2163	C2164	G2165	G2166	U2167	G2168	A2169	A2170	U2171	U2172	A2173	U2180	G2181	G2182	C2183	G2184	C2185	G2186	G2187	C2188	U2189	G2190	G2191	G2192	G2193	A2198	C2202	C2206
G2207	A2208	A2225	G2228	U2232	U2233	G2238	G2239	G2242	U2243	U2244	C2248	U2249	G2250	G2251	C2254	C2258	C2264	A2268	A2273	A2274	C2275	G2276	A2277	A2278	G2279	G2280	C2281	G2282	C2283	A2286	A2287	A2288	G2289	G2290	U2291	C2292	G2303	G2304	A2305	G2308	U2309	A2310	U2311	U2312	U2313	C2202	C2206					
C2314	G2315	C2316	C2319	A2320	G2325	G2326	A2327	A2328	G2329	G2330	G2331	G2334	A2335	A2336	G2341	G2345	A2346	C2347	U2348	G2349	C2350	G2353	C2354	C2355	C2356	U2357	C2364	G2365	G2372	C2373	C2374	A2375	A2376	A2377	A2378	C2381	G2382	G2383	G2384	C2385	C2386	U2390	A2393	G2396	G2405	U2406	C2313					
G2421	A2422	U2423	A2424	A2425	A2426	A2427	G2428	G2429	A2430	A2435	U2438	A2439	C2440	C2441	C2442	C2443	C2444	G2445	G2446	G2447	A2448	G2453	C2464	C2465	C2467	G2468	A2469	C2475	A2476	C2477	C2478	A2479	C2480	C2483	G2484	G2485	G2486	G2487	U2491	U2492	C2493	C2498	C2499	G2502	A2503	U2504	G2505	U2506	G2509	C2510		

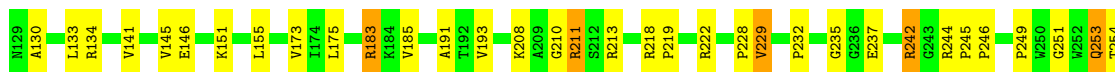
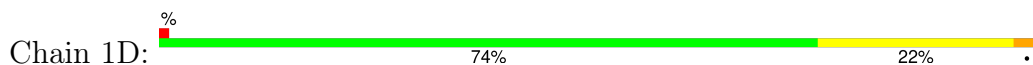




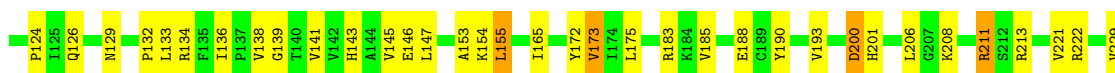




• Molecule 3: 50S ribosomal protein L2



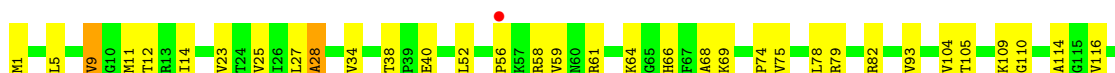
• Molecule 3: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L3



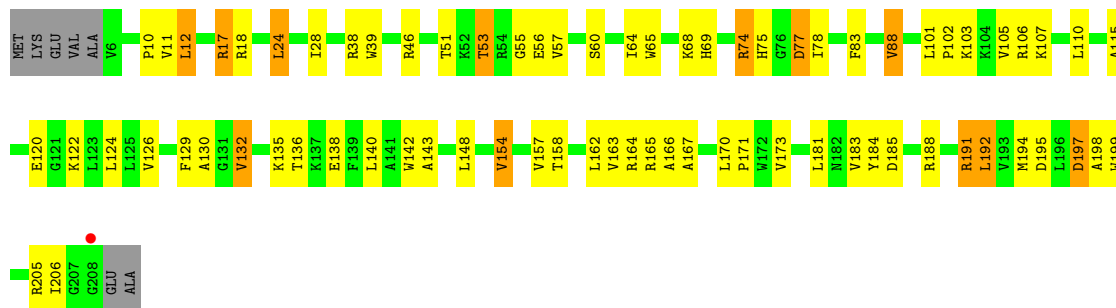
• Molecule 4: 50S ribosomal protein L3





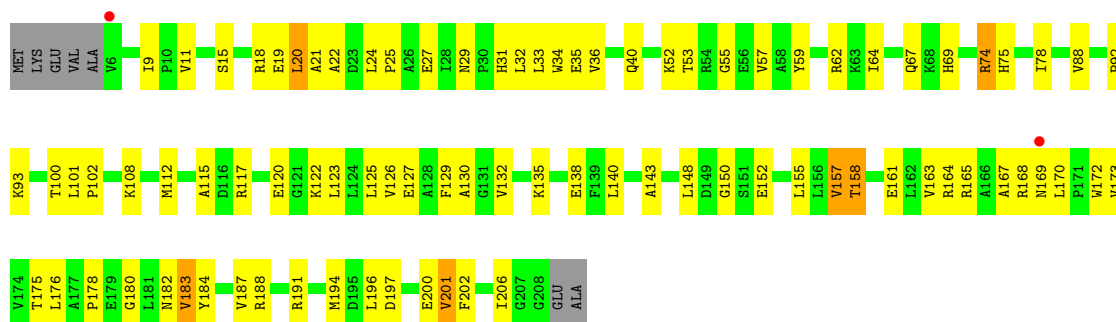
- Molecule 5: 50S ribosomal protein L4

Chain 1F: 61% 30% 6%



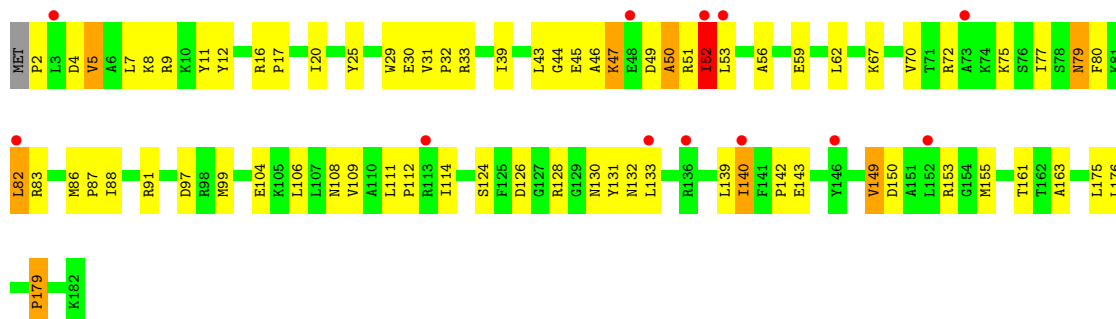
- Molecule 5: 50S ribosomal protein L4

Chain 2F: 55% 39%



- Molecule 6: 50S ribosomal protein L5

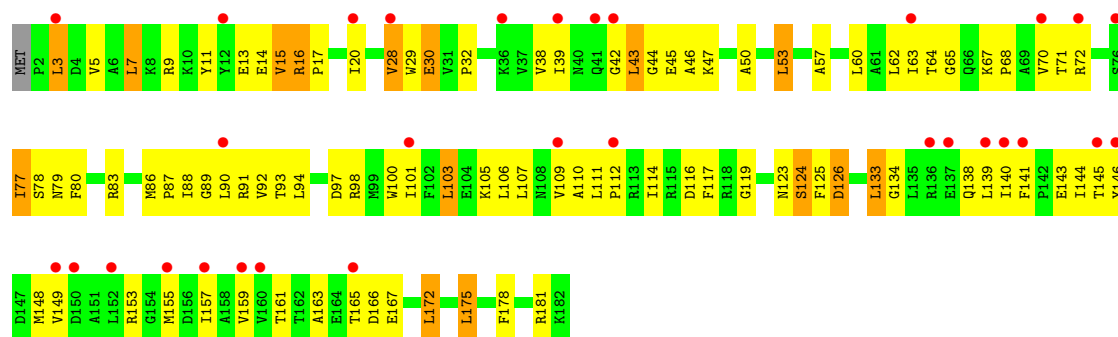
Chain 1G: 7% 59% 35%



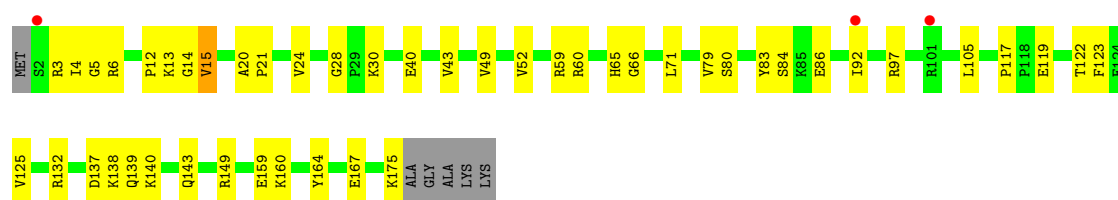
- Molecule 6: 50S ribosomal protein L5

Chain 2G: 17% 47% 44% 8%

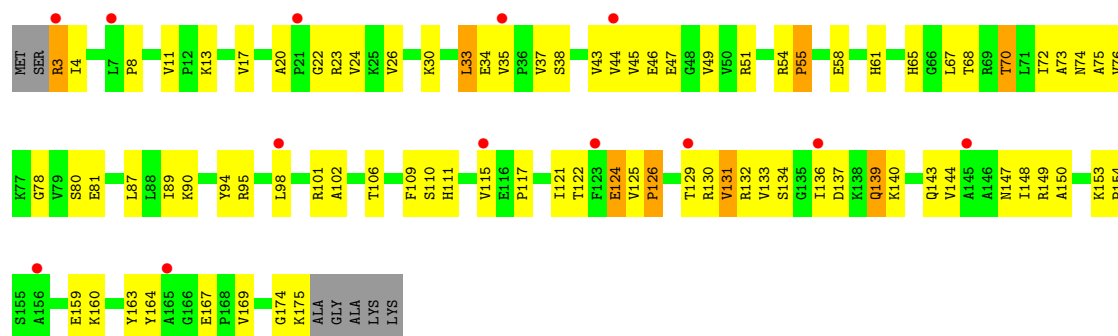




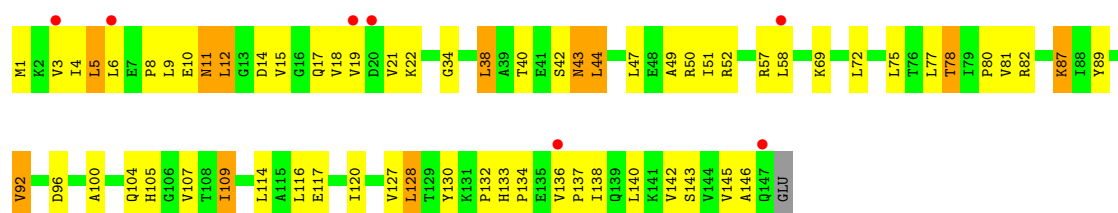
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

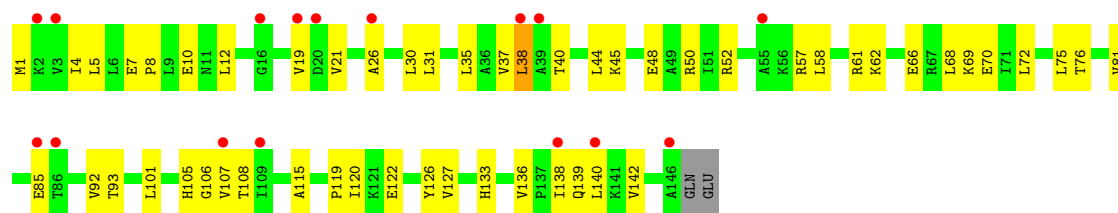


• Molecule 8: 50S ribosomal protein L9



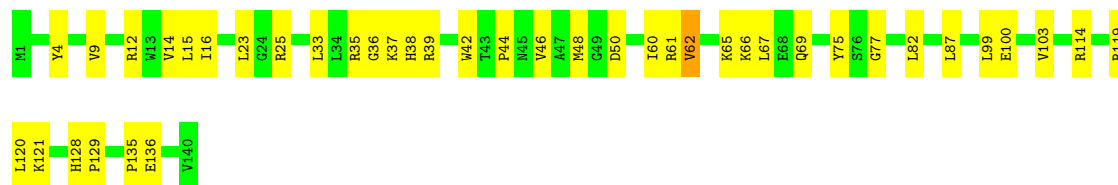
• Molecule 8: 50S ribosomal protein L9





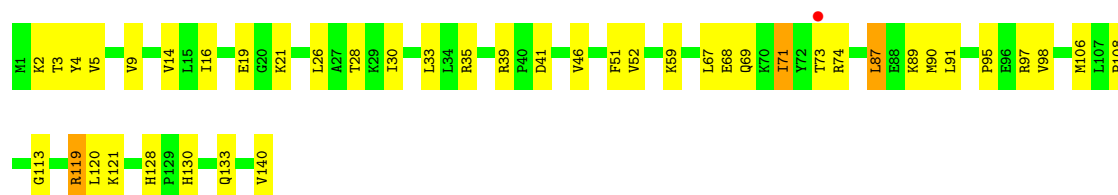
• Molecule 9: 50S ribosomal protein L13

Chain 1N: 71% 29% .



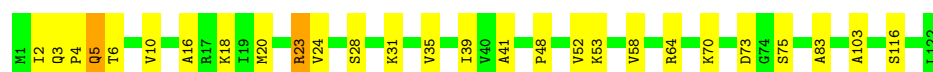
• Molecule 9: 50S ribosomal protein L13

Chain 2N: 69% 29% .



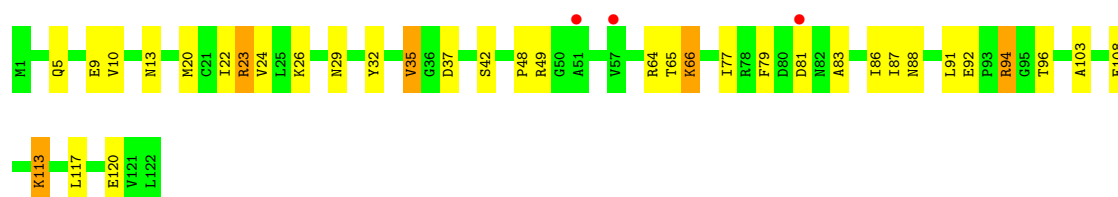
• Molecule 10: 50S ribosomal protein L14

Chain 1O: 78% 20% .



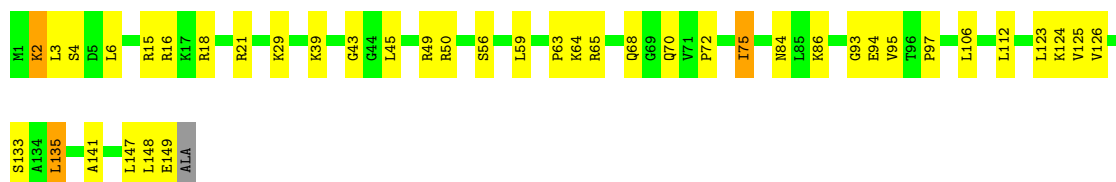
• Molecule 10: 50S ribosomal protein L14

Chain 2O: 71% 25% .

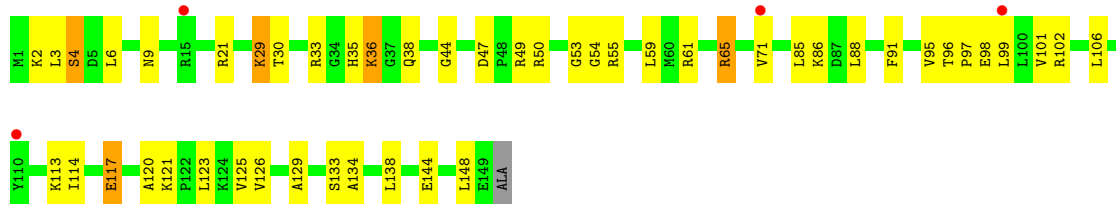


• Molecule 11: 50S ribosomal protein L15

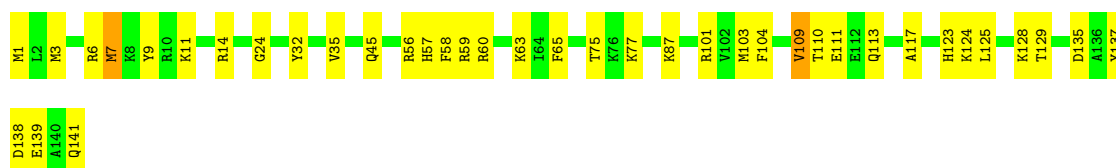
Chain 1P: 72% 25% ..



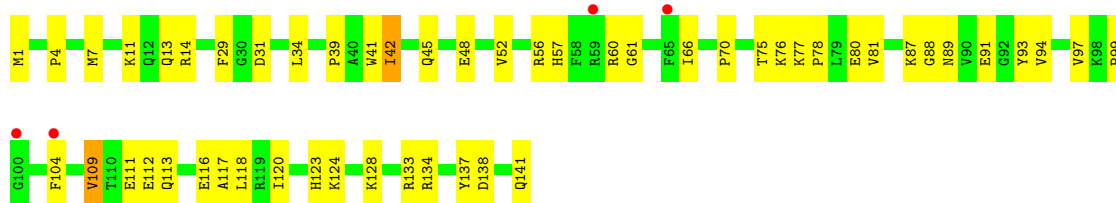
- Molecule 11: 50S ribosomal protein L15



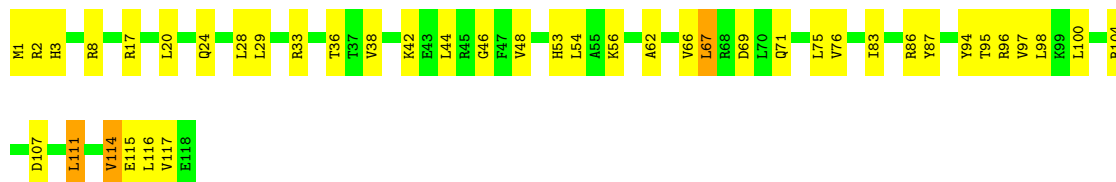
- Molecule 12: 50S ribosomal protein L16



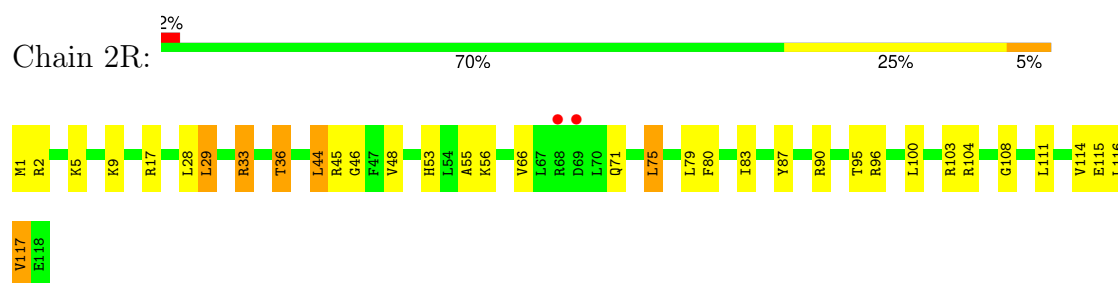
- Molecule 12: 50S ribosomal protein L16



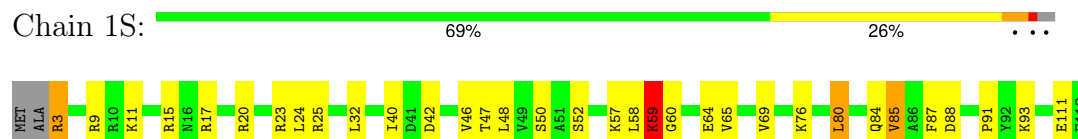
- Molecule 13: 50S ribosomal protein L17



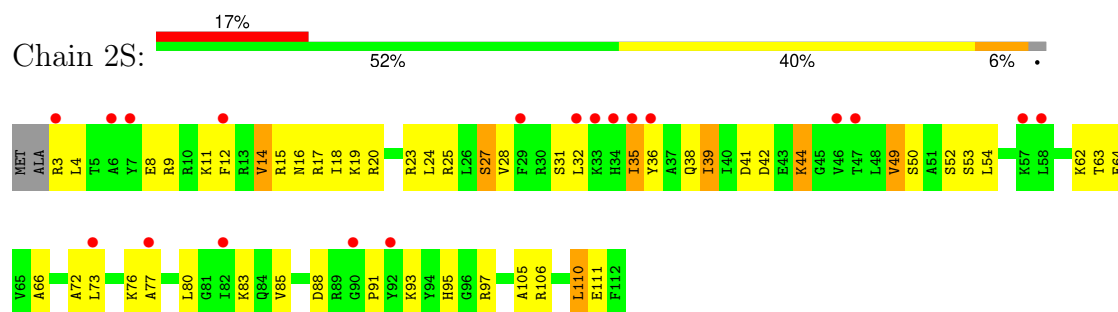
- Molecule 13: 50S ribosomal protein L17



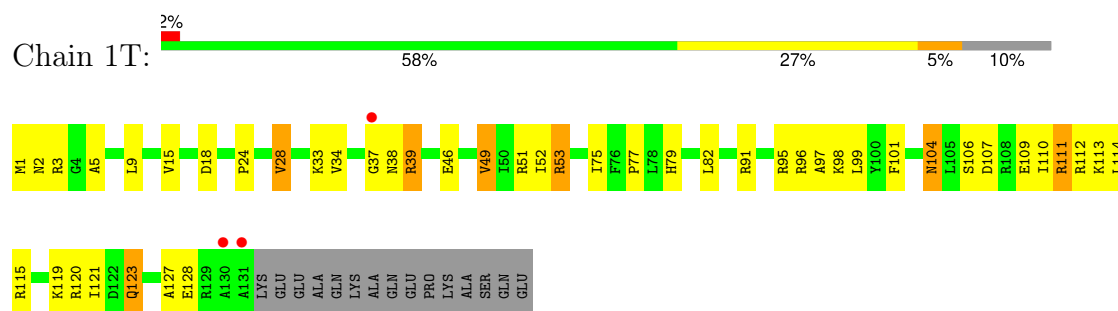
- Molecule 14: 50S ribosomal protein L18



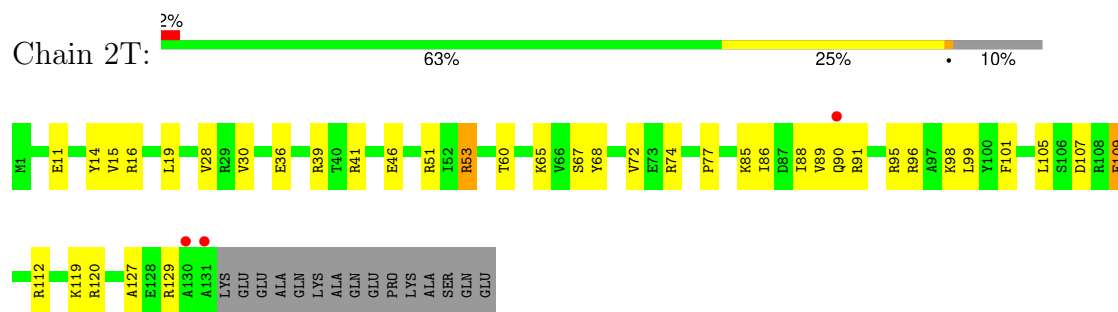
- Molecule 14: 50S ribosomal protein L18



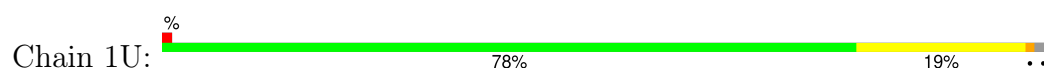
- Molecule 15: 50S ribosomal protein L19



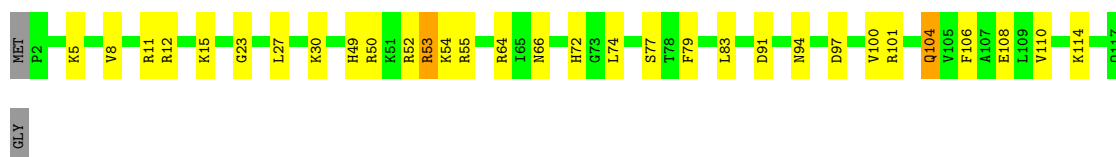
- Molecule 15: 50S ribosomal protein L19



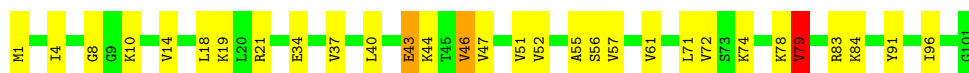
- Molecule 16: 50S ribosomal protein L20



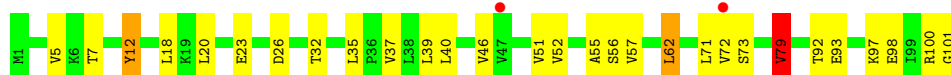
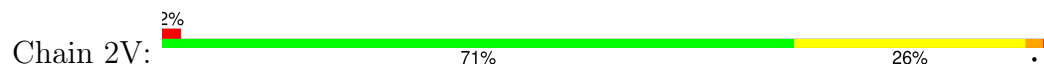
• Molecule 16: 50S ribosomal protein L20



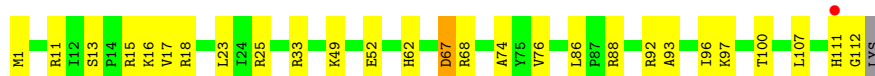
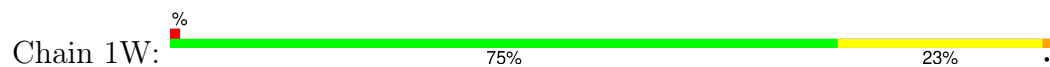
• Molecule 17: 50S ribosomal protein L21



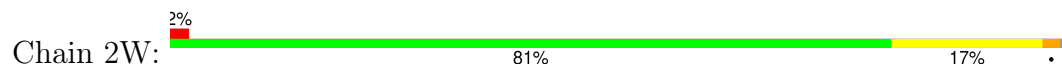
• Molecule 17: 50S ribosomal protein L21



• Molecule 18: 50S ribosomal protein L22

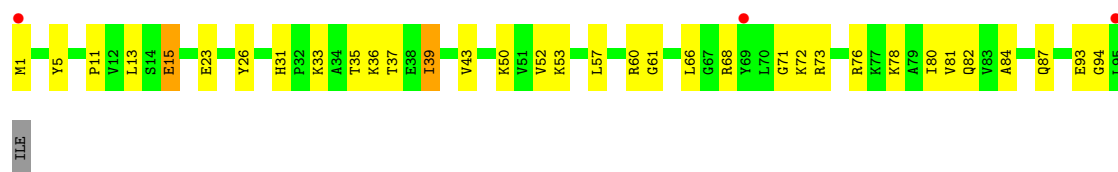


• Molecule 18: 50S ribosomal protein L22



• Molecule 19: 50S ribosomal protein L23

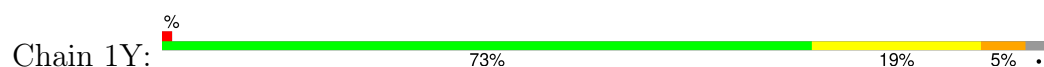




- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25





- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27



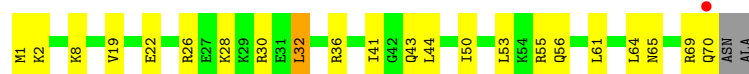
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28

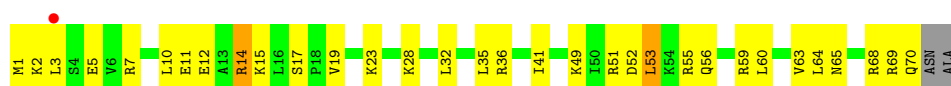


- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29





- Molecule 25: 50S ribosomal protein L30

Chain 13: 63% 30% 5% .



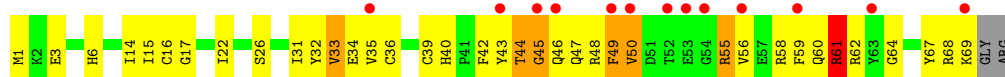
- Molecule 25: 50S ribosomal protein L30

Chain 23: 7% 73% 23% . .



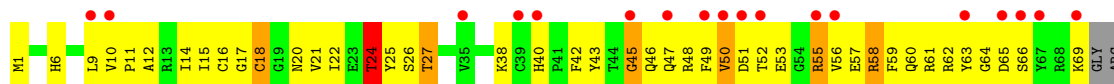
- Molecule 26: 50S ribosomal protein L31

Chain 14: 18% 45% 42% 8% . .



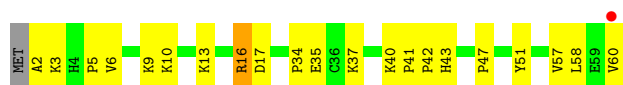
- Molecule 26: 50S ribosomal protein L31

Chain 24: 25% 35% 52% 8% . .



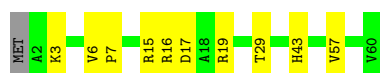
- Molecule 27: 50S ribosomal protein L32

Chain 15: 2% 63% 33% . .



- Molecule 27: 50S ribosomal protein L32

Chain 25: 82% 17% .



- Molecule 28: 50S ribosomal protein L33

Chain 16:  59% 35% ..



- Molecule 28: 50S ribosomal protein L33

Chain 26:  2% 67% 20% 11% ..



- Molecule 29: 50S ribosomal protein L34

Chain 17:  4% 67% 29% ..



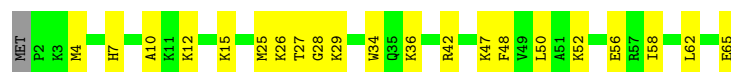
- Molecule 29: 50S ribosomal protein L34

Chain 27:  2% 73% 20% ..



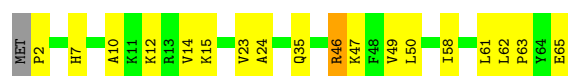
- Molecule 30: 50S ribosomal protein L35

Chain 18:  66% 32% ..



- Molecule 30: 50S ribosomal protein L35

Chain 28:  71% 26% ..

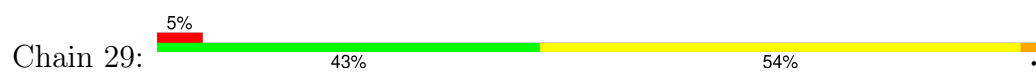


- Molecule 31: 50S ribosomal protein L36

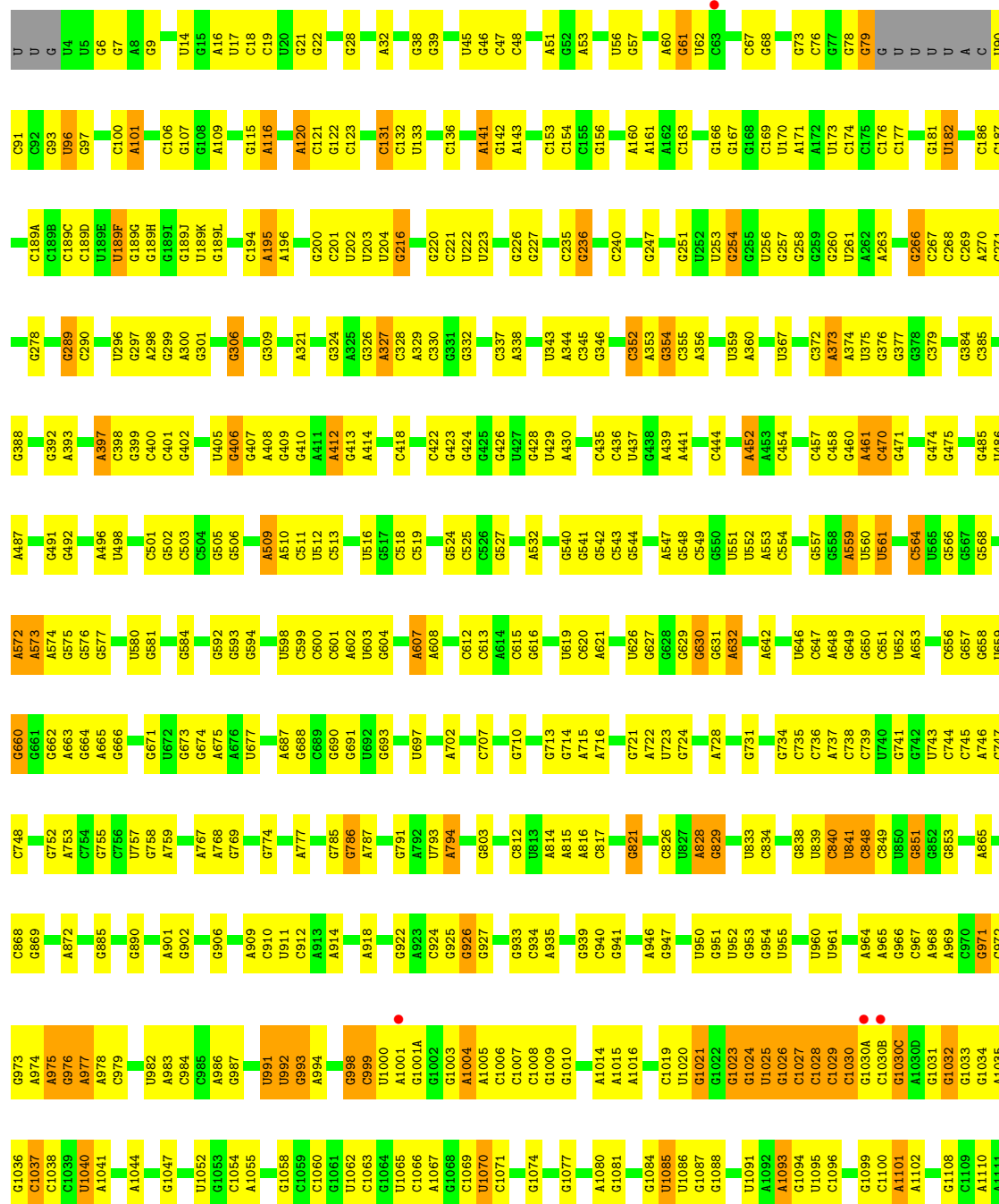
Chain 19:  81% 16% ..



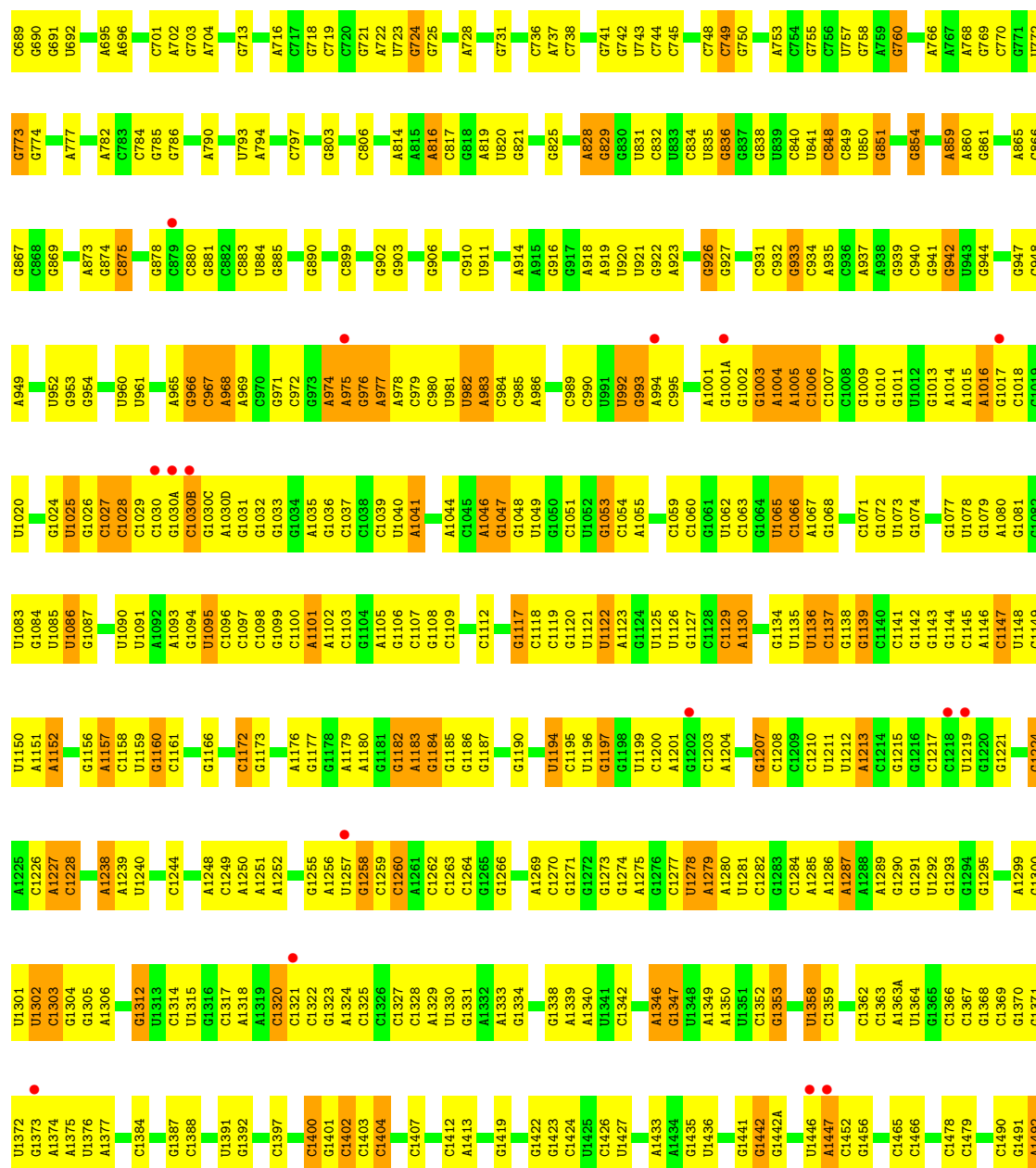
- Molecule 31: 50S ribosomal protein L36



• Molecule 32: 16S Ribosomal RNA

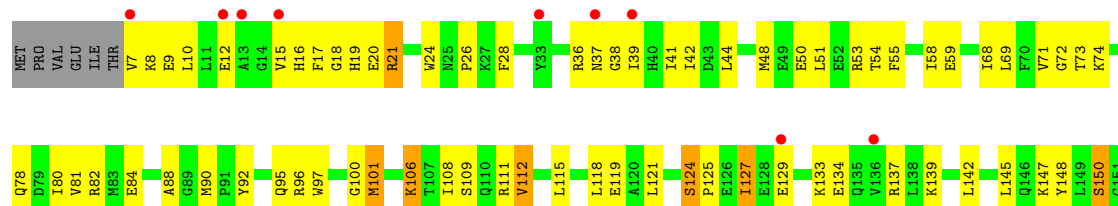


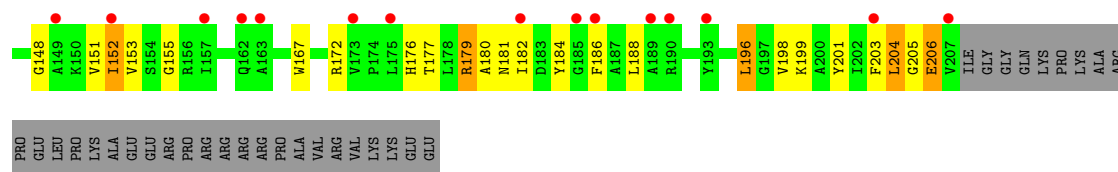




• Molecule 33: 30S ribosomal protein S2

Chain 1b: 5% 48% 37% 6% 10%





• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

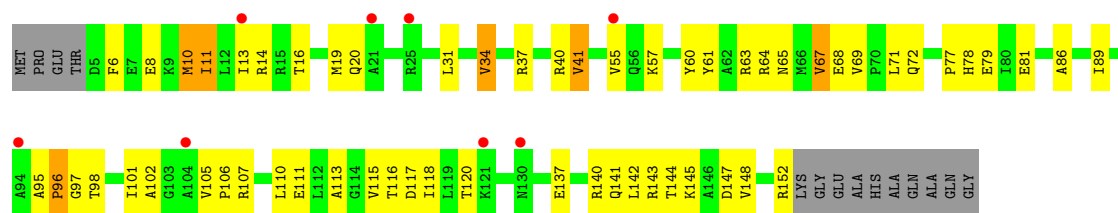


• Molecule 36: 30S ribosomal protein S5

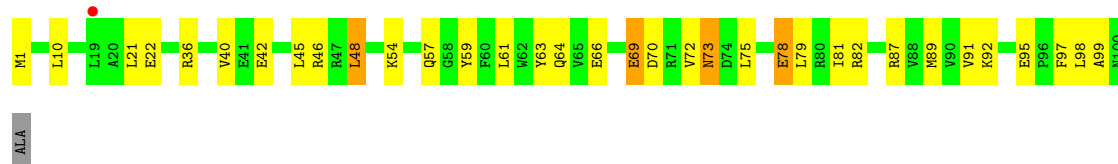


• Molecule 36: 30S ribosomal protein S5





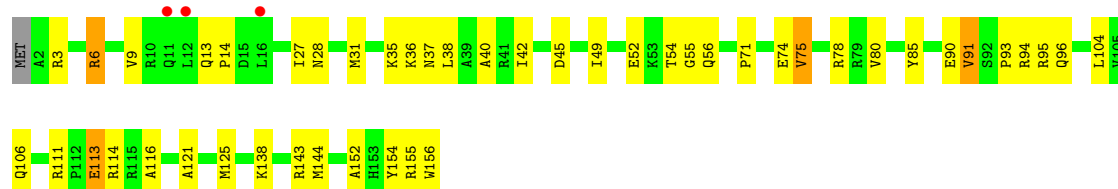
• Molecule 37: 30S ribosomal protein S6



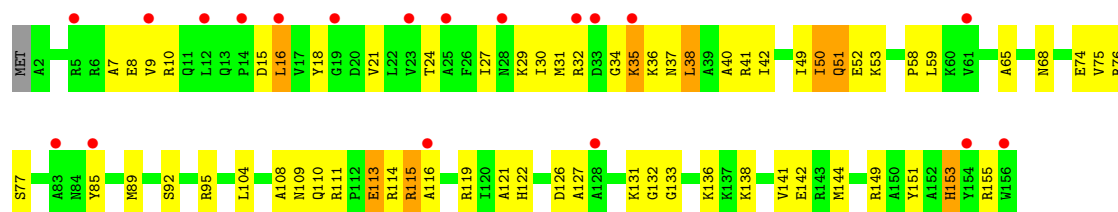
• Molecule 37: 30S ribosomal protein S6



• Molecule 38: 30S ribosomal protein S7

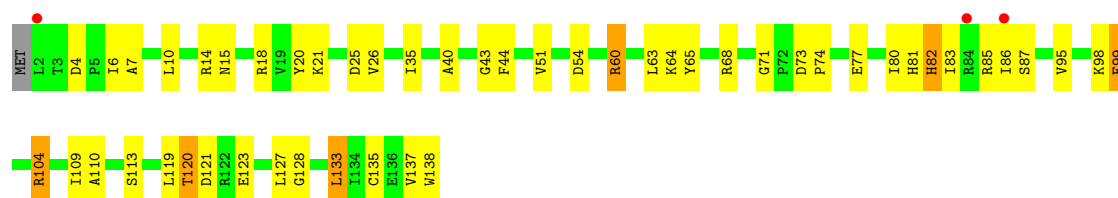


• Molecule 38: 30S ribosomal protein S7

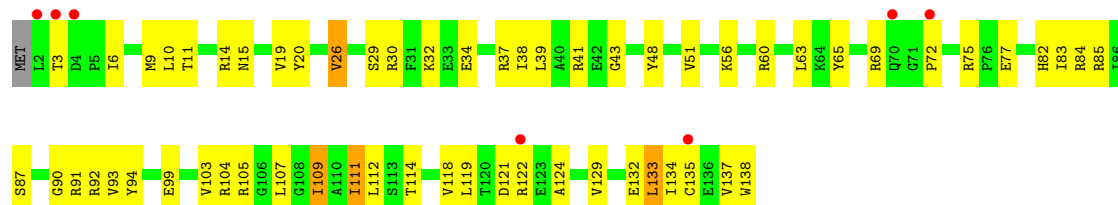


• Molecule 39: 30S ribosomal protein S8

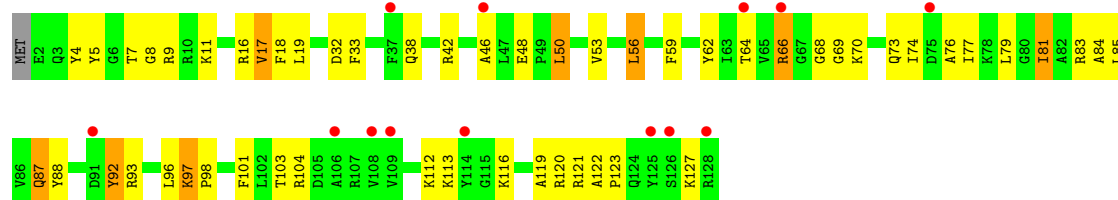




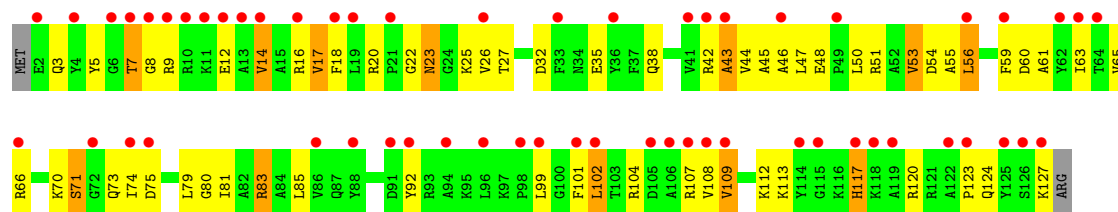
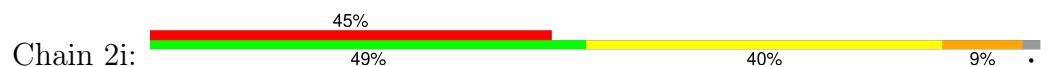
• Molecule 39: 30S ribosomal protein S8



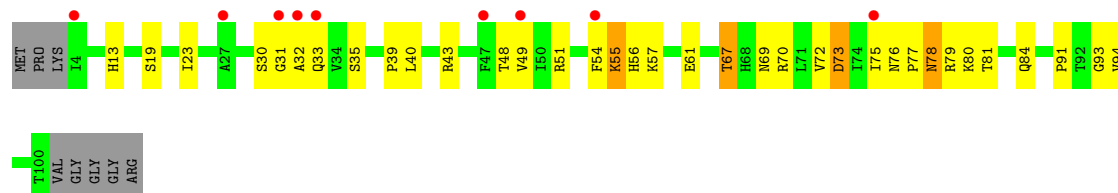
• Molecule 40: 30S ribosomal protein S9



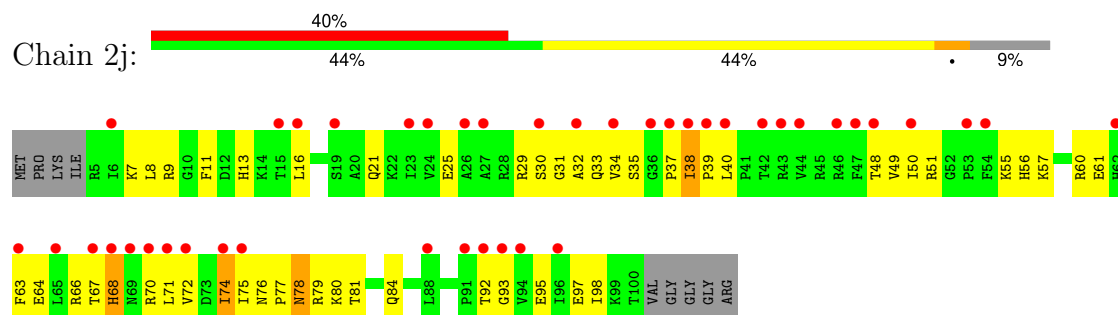
• Molecule 40: 30S ribosomal protein S9



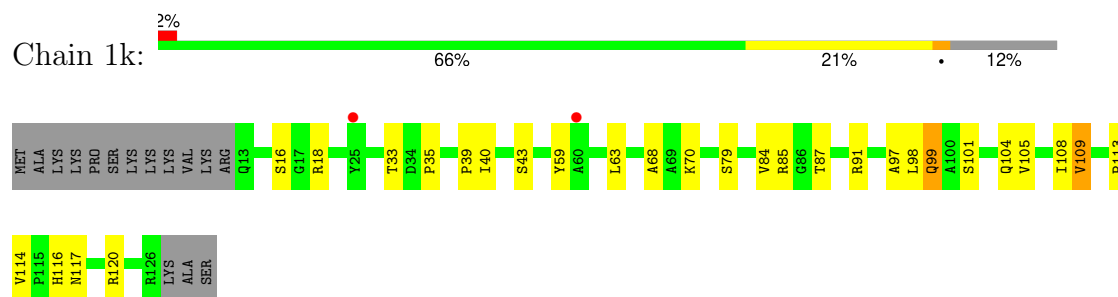
• Molecule 41: 30S ribosomal protein S10



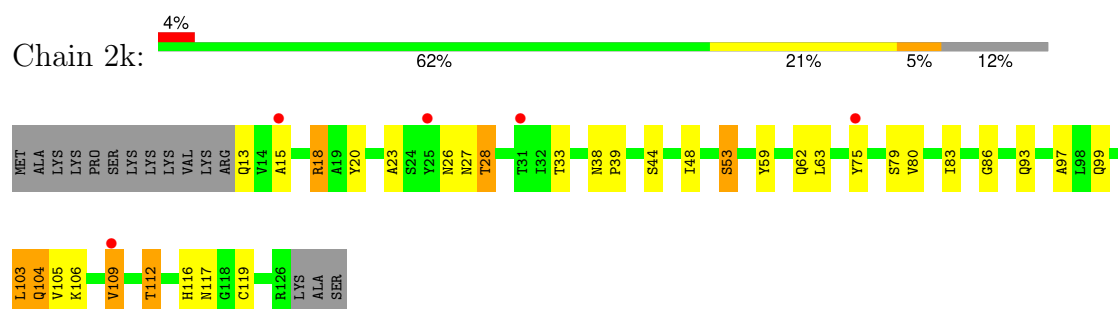
- Molecule 41: 30S ribosomal protein S10



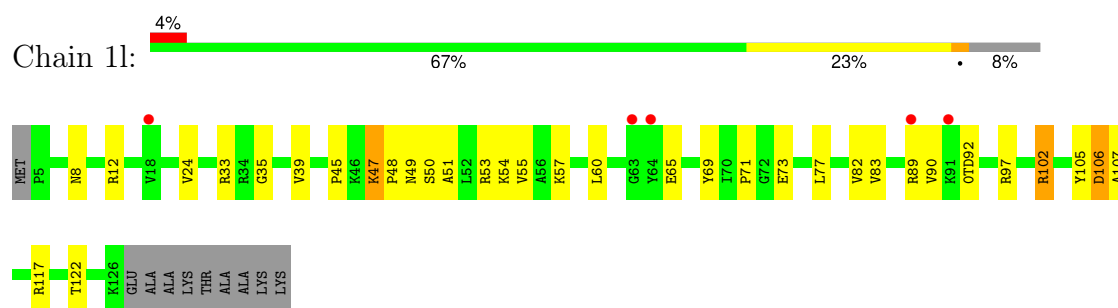
- Molecule 42: 30S ribosomal protein S11



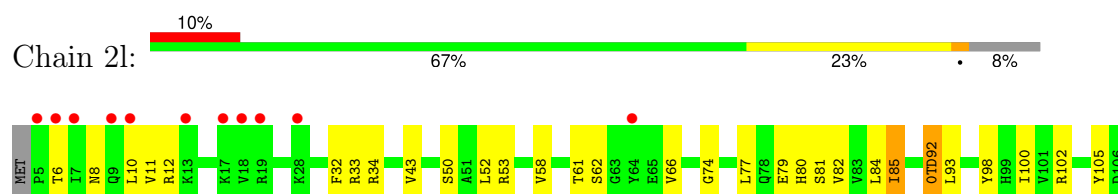
- Molecule 42: 30S ribosomal protein S11

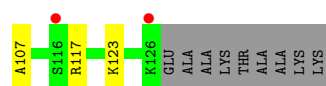


- Molecule 43: 30S ribosomal protein S12

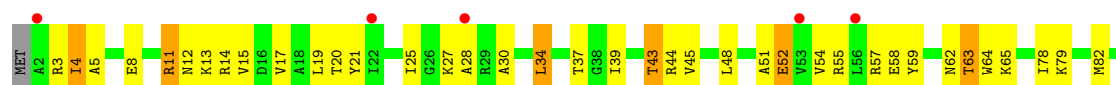


- Molecule 43: 30S ribosomal protein S12

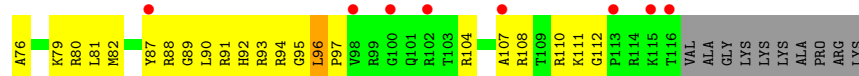
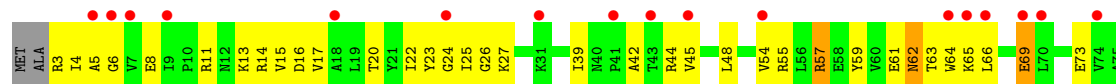




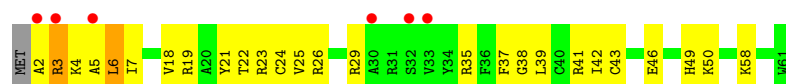
- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13



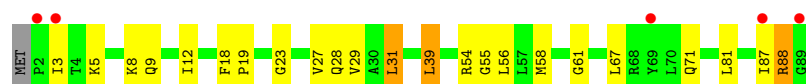
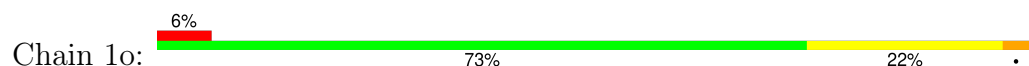
- Molecule 45: 30S ribosomal protein S14 type Z



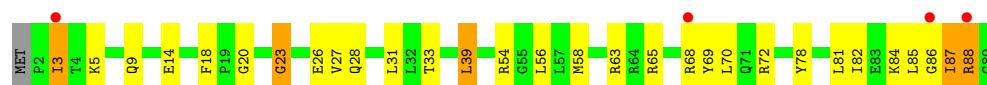
- Molecule 45: 30S ribosomal protein S14 type Z



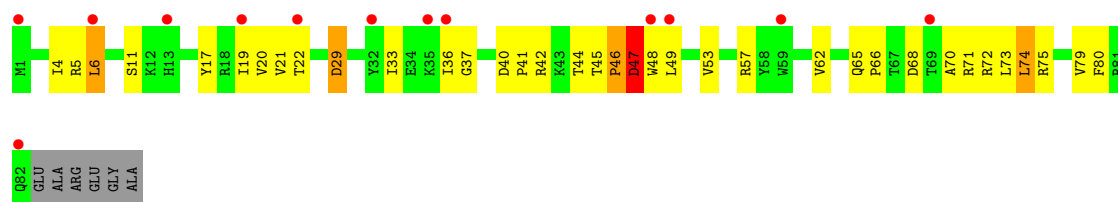
- Molecule 46: 30S ribosomal protein S15



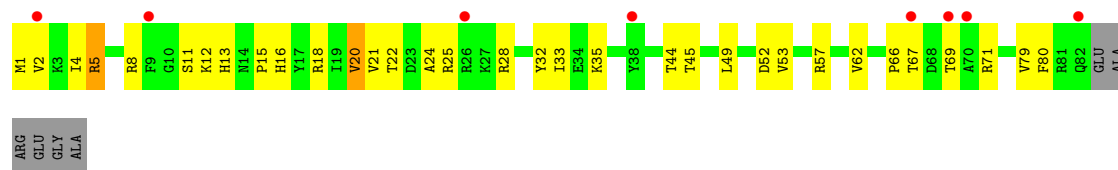
- Molecule 46: 30S ribosomal protein S15



• Molecule 47: 30S ribosomal protein S16



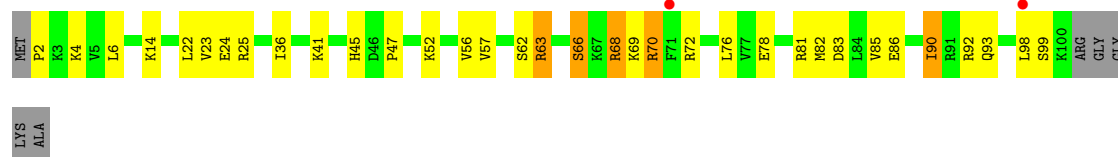
• Molecule 47: 30S ribosomal protein S16



• Molecule 48: 30S ribosomal protein S17

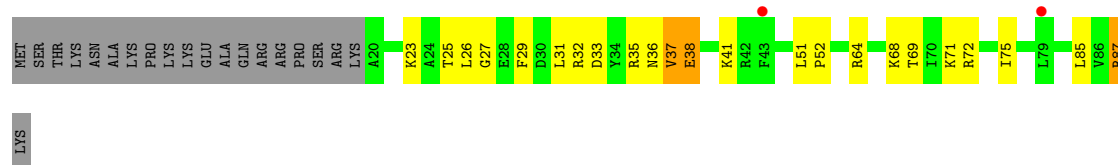


• Molecule 48: 30S ribosomal protein S17

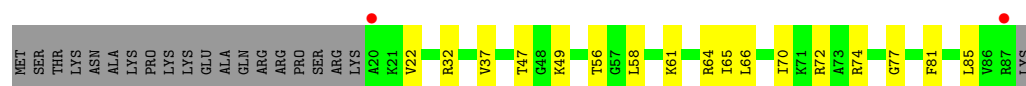


• Molecule 49: 30S ribosomal protein S18

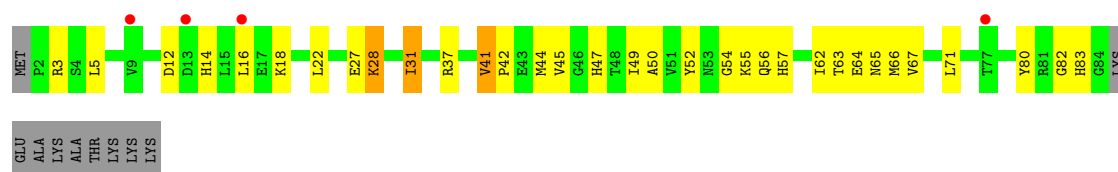




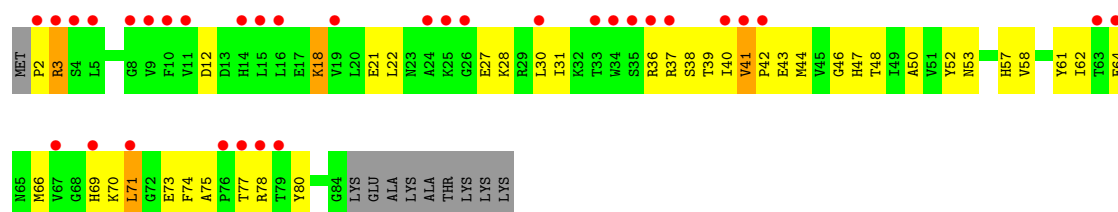
- Molecule 49: 30S ribosomal protein S18



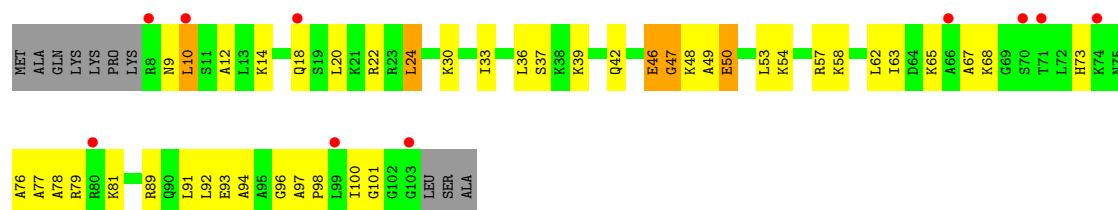
- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19

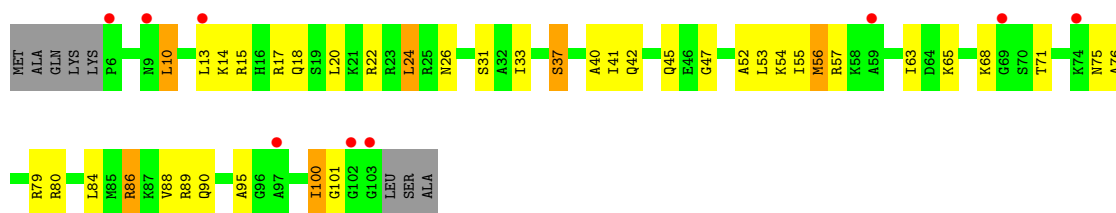


- Molecule 51: 30S ribosomal protein S20

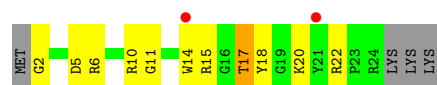
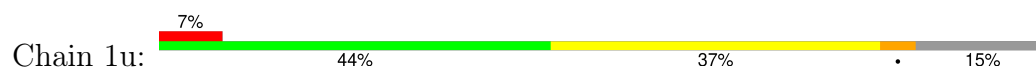


- Molecule 51: 30S ribosomal protein S20

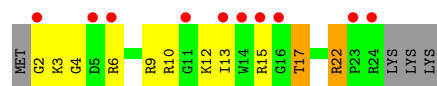
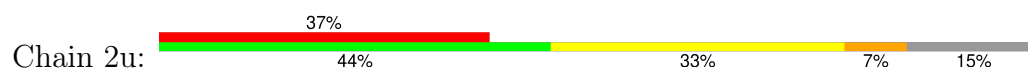




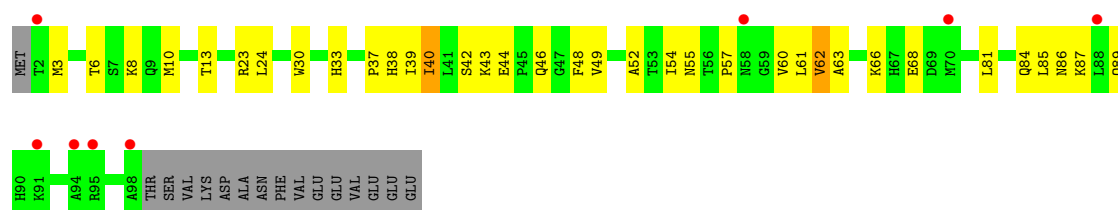
- Molecule 52: 30S ribosomal protein Thx



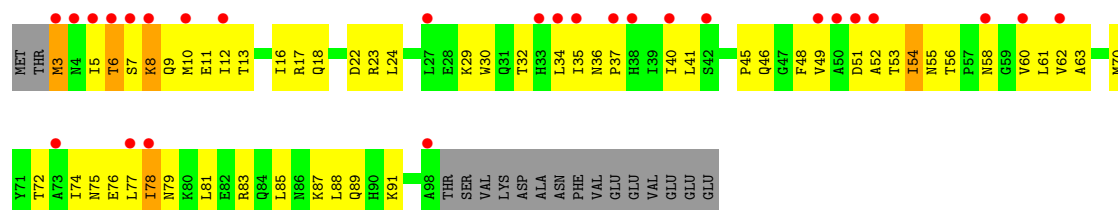
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: 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	209.51Å 448.86Å 619.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.43 – 2.55 224.43 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (224.43-2.55) 99.9 (224.43-2.55)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.222 , 0.272 0.228 , 0.275	Depositor DCC
R_{free} test set	93828 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 82.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	296819	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: 2MG, SF4, MG, 0TD, 5MU, MPD, UR3, 2MU, 2MA, ERY, 5MC, 7MG, MA6, 4OC, OMG, M2G, ZN, PSU

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	0/69029	0.50	4/107746 (0.0%)
1	2A	0.24	0/68901	0.43	1/107544 (0.0%)
2	1B	0.25	0/2876	0.45	0/4486
2	2B	0.20	0/2878	0.38	0/4490
3	1D	0.29	0/2181	0.55	0/2940
3	2D	0.25	0/2186	0.48	0/2944
4	1E	0.28	0/1592	0.51	0/2149
4	2E	0.22	0/1592	0.50	1/2149 (0.0%)
5	1F	0.26	0/1619	0.47	0/2193
5	2F	0.22	0/1615	0.51	0/2188
6	1G	0.22	0/1451	0.45	0/1961
6	2G	0.22	0/1449	0.47	0/1957
7	1H	0.24	0/1356	0.43	0/1834
7	2H	0.19	0/1350	0.41	0/1826
8	1I	0.20	0/1109	0.43	0/1512
8	2I	0.18	0/1091	0.40	0/1490
9	1N	0.27	0/1148	0.48	0/1547
9	2N	0.21	0/1144	0.39	0/1543
10	1O	0.30	0/943	0.53	0/1269
10	2O	0.21	0/943	0.45	0/1269
11	1P	0.29	0/1152	0.55	0/1533
11	2P	0.23	0/1152	0.47	0/1533
12	1Q	0.28	0/1143	0.50	0/1527
12	2Q	0.21	0/1143	0.45	0/1527
13	1R	0.30	0/982	0.52	0/1312
13	2R	0.23	0/982	0.48	0/1312
14	1S	0.24	0/887	0.49	0/1180
14	2S	0.21	0/880	0.46	0/1172
15	1T	0.26	0/1105	0.50	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	0.41	0/1301
17	1V	0.26	0/786	0.46	0/1053
17	2V	0.20	0/782	0.46	0/1049
18	1W	0.28	0/897	0.49	0/1205
18	2W	0.23	0/897	0.43	0/1205
19	1X	0.27	0/764	0.55	0/1025
19	2X	0.22	0/764	0.45	0/1025
20	1Y	0.28	0/823	0.56	0/1099
20	2Y	0.22	0/823	0.46	0/1100
21	1Z	0.24	0/1620	0.44	0/2200
21	2Z	0.21	0/1590	0.46	0/2162
22	10	0.29	0/616	0.52	0/821
22	20	0.22	0/616	0.47	0/821
23	11	0.27	0/761	0.45	0/1013
23	21	0.24	0/766	0.49	0/1018
24	12	0.26	0/590	0.52	0/781
24	22	0.21	0/594	0.40	0/785
25	13	0.30	0/474	0.53	0/635
25	23	0.21	0/469	0.44	0/630
26	14	0.22	0/559	0.58	0/754
26	24	0.28	0/549	0.63	0/741
27	15	0.29	0/473	0.55	0/639
27	25	0.23	0/469	0.48	0/635
28	16	0.26	0/460	0.48	0/613
28	26	0.23	0/456	0.43	0/608
29	17	0.32	0/426	0.54	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.29	0/525	0.49	0/691
30	28	0.22	0/525	0.38	0/691
31	19	0.25	0/310	0.48	0/407
31	29	0.22	0/310	0.43	0/407
32	1a	0.21	0/35795	0.40	1/55864 (0.0%)
32	2a	0.21	0/35890	0.40	1/56012 (0.0%)
33	1b	0.21	0/1876	0.48	0/2533
33	2b	0.24	0/1860	0.49	0/2518
34	1c	0.20	0/1582	0.41	0/2137
34	2c	0.23	0/1566	0.43	0/2119
35	1d	0.21	0/1695	0.46	0/2274
35	2d	0.22	0/1698	0.48	0/2277
36	1e	0.22	0/1149	0.45	0/1548
36	2e	0.21	0/1149	0.45	0/1548
37	1f	0.21	0/827	0.41	0/1120
37	2f	0.20	0/829	0.43	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.20	0/1254	0.40	0/1683
38	2g	0.19	0/1248	0.41	0/1676
39	1h	0.21	0/1118	0.43	0/1506
39	2h	0.18	0/1108	0.41	0/1494
40	1i	0.20	0/1005	0.47	0/1351
40	2i	0.21	0/985	0.47	0/1329
41	1j	0.19	0/732	0.43	0/993
41	2j	0.22	0/723	0.50	0/984
42	1k	0.18	0/849	0.40	0/1150
42	2k	0.19	0/848	0.50	0/1149
43	1l	0.21	0/937	0.44	0/1260
43	2l	0.20	0/937	0.41	0/1260
44	1m	0.22	0/924	0.46	0/1242
44	2m	0.23	0/905	0.53	0/1217
45	1n	0.21	0/501	0.49	0/664
45	2n	0.21	0/501	0.48	0/664
46	1o	0.21	0/739	0.40	0/985
46	2o	0.21	0/739	0.38	0/985
47	1p	0.20	0/697	0.46	0/939
47	2p	0.20	0/693	0.45	0/935
48	1q	0.22	0/836	0.47	0/1117
48	2q	0.21	0/836	0.46	0/1117
49	1r	0.22	0/560	0.45	0/746
49	2r	0.22	0/560	0.41	0/746
50	1s	0.20	0/663	0.44	0/895
50	2s	0.21	0/660	0.41	0/893
51	1t	0.24	0/734	0.50	0/969
51	2t	0.21	0/736	0.45	0/976
52	1u	0.21	0/203	0.42	0/266
52	2u	0.21	0/203	0.52	0/266
53	1y	0.22	0/776	0.41	0/1048
53	2y	0.18	0/761	0.37	0/1030
All	All	0.24	0/309937	0.45	8/463223 (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
21	2Z	0	1
26	24	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	1i	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1042	G	OP1-P-O3'	-9.78	78.67	108.00
1	1A	1042	G	OP2-P-O3'	-6.38	88.85	108.00
4	2E	142	GLY	N-CA-C	6.32	118.38	110.29
1	2A	1992	G	C2'-C3'-O3'	5.36	117.53	109.50
32	2a	266	G	P-O3'-C3'	5.30	128.15	120.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	1i	59	PHE	Peptide
26	24	18	CYS	Peptide
21	2Z	136	PHE	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	61869	0	31202	739	0
1	2A	61758	0	31148	905	0
2	1B	2572	0	1305	28	0
2	2B	2573	0	1306	40	0
3	1D	2131	0	2207	58	0
3	2D	2136	0	2218	59	0
4	1E	1559	0	1618	38	0
4	2E	1559	0	1618	38	0
5	1F	1584	0	1625	57	0
5	2F	1580	0	1619	55	0
6	1G	1426	0	1445	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	2G	1424	0	1441	67	0
7	1H	1330	0	1407	31	0
7	2H	1324	0	1402	41	0
8	1I	1094	0	1127	41	1
8	2I	1076	0	1094	34	0
9	1N	1121	0	1195	26	0
9	2N	1117	0	1184	25	0
10	1O	933	0	996	16	0
10	2O	933	0	996	26	0
11	1P	1135	0	1212	35	0
11	2P	1135	0	1212	36	0
12	1Q	1122	0	1179	30	0
12	2Q	1122	0	1179	35	0
13	1R	968	0	1033	29	0
13	2R	968	0	1033	23	0
14	1S	877	0	938	24	0
14	2S	870	0	923	39	0
15	1T	1091	0	1151	35	0
15	2T	1083	0	1136	26	0
16	1U	959	0	1019	19	0
16	2U	959	0	1019	26	0
17	1V	775	0	841	22	0
17	2V	771	0	829	12	0
18	1W	886	0	940	16	0
18	2W	886	0	940	18	0
19	1X	750	0	814	23	0
19	2X	750	0	814	18	0
20	1Y	810	0	892	18	0
20	2Y	810	0	887	27	0
21	1Z	1587	0	1598	38	0
21	2Z	1557	0	1564	59	0
22	10	608	0	622	17	0
22	20	608	0	622	17	0
23	11	754	0	823	22	0
23	21	759	0	837	24	0
24	12	588	0	643	12	0
24	22	592	0	654	22	0
25	13	469	0	518	13	0
25	23	464	0	514	9	0
26	14	546	0	522	30	0
26	24	536	0	514	34	0
27	15	459	0	476	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	25	455	0	465	10	0
28	16	453	0	473	13	0
28	26	449	0	469	10	0
29	17	418	0	467	12	0
29	27	418	0	467	10	0
30	18	517	0	582	20	0
30	28	517	0	582	13	0
31	19	307	0	335	5	0
31	29	307	0	335	14	0
32	1a	32246	0	16296	489	0
32	2a	32331	0	16339	601	1
33	1b	1842	0	1862	70	0
33	2b	1825	0	1828	82	0
34	1c	1558	0	1557	40	0
34	2c	1542	0	1517	75	0
35	1d	1665	0	1687	65	0
35	2d	1668	0	1703	67	0
36	1e	1133	0	1191	29	0
36	2e	1133	0	1191	43	0
37	1f	814	0	808	29	0
37	2f	816	0	808	12	0
38	1g	1235	0	1249	33	0
38	2g	1229	0	1238	41	0
39	1h	1098	0	1143	37	0
39	2h	1088	0	1126	37	0
40	1i	986	0	990	36	0
40	2i	966	0	953	59	0
41	1j	719	0	672	22	0
41	2j	710	0	661	37	0
42	1k	834	0	838	16	0
42	2k	833	0	836	23	0
43	1l	932	0	981	19	0
43	2l	932	0	981	17	0
44	1m	914	0	954	38	0
44	2m	895	0	920	41	0
45	1n	492	0	528	20	0
45	2n	492	0	529	36	0
46	1o	728	0	760	15	0
46	2o	728	0	760	20	0
47	1p	681	0	697	24	0
47	2p	677	0	686	22	0
48	1q	823	0	891	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	2q	823	0	891	22	0
49	1r	555	0	618	23	0
49	2r	555	0	618	11	0
50	1s	648	0	658	26	0
50	2s	645	0	635	32	0
51	1t	732	0	809	26	0
51	2t	733	0	795	24	0
52	1u	199	0	208	9	0
52	2u	199	0	208	9	0
53	1y	764	0	786	23	0
53	2y	749	0	757	38	0
54	10	7	0	0	0	0
54	11	4	0	0	0	0
54	13	4	0	0	0	0
54	15	6	0	0	0	0
54	17	5	0	0	0	0
54	18	2	0	0	0	0
54	19	1	0	0	0	0
54	1A	1020	0	0	0	0
54	1B	32	0	0	0	0
54	1D	16	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	6	0	0	0	0
54	1Q	4	0	0	0	0
54	1R	5	0	0	0	0
54	1T	3	0	0	0	0
54	1U	8	0	0	0	0
54	1V	7	0	0	0	0
54	1W	4	0	0	0	0
54	1Y	2	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	274	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	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	2	0	0	0	0
54	1y	3	0	0	0	0
54	20	2	0	0	0	0
54	21	1	0	0	0	0
54	23	1	0	0	0	0
54	25	2	0	0	0	0
54	27	1	0	0	0	0
54	28	2	0	0	0	0
54	2A	733	0	0	0	0
54	2B	18	0	0	0	0
54	2D	10	0	0	0	0
54	2E	7	0	0	0	0
54	2F	4	0	0	0	0
54	2G	3	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	2	0	0	0	0
54	2Q	2	0	0	0	0
54	2R	2	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	2a	183	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	2l	1	0	0	0	0
54	2n	1	0	0	0	0
54	2o	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	51	0	67	4	0
55	2A	51	0	67	2	0
56	18	8	0	14	4	0
56	1A	8	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1T	8	0	14	1	0
56	1a	8	0	14	3	0
56	2A	16	0	28	3	0
56	2B	8	0	14	0	0
57	1B	12	0	12	2	0
57	1F	12	0	12	4	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	1	0
59	2d	8	0	0	1	0
60	10	20	0	0	1	0
60	11	25	0	0	3	0
60	12	12	0	0	0	0
60	13	26	0	0	2	0
60	14	2	0	0	0	0
60	15	28	0	0	1	0
60	16	19	0	0	1	0
60	17	14	0	0	2	0
60	18	28	0	0	2	0
60	19	5	0	0	0	0
60	1A	3765	0	0	169	0
60	1B	106	0	0	2	0
60	1D	90	0	0	4	0
60	1E	74	0	0	5	0
60	1F	67	0	0	2	0
60	1G	18	0	0	0	0
60	1H	14	0	0	0	0
60	1I	8	0	0	2	0
60	1N	51	0	0	3	0
60	1O	26	0	0	2	0
60	1P	57	0	0	3	0
60	1Q	41	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1R	32	0	0	3	0
60	1S	14	0	0	5	0
60	1T	33	0	0	4	0
60	1U	42	0	0	3	0
60	1V	39	0	0	0	0
60	1W	27	0	0	2	0
60	1X	24	0	0	2	0
60	1Y	18	0	0	2	0
60	1Z	13	0	0	1	0
60	1a	465	0	0	27	0
60	1d	9	0	0	1	0
60	1e	1	0	0	0	0
60	1f	2	0	0	0	0
60	1h	1	0	0	0	0
60	1i	1	0	0	0	0
60	1j	1	0	0	0	0
60	1k	1	0	0	0	0
60	1l	5	0	0	1	0
60	1m	3	0	0	1	0
60	1o	3	0	0	0	0
60	1p	1	0	0	0	0
60	1u	1	0	0	0	0
60	1y	3	0	0	0	0
60	20	10	0	0	0	0
60	21	20	0	0	1	0
60	22	2	0	0	1	0
60	23	3	0	0	0	0
60	25	6	0	0	2	0
60	26	5	0	0	0	0
60	27	9	0	0	1	0
60	28	9	0	0	0	0
60	29	1	0	0	0	0
60	2A	1860	0	0	176	0
60	2B	53	0	0	9	0
60	2D	40	0	0	4	0
60	2E	19	0	0	2	0
60	2F	22	0	0	1	0
60	2G	7	0	0	0	0
60	2H	4	0	0	0	0
60	2I	4	0	0	4	0
60	2N	3	0	0	1	0
60	2O	19	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2P	19	0	0	3	0
60	2Q	18	0	0	1	0
60	2R	17	0	0	3	0
60	2S	3	0	0	0	0
60	2T	8	0	0	0	0
60	2U	16	0	0	3	0
60	2V	3	0	0	1	0
60	2W	13	0	0	0	0
60	2X	6	0	0	1	0
60	2Y	5	0	0	0	0
60	2Z	7	0	0	0	0
60	2a	303	0	0	34	0
60	2d	2	0	0	0	0
60	2e	1	0	0	0	0
60	2f	2	0	0	0	0
60	2j	2	0	0	1	0
60	2l	2	0	0	0	0
60	2m	3	0	0	0	0
60	2n	1	0	0	0	0
60	2o	2	0	0	0	0
60	2p	2	0	0	0	0
60	2q	1	0	0	0	0
60	2r	4	0	0	0	0
60	2y	3	0	0	0	0
All	All	296819	0	194645	5059	1

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 11.

The worst 5 of 5059 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	1.39	1.19
1:2A:2139:C:N4	1:2A:2152:G:H1	1.50	1.08
32:1a:1003:G:H2'	32:1a:1004:A:H4'	1.42	1.02
32:2a:1003:G:H2'	32:2a:1004:A:H4'	1.45	0.98
1:2A:2139:C:N3	1:2A:2152:G:N2	2.13	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:82:ARG:NH2	32:2a:56:U:O2'[3_654]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	252 (92%)	21 (8%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	7 (4%)	3 (2%)	8	10
4	2E	202/206 (98%)	186 (92%)	14 (7%)	2 (1%)	12	17
5	1F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	24	34
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	34
6	1G	179/182 (98%)	157 (88%)	17 (10%)	5 (3%)	4	3
6	2G	179/182 (98%)	152 (85%)	24 (13%)	3 (2%)	7	8
7	1H	172/180 (96%)	161 (94%)	9 (5%)	2 (1%)	10	13
7	2H	171/180 (95%)	153 (90%)	13 (8%)	5 (3%)	3	3
8	1I	145/148 (98%)	126 (87%)	18 (12%)	1 (1%)	18	25
8	2I	144/148 (97%)	133 (92%)	9 (6%)	2 (1%)	9	11
9	1N	138/140 (99%)	134 (97%)	3 (2%)	1 (1%)	18	25
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	22
10	2O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	22
11	1P	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
11	2P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	9	11
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18	25
12	2Q	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	14	20
14	2S	108/112 (96%)	95 (88%)	13 (12%)	0	100	100
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	6
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	17
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	15
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	15
20	1Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	12	17
20	2Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	12	17
21	1Z	201/206 (98%)	185 (92%)	15 (8%)	1 (0%)	24	34
21	2Z	199/206 (97%)	177 (89%)	19 (10%)	3 (2%)	8	10
22	10	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
22	20	75/85 (88%)	69 (92%)	6 (8%)	0	100	100
23	11	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
23	21	95/98 (97%)	88 (93%)	6 (6%)	1 (1%)	11	15
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	0	0
26	24	67/71 (94%)	44 (66%)	16 (24%)	7 (10%)	0	0
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	191 (83%)	28 (12%)	10 (4%)	2	1
33	2b	229/256 (90%)	197 (86%)	27 (12%)	5 (2%)	5	5
34	1c	204/239 (85%)	186 (91%)	18 (9%)	0	100	100
34	2c	204/239 (85%)	175 (86%)	27 (13%)	2 (1%)	12	17
35	1d	206/209 (99%)	193 (94%)	12 (6%)	1 (0%)	24	34
35	2d	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	24	34
36	1e	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
36	2e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	9	11
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
38	1g	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	18	25
38	2g	153/156 (98%)	131 (86%)	19 (12%)	3 (2%)	6	6
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	122 (90%)	11 (8%)	2 (2%)	8	10
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	22
40	2i	124/128 (97%)	106 (86%)	15 (12%)	3 (2%)	4	4
41	1j	95/105 (90%)	77 (81%)	13 (14%)	5 (5%)	1	0
41	2j	94/105 (90%)	75 (80%)	12 (13%)	7 (7%)	1	0
42	1k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	14	20
42	2k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	6	7
43	1l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16	22
43	2l	119/132 (90%)	107 (90%)	11 (9%)	1 (1%)	16	22
44	1m	114/126 (90%)	100 (88%)	11 (10%)	3 (3%)	4	3
44	2m	112/126 (89%)	95 (85%)	16 (14%)	1 (1%)	14	20
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	2n	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	8
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	13
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	13
47	1p	80/88 (91%)	71 (89%)	6 (8%)	3 (4%)	2	1
47	2p	80/88 (91%)	67 (84%)	12 (15%)	1 (1%)	9	12
48	1q	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
48	2q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	12	17
49	1r	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	8	10
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
50	2s	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
51	1t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5	5
51	2t	96/106 (91%)	84 (88%)	9 (9%)	3 (3%)	3	2
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	16 (76%)	4 (19%)	1 (5%)	2	1
53	1y	95/113 (84%)	93 (98%)	1 (1%)	1 (1%)	11	15
53	2y	94/113 (83%)	88 (94%)	4 (4%)	2 (2%)	5	5
All	All	11629/12354 (94%)	10669 (92%)	832 (7%)	128 (1%)	11	15

5 of 128 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	71	GLY
6	1G	47	LYS
7	1H	92	ILE
14	1S	59	LYS
26	14	44	THR

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	16
3	2D	215/218 (99%)	193 (90%)	22 (10%)	7	8
4	1E	164/166 (99%)	151 (92%)	13 (8%)	11	16
4	2E	164/166 (99%)	156 (95%)	8 (5%)	22	34
5	1F	160/166 (96%)	139 (87%)	21 (13%)	4	4
5	2F	159/166 (96%)	140 (88%)	19 (12%)	5	5
6	1G	144/156 (92%)	132 (92%)	12 (8%)	10	14
6	2G	142/156 (91%)	117 (82%)	25 (18%)	2	1
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12	17
7	2H	143/148 (97%)	118 (82%)	25 (18%)	2	1
8	1I	111/124 (90%)	89 (80%)	22 (20%)	1	1
8	2I	108/124 (87%)	98 (91%)	10 (9%)	8	10
9	1N	119/119 (100%)	109 (92%)	10 (8%)	10	14
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6	6
10	1O	100/100 (100%)	94 (94%)	6 (6%)	17	26
10	2O	100/100 (100%)	92 (92%)	8 (8%)	11	15
11	1P	115/116 (99%)	107 (93%)	8 (7%)	14	19
11	2P	115/116 (99%)	109 (95%)	6 (5%)	21	32
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	20	30
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	23
13	1R	101/101 (100%)	91 (90%)	10 (10%)	7	9
13	2R	101/101 (100%)	91 (90%)	10 (10%)	7	9
14	1S	87/88 (99%)	77 (88%)	10 (12%)	5	6
14	2S	85/88 (97%)	73 (86%)	12 (14%)	3	3
15	1T	115/127 (91%)	105 (91%)	10 (9%)	9	13
15	2T	113/127 (89%)	103 (91%)	10 (9%)	9	12
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	13
16	2U	93/94 (99%)	87 (94%)	6 (6%)	15	22
17	1V	81/82 (99%)	74 (91%)	7 (9%)	10	13
17	2V	80/82 (98%)	65 (81%)	15 (19%)	1	1
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	16
18	2W	90/92 (98%)	85 (94%)	5 (6%)	19	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	1X	77/78 (99%)	69 (90%)	8 (10%)	7	8
19	2X	77/78 (99%)	72 (94%)	5 (6%)	15	22
20	1Y	86/91 (94%)	78 (91%)	8 (9%)	8	10
20	2Y	86/91 (94%)	74 (86%)	12 (14%)	3	3
21	1Z	169/179 (94%)	150 (89%)	19 (11%)	6	6
21	2Z	165/179 (92%)	145 (88%)	20 (12%)	5	5
22	10	61/67 (91%)	59 (97%)	2 (3%)	33	50
22	20	61/67 (91%)	58 (95%)	3 (5%)	22	34
23	11	79/83 (95%)	76 (96%)	3 (4%)	29	44
23	21	81/83 (98%)	77 (95%)	4 (5%)	22	34
24	12	65/67 (97%)	57 (88%)	8 (12%)	4	4
24	22	66/67 (98%)	61 (92%)	5 (8%)	12	17
25	13	51/52 (98%)	46 (90%)	5 (10%)	7	9
25	23	50/52 (96%)	44 (88%)	6 (12%)	5	5
26	14	58/63 (92%)	51 (88%)	7 (12%)	5	5
26	24	54/63 (86%)	44 (82%)	10 (18%)	1	1
27	15	51/52 (98%)	48 (94%)	3 (6%)	18	27
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	42
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	5
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	3
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	34
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	9
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	29
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	17
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	55
31	29	34/34 (100%)	30 (88%)	4 (12%)	5	5
33	1b	191/220 (87%)	166 (87%)	25 (13%)	4	4
33	2b	187/220 (85%)	167 (89%)	20 (11%)	6	7
34	1c	144/188 (77%)	131 (91%)	13 (9%)	9	11
34	2c	140/188 (74%)	123 (88%)	17 (12%)	5	5
35	1d	171/181 (94%)	150 (88%)	21 (12%)	4	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	2d	172/181 (95%)	146 (85%)	26 (15%)	3	2
36	1e	114/123 (93%)	106 (93%)	8 (7%)	14	19
36	2e	114/123 (93%)	102 (90%)	12 (10%)	6	8
37	1f	85/90 (94%)	74 (87%)	11 (13%)	4	4
37	2f	85/90 (94%)	77 (91%)	8 (9%)	8	10
38	1g	120/127 (94%)	111 (92%)	9 (8%)	12	17
38	2g	119/127 (94%)	100 (84%)	19 (16%)	2	2
39	1h	116/119 (98%)	104 (90%)	12 (10%)	7	8
39	2h	114/119 (96%)	98 (86%)	16 (14%)	3	3
40	1i	91/99 (92%)	79 (87%)	12 (13%)	4	4
40	2i	88/99 (89%)	71 (81%)	17 (19%)	1	1
41	1j	68/92 (74%)	63 (93%)	5 (7%)	13	17
41	2j	68/92 (74%)	62 (91%)	6 (9%)	9	12
42	1k	83/99 (84%)	77 (93%)	6 (7%)	13	18
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	9
43	1l	96/108 (89%)	88 (92%)	8 (8%)	10	14
43	2l	96/108 (89%)	86 (90%)	10 (10%)	7	8
44	1m	90/101 (89%)	75 (83%)	15 (17%)	2	2
44	2m	87/101 (86%)	80 (92%)	7 (8%)	11	15
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	8
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	8
46	1o	78/80 (98%)	72 (92%)	6 (8%)	12	17
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9	11
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	4
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2	2
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20	31
48	2q	94/97 (97%)	83 (88%)	11 (12%)	5	6
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14	20
49	2r	59/77 (77%)	55 (93%)	4 (7%)	14	20
50	1s	68/80 (85%)	63 (93%)	5 (7%)	13	17
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	1t	71/82 (87%)	64 (90%)	7 (10%)	7	9
51	2t	70/82 (85%)	61 (87%)	9 (13%)	4	4
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	29
52	2u	18/22 (82%)	15 (83%)	3 (17%)	2	2
53	1y	82/98 (84%)	77 (94%)	5 (6%)	17	25
53	2y	79/98 (81%)	64 (81%)	15 (19%)	1	1
All	All	9524/10260 (93%)	8552 (90%)	972 (10%)	7	8

5 of 972 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2D	229	VAL
43	2l	66	VAL
10	2O	108	GLU
42	2k	103	LEU
51	2t	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
30	28	35	GLN
40	2i	58	HIS
34	2c	3	ASN
35	2d	201	GLN
42	2k	62	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	434 (15%)	33 (1%)
1	2A	2858/2915 (98%)	487 (17%)	31 (1%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	119/121 (98%)	16 (13%)	0
32	1a	1497/1521 (98%)	258 (17%)	0
32	2a	1501/1521 (98%)	290 (19%)	0
All	All	8959/9114 (98%)	1495 (16%)	64 (0%)

5 of 1495 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	45	C

5 of 64 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	2171	A
1	2A	2321	G
1	1A	1653	G
1	1A	1608	A
1	2A	2406	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	5MC	1a	1407	32	19,22,23	1.72	2 (10%)	26,32,35	1.11	3 (11%)
32	5MC	2a	1404	32	19,22,23	1.71	3 (15%)	26,32,35	1.16	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.37	3 (16%)	21,30,33	2.05	5 (23%)
32	5MC	2a	967	32	19,22,23	1.77	2 (10%)	26,32,35	1.03	2 (7%)
1	2MA	1A	2503	54,1	22,25,26	1.47	4 (18%)	32,37,40	2.29	8 (25%)
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.05	3 (14%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.08	10 (30%)
43	0TD	1l	92	43	8,9,10	4.47	1 (12%)	6,11,13	5.36	3 (50%)
1	5MU	1A	1939	1	19,22,23	1.50	6 (31%)	27,32,35	2.11	8 (29%)
1	5MC	2A	1962	54,1	19,22,23	1.59	2 (10%)	26,32,35	1.16	2 (7%)
32	7MG	2a	527	32	23,26,27	1.42	4 (17%)	27,39,42	2.49	6 (22%)
1	5MC	1A	1962	54,1	19,22,23	1.54	3 (15%)	26,32,35	1.11	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	2A	1920	1	19,22,24	0.82	0	25,31,35	0.96	1 (4%)
1	5MC	1A	1942	1	19,22,23	1.68	3 (15%)	26,32,35	1.19	3 (11%)
1	4OC	1A	1920	1	19,22,24	0.84	0	25,31,35	1.01	1 (4%)
32	MA6	1a	1518	32	23,26,27	0.39	0	33,38,41	1.89	10 (30%)
32	5MC	1a	1404	32	19,22,23	1.68	3 (15%)	26,32,35	1.17	2 (7%)
32	PSU	1a	516	32,54	18,21,22	1.37	2 (11%)	21,30,33	2.00	5 (23%)
1	5MU	2A	1915	1	19,22,23	1.37	4 (21%)	27,32,35	2.19	7 (25%)
1	OMG	1A	2251	54,1	23,26,27	1.26	3 (13%)	32,38,41	2.00	5 (15%)
1	PSU	2A	1911	1	18,21,22	1.41	3 (16%)	21,30,33	2.03	3 (14%)
1	2MU	1A	2552	54,1	19,22,24	1.33	4 (21%)	25,31,36	1.88	5 (20%)
32	2MG	1a	1207	32,54	23,26,27	1.21	2 (8%)	33,38,41	2.43	12 (36%)
32	MA6	2a	1518	32	23,26,27	0.38	0	33,38,41	2.03	9 (27%)
32	PSU	2a	516	32,54	18,21,22	1.35	2 (11%)	21,30,33	2.17	5 (23%)
32	M2G	1a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.85	6 (18%)
1	5MU	2A	1939	54,1	19,22,23	1.45	6 (31%)	27,32,35	2.17	8 (29%)
1	2MA	2A	2503	54,1	22,25,26	1.50	4 (18%)	32,37,40	2.48	9 (28%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.06	10 (30%)
1	PSU	1A	2605	54,1	18,21,22	1.43	3 (16%)	21,30,33	1.93	4 (19%)
32	UR3	1a	1498	32	19,22,23	0.96	1 (5%)	26,32,35	1.85	4 (15%)
32	5MC	2a	1400	32	19,22,23	1.72	3 (15%)	26,32,35	1.18	2 (7%)
1	5MC	2A	1942	1	19,22,23	1.71	3 (15%)	26,32,35	1.22	2 (7%)
32	5MC	1a	967	32	19,22,23	1.64	3 (15%)	26,32,35	1.15	3 (11%)
1	OMG	2A	2251	54,1	23,26,27	1.21	3 (13%)	32,38,41	1.92	5 (15%)
32	5MC	2a	1407	32	19,22,23	1.64	2 (10%)	26,32,35	1.17	3 (11%)
32	2MG	2a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.14	7 (21%)
32	4OC	2a	1402	32	20,23,24	0.78	0	25,32,35	1.04	1 (4%)
1	5MU	1A	1915	1	19,22,23	1.41	4 (21%)	27,32,35	2.20	9 (33%)
1	2MU	2A	2552	54,1	19,22,24	1.22	2 (10%)	25,31,36	1.92	6 (24%)
43	0TD	2l	92	43	8,9,10	4.38	1 (12%)	6,11,13	6.38	2 (33%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.06	3 (14%)
32	M2G	2a	966	32	24,27,28	1.33	4 (16%)	33,40,43	1.88	5 (15%)
32	7MG	1a	527	32,54	23,26,27	1.33	3 (13%)	27,39,42	2.57	7 (25%)
32	UR3	2a	1498	32	19,22,23	1.03	2 (10%)	26,32,35	1.69	4 (15%)
32	5MC	1a	1400	32	19,22,23	1.74	3 (15%)	26,32,35	1.19	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.77	1 (5%)	25,32,35	0.96	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	1.93	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	54,1	-	1/7/25/26	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	2/11/29/30	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	54,1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	2/7/37/38	0/3/3/3
1	5MC	1A	1962	54,1	-	2/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	1/9/27/30	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	OMG	1A	2251	54,1	-	1/9/27/28	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	54,1	-	0/9/27/28	0/2/2/2
32	2MG	1a	1207	32,54	-	2/9/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1939	54,1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	54,1	-	0/7/25/26	0/3/3/3
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
1	PSU	1A	2605	54,1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	4/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	54,1	-	1/9/27/28	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/9/27/28	0/3/3/3
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	2MU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	7MG	1a	527	32,54	-	2/7/37/38	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.23	1.69	1.82
43	2l	92	0TD	CB-SB	-12.00	1.70	1.82
32	2a	967	5MC	C5-C4	6.60	1.49	1.44
32	2a	1400	5MC	C5-C4	6.28	1.48	1.44
32	1a	1407	5MC	C5-C4	6.28	1.48	1.44

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-15.12	75.19	102.36
43	1l	92	0TD	CSB-SB-CB	-12.41	80.06	102.36
32	1a	527	7MG	N9-C4-N3	8.74	138.27	125.46
1	2A	2503	2MA	C5-C4-N3	-8.65	118.07	127.18
32	2a	527	7MG	N9-C4-N3	8.48	137.89	125.46

There are no chirality outliers.

5 of 28 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
32	1a	1207	2MG	N1-C2-N2-CM2

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Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N3-C2-N2-CM2
1	2A	1915	5MU	O4'-C1'-N1-C2

There are no ring outliers.

24 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1404	5MC	1	0
32	2a	967	5MC	1	0
1	1A	2503	2MA	1	0
32	2a	1519	MA6	3	0
1	1A	1939	5MU	1	0
1	2A	1920	4OC	1	0
1	1A	1920	4OC	2	0
32	1a	1518	MA6	1	0
32	1a	1404	5MC	1	0
1	1A	2251	OMG	1	0
1	2A	1911	PSU	1	0
32	2a	1518	MA6	2	0
1	2A	1939	5MU	3	0
1	2A	2503	2MA	1	0
32	1a	1519	MA6	3	0
32	1a	1498	UR3	1	0
32	2a	1400	5MC	1	0
32	2a	1207	2MG	4	0
32	2a	1402	4OC	4	0
1	2A	2552	2MU	1	0
43	2l	92	0TD	1	0
32	2a	1498	UR3	1	0
32	1a	1400	5MC	1	0
32	1a	1402	4OC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2499 ligands modelled in this entry, 2486 are monoatomic - leaving 13 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
55	ERY	1A	4021	-	53,53,53	0.93	2 (3%)	82,82,82	1.47	13 (15%)
56	MPD	2A	3735	-	7,7,7	0.30	0	9,10,10	0.21	0
55	ERY	2A	3734	-	53,53,53	0.94	2 (3%)	82,82,82	1.62	13 (15%)
56	MPD	1T	204	-	7,7,7	0.34	0	9,10,10	0.23	0
57	ARG	1F	319	54	10,11,11	0.75	1 (10%)	9,13,13	0.86	1 (11%)
57	ARG	1B	233	54	10,11,11	0.72	1 (10%)	9,13,13	0.92	1 (11%)
56	MPD	2A	3736	-	7,7,7	0.34	0	9,10,10	0.36	0
59	SF4	1d	306	35	0,12,12	-	-	-	-	-
56	MPD	2B	219	-	7,7,7	0.30	0	9,10,10	0.30	0
59	SF4	2d	501	35	0,12,12	-	-	-	-	-
56	MPD	18	103	-	7,7,7	0.35	0	9,10,10	0.49	0
56	MPD	1a	1875	-	7,7,7	0.40	0	9,10,10	0.45	0
56	MPD	1A	4022	54	7,7,7	0.29	0	9,10,10	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	ERY	1A	4021	-	-	8/72/107/107	0/3/3/3
56	MPD	2A	3735	-	-	3/5/5/5	-
55	ERY	2A	3734	-	-	8/72/107/107	0/3/3/3
56	MPD	1T	204	-	-	3/5/5/5	-
57	ARG	1F	319	54	-	0/11/11/11	-
57	ARG	1B	233	54	-	4/11/11/11	-
56	MPD	2A	3736	-	-	4/5/5/5	-
59	SF4	1d	306	35	-	-	0/6/5/5
56	MPD	2B	219	-	-	2/5/5/5	-
59	SF4	2d	501	35	-	-	0/6/5/5
56	MPD	18	103	-	-	1/5/5/5	-
56	MPD	1a	1875	-	-	5/5/5/5	-
56	MPD	1A	4022	54	-	3/5/5/5	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3734	ERY	O2-C1	4.87	1.45	1.34
55	1A	4021	ERY	O2-C1	4.75	1.45	1.34
55	1A	4021	ERY	O2-C13	-2.61	1.42	1.46
57	1B	233	ARG	OXT-C	-2.12	1.23	1.30
55	2A	3734	ERY	O2-C13	-2.08	1.42	1.46

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3734	ERY	O5-C16-C17	4.39	110.22	103.86
55	2A	3734	ERY	C13-O2-C1	-4.23	110.81	118.20
55	1A	4021	ERY	O7-C5-C4	-4.00	105.80	111.58
55	2A	3734	ERY	O5-C16-C15	-3.71	107.24	112.95
55	2A	3734	ERY	C6-C5-C4	-3.62	108.64	113.89

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

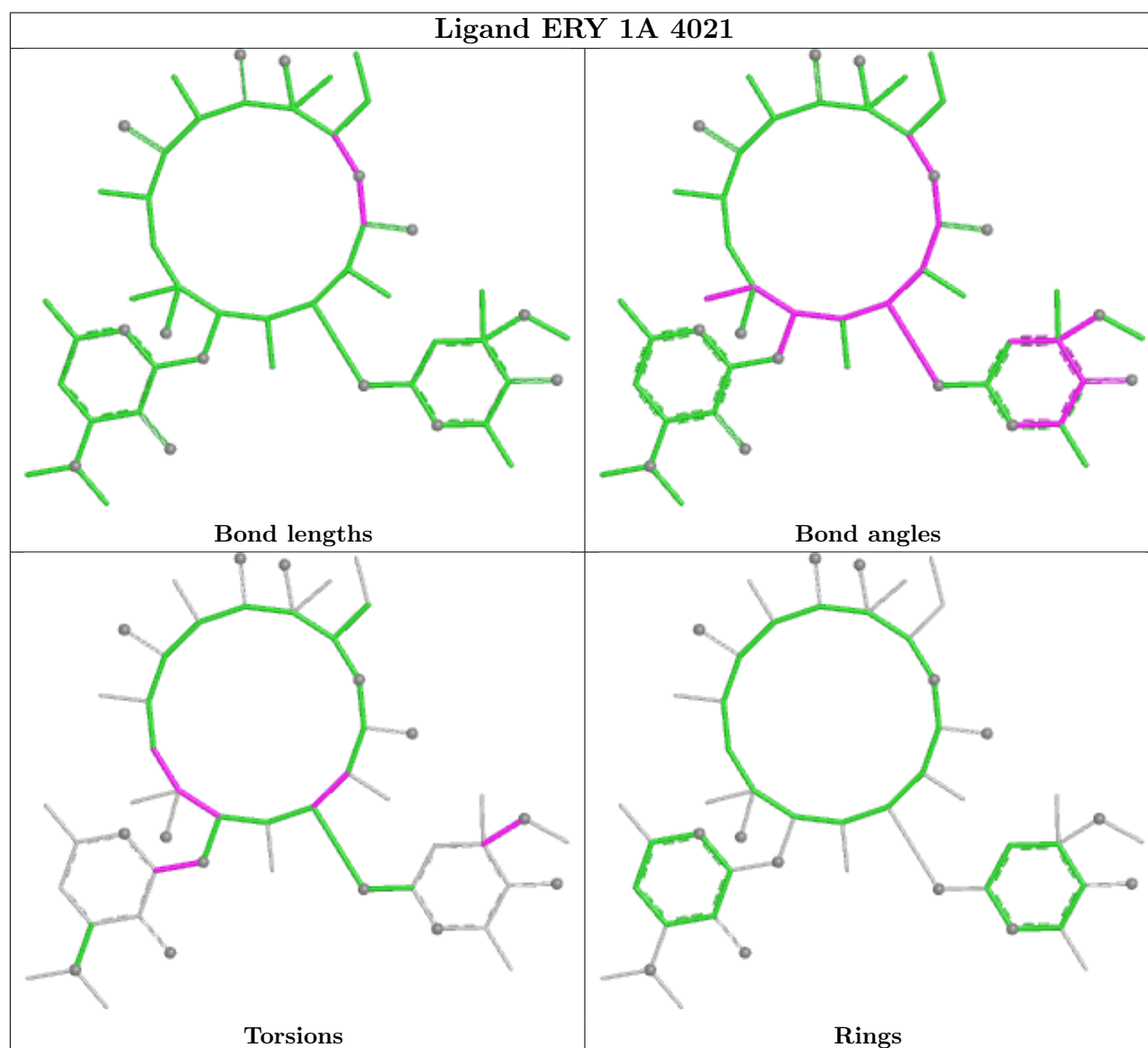
Mol	Chain	Res	Type	Atoms
55	1A	4021	ERY	C15-C16-O5-C20
55	1A	4021	ERY	C17-C16-O5-C20
55	1A	4021	ERY	C19-C16-O5-C20
55	2A	3734	ERY	C32-C6-C7-C8
55	2A	3734	ERY	C15-C16-O5-C20

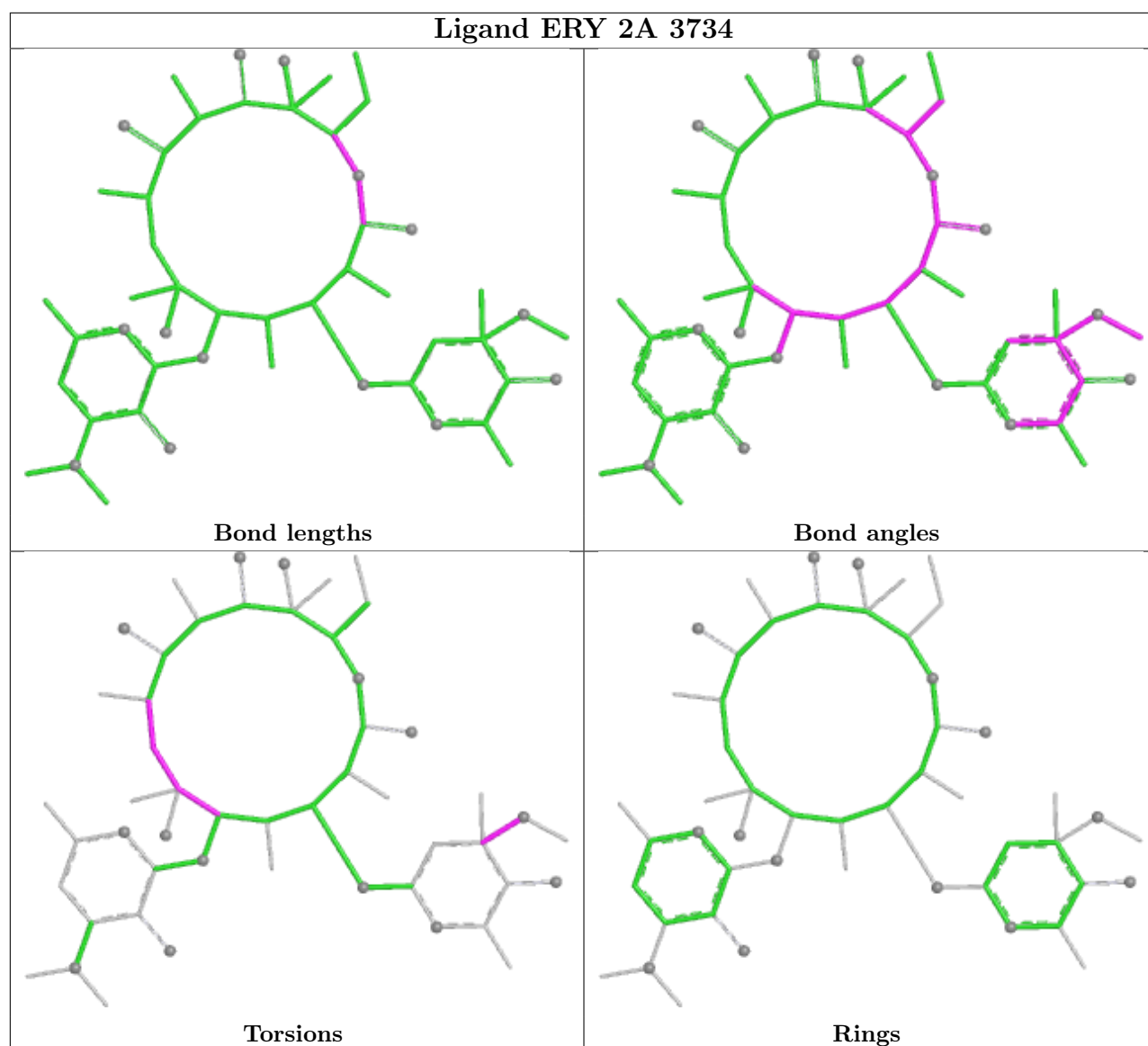
There are no ring outliers.

11 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1A	4021	ERY	4	0
56	2A	3735	MPD	3	0
55	2A	3734	ERY	2	0
56	1T	204	MPD	1	0
57	1F	319	ARG	4	0
57	1B	233	ARG	2	0
59	1d	306	SF4	1	0
59	2d	501	SF4	1	0
56	18	103	MPD	4	0
56	1a	1875	MPD	3	0
56	1A	4022	MPD	2	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.





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	2861/2915 (98%)	-0.65	62 (2%) 62 63	22, 39, 89, 104	0
1	2A	2856/2915 (97%)	-0.23	51 (1%) 67 68	35, 58, 91, 103	0
2	1B	120/121 (99%)	-0.50	0 100 100	30, 52, 65, 78	0
2	2B	120/121 (99%)	0.24	1 (0%) 82 84	60, 75, 83, 87	0
3	1D	275/276 (99%)	-0.04	2 (0%) 84 86	25, 41, 54, 72	0
3	2D	275/276 (99%)	0.34	1 (0%) 88 90	36, 53, 65, 78	0
4	1E	204/206 (99%)	-0.05	0 100 100	23, 44, 60, 70	0
4	2E	204/206 (99%)	0.31	2 (0%) 79 80	32, 58, 73, 81	0
5	1F	203/210 (96%)	-0.07	1 (0%) 87 89	22, 46, 68, 84	0
5	2F	203/210 (96%)	0.50	2 (0%) 79 80	36, 65, 77, 83	0
6	1G	181/182 (99%)	0.74	12 (6%) 24 24	47, 63, 74, 79	0
6	2G	181/182 (99%)	1.37	31 (17%) 4 3	70, 79, 86, 89	0
7	1H	174/180 (96%)	0.23	3 (1%) 69 69	38, 55, 66, 74	0
7	2H	173/180 (96%)	1.01	13 (7%) 20 19	66, 77, 83, 87	0
8	1I	147/148 (99%)	0.69	7 (4%) 35 35	46, 71, 79, 82	0
8	2I	146/148 (98%)	1.11	16 (10%) 10 10	60, 72, 81, 85	0
9	1N	140/140 (100%)	0.01	0 100 100	29, 42, 62, 79	0
9	2N	140/140 (100%)	0.51	1 (0%) 84 86	45, 62, 74, 80	0
10	1O	122/122 (100%)	-0.12	0 100 100	32, 44, 58, 64	0
10	2O	122/122 (100%)	0.39	3 (2%) 58 59	49, 58, 68, 77	0
11	1P	149/150 (99%)	0.14	0 100 100	23, 48, 66, 76	0
11	2P	149/150 (99%)	0.56	4 (2%) 56 57	39, 65, 77, 83	0
12	1Q	141/141 (100%)	0.06	0 100 100	30, 44, 54, 65	0
12	2Q	141/141 (100%)	0.74	4 (2%) 55 56	47, 62, 72, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.06	0 100 100	30, 39, 53, 62	0
13	2R	118/118 (100%)	0.35	2 (1%) 69 69	42, 54, 63, 72	0
14	1S	110/112 (98%)	0.32	0 100 100	39, 51, 64, 69	0
14	2S	110/112 (98%)	1.16	19 (17%) 4 3	63, 70, 76, 79	0
15	1T	131/146 (89%)	0.08	3 (2%) 61 62	34, 48, 66, 80	0
15	2T	131/146 (89%)	0.48	3 (2%) 61 62	49, 60, 73, 78	0
16	1U	116/118 (98%)	-0.16	1 (0%) 81 83	24, 35, 49, 67	0
16	2U	116/118 (98%)	0.55	0 100 100	41, 59, 71, 76	0
17	1V	101/101 (100%)	-0.01	0 100 100	27, 44, 60, 67	0
17	2V	101/101 (100%)	0.46	2 (1%) 65 65	44, 65, 73, 78	0
18	1W	112/113 (99%)	-0.12	1 (0%) 81 83	26, 34, 55, 80	0
18	2W	112/113 (99%)	0.20	2 (1%) 67 68	39, 50, 65, 88	0
19	1X	95/96 (98%)	-0.04	3 (3%) 50 51	30, 39, 60, 69	0
19	2X	95/96 (98%)	0.80	4 (4%) 40 41	48, 60, 71, 76	0
20	1Y	107/110 (97%)	0.20	1 (0%) 81 83	35, 50, 65, 70	0
20	2Y	107/110 (97%)	0.92	6 (5%) 30 29	57, 67, 76, 81	0
21	1Z	203/206 (98%)	0.47	3 (1%) 72 73	41, 58, 71, 80	0
21	2Z	201/206 (97%)	1.05	15 (7%) 20 19	65, 73, 79, 84	0
22	10	77/85 (90%)	-0.01	1 (1%) 75 75	31, 40, 56, 60	0
22	20	77/85 (90%)	0.95	8 (10%) 11 11	50, 62, 70, 74	0
23	11	97/98 (98%)	0.17	1 (1%) 79 80	30, 46, 65, 72	0
23	21	97/98 (98%)	0.68	3 (3%) 51 52	43, 58, 72, 75	0
24	12	70/72 (97%)	0.21	1 (1%) 73 74	36, 50, 61, 76	0
24	22	70/72 (97%)	0.68	1 (1%) 73 74	57, 66, 73, 76	0
25	13	59/60 (98%)	-0.04	0 100 100	30, 40, 60, 65	0
25	23	59/60 (98%)	0.66	4 (6%) 23 22	50, 61, 75, 80	0
26	14	69/71 (97%)	1.13	13 (18%) 3 2	55, 77, 87, 90	0
26	24	69/71 (97%)	1.63	18 (26%) 1 1	74, 84, 89, 94	0
27	15	59/60 (98%)	-0.14	1 (1%) 69 69	23, 38, 56, 63	0
27	25	59/60 (98%)	0.02	0 100 100	37, 52, 66, 70	0
28	16	53/54 (98%)	0.03	0 100 100	35, 46, 59, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.46	1 (1%) 66 66	52, 60, 68, 71	0
29	17	48/49 (97%)	-0.17	2 (4%) 40 41	23, 31, 55, 62	0
29	27	48/49 (97%)	0.14	1 (2%) 63 64	34, 43, 63, 68	0
30	18	64/65 (98%)	-0.04	0 100 100	30, 37, 45, 60	0
30	28	64/65 (98%)	0.54	0 100 100	44, 56, 64, 70	0
31	19	37/37 (100%)	0.22	0 100 100	35, 46, 62, 63	0
31	29	37/37 (100%)	0.83	2 (5%) 31 31	57, 64, 76, 80	0
32	1a	1488/1521 (97%)	-0.02	6 (0%) 88 90	42, 69, 88, 101	0
32	2a	1492/1521 (98%)	0.25	16 (1%) 78 79	55, 76, 91, 100	0
33	1b	231/256 (90%)	0.83	13 (5%) 30 29	66, 75, 82, 88	0
33	2b	231/256 (90%)	1.23	36 (15%) 5 4	71, 80, 86, 89	0
34	1c	206/239 (86%)	0.66	6 (2%) 53 55	57, 71, 78, 84	0
34	2c	206/239 (86%)	1.46	48 (23%) 2 1	72, 80, 86, 90	0
35	1d	208/209 (99%)	0.74	13 (6%) 26 25	58, 70, 77, 86	0
35	2d	208/209 (99%)	1.11	15 (7%) 21 20	64, 72, 79, 81	0
36	1e	148/162 (91%)	0.58	1 (0%) 84 86	56, 65, 73, 80	0
36	2e	148/162 (91%)	0.92	8 (5%) 31 31	63, 73, 80, 85	0
37	1f	100/101 (99%)	0.55	1 (1%) 79 80	58, 65, 73, 77	0
37	2f	100/101 (99%)	0.49	0 100 100	59, 70, 76, 79	0
38	1g	155/156 (99%)	0.67	3 (1%) 66 66	61, 70, 77, 87	0
38	2g	155/156 (99%)	1.18	19 (12%) 8 7	69, 78, 83, 87	0
39	1h	137/138 (99%)	0.65	3 (2%) 62 63	59, 68, 74, 77	0
39	2h	137/138 (99%)	0.81	7 (5%) 33 33	65, 73, 78, 87	0
40	1i	127/128 (99%)	1.12	13 (10%) 12 11	58, 75, 81, 84	0
40	2i	126/128 (98%)	1.94	57 (45%) 0 0	74, 80, 84, 89	0
41	1j	97/105 (92%)	1.11	9 (9%) 14 13	64, 73, 83, 85	0
41	2j	96/105 (91%)	1.98	42 (43%) 0 0	71, 81, 86, 88	0
42	1k	114/129 (88%)	0.32	2 (1%) 67 68	44, 64, 71, 76	0
42	2k	114/129 (88%)	0.75	5 (4%) 39 39	61, 72, 79, 84	0
43	1l	121/132 (91%)	0.62	5 (4%) 41 42	53, 60, 69, 74	0
43	2l	121/132 (91%)	0.84	13 (10%) 11 10	59, 68, 76, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.89	6 (5%) 33 32	58, 72, 78, 84	0
44	2m	114/126 (90%)	1.47	25 (21%) 2 2	74, 80, 84, 85	0
45	1n	60/61 (98%)	1.09	6 (10%) 12 12	63, 69, 75, 75	0
45	2n	60/61 (98%)	2.00	31 (51%) 0 0	73, 80, 85, 87	0
46	1o	88/89 (98%)	0.69	5 (5%) 29 29	50, 65, 75, 78	0
46	2o	88/89 (98%)	0.95	4 (4%) 38 38	65, 73, 78, 84	0
47	1p	82/88 (93%)	1.23	13 (15%) 5 4	61, 70, 77, 81	0
47	2p	82/88 (93%)	1.06	8 (9%) 13 12	63, 71, 75, 80	0
48	1q	99/105 (94%)	0.67	1 (1%) 79 80	58, 66, 75, 77	0
48	2q	99/105 (94%)	0.67	2 (2%) 65 65	61, 70, 77, 82	0
49	1r	68/88 (77%)	0.49	2 (2%) 53 55	58, 65, 74, 80	0
49	2r	68/88 (77%)	0.82	2 (2%) 53 55	65, 73, 80, 82	0
50	1s	83/93 (89%)	0.96	4 (4%) 35 35	65, 73, 80, 83	0
50	2s	83/93 (89%)	1.72	33 (39%) 1 0	71, 81, 86, 88	0
51	1t	96/106 (90%)	1.00	10 (10%) 11 11	62, 69, 79, 84	0
51	2t	98/106 (92%)	0.82	9 (9%) 14 14	59, 69, 76, 81	0
52	1u	23/27 (85%)	1.22	2 (8%) 16 15	67, 72, 78, 79	0
52	2u	23/27 (85%)	2.09	10 (43%) 0 0	74, 78, 82, 83	0
53	1y	97/113 (85%)	0.82	8 (8%) 17 17	54, 63, 73, 75	0
53	2y	96/113 (84%)	1.59	27 (28%) 1 1	67, 76, 82, 84	0
All	All	20766/21468 (96%)	0.26	887 (4%) 40 40	22, 64, 84, 104	0

The worst 5 of 887 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1087	G	8.7
1	1A	1090	U	7.8
45	2n	2	ALA	6.5
1	1A	1091	G	6.2
1	1A	1089	G	6.0

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MU	2A	1915	21/22	0.86	0.11	80,84,88,102	0
32	M2G	2a	966	25/26	0.86	0.17	69,76,86,98	0
1	PSU	2A	1917	20/21	0.87	0.09	73,79,95,99	0
32	2MG	2a	1207	24/25	0.87	0.10	77,85,88,97	0
1	5MU	1A	1915	21/22	0.88	0.10	68,75,80,84	0
32	PSU	2a	516	20/21	0.88	0.10	76,79,84,89	0
32	5MC	2a	967	21/22	0.89	0.14	71,76,81,84	0
1	PSU	2A	1911	20/21	0.89	0.09	68,74,86,88	0
32	2MG	1a	1207	24/25	0.90	0.10	63,72,76,80	0
43	0TD	2l	92	10/11	0.90	0.14	67,70,73,81	0
1	4OC	2A	1920	21/23	0.92	0.10	67,70,73,76	0
1	PSU	1A	1917	20/21	0.93	0.08	65,72,76,79	0
32	7MG	2a	527	24/25	0.93	0.12	64,69,71,76	0
43	0TD	1l	92	10/11	0.93	0.12	51,59,63,68	0
1	PSU	1A	1911	20/21	0.94	0.08	61,69,76,82	0
32	5MC	2a	1400	21/22	0.94	0.12	67,74,78,81	0
32	4OC	2a	1402	22/23	0.94	0.11	62,69,73,81	0
32	PSU	1a	516	20/21	0.94	0.08	61,67,71,77	0
32	5MC	1a	1407	21/22	0.95	0.09	46,56,62,67	0
32	MA6	1a	1519	24/25	0.95	0.11	48,54,58,62	0
32	5MC	2a	1407	21/22	0.95	0.09	60,68,72,78	0
32	UR3	2a	1498	21/22	0.95	0.10	57,64,70,75	0
32	MA6	2a	1519	24/25	0.95	0.11	62,67,71,76	0
32	5MC	1a	967	21/22	0.95	0.09	65,71,75,80	0
1	PSU	2A	2605	20/21	0.96	0.10	37,41,48,49	0
32	7MG	1a	527	24/25	0.96	0.09	50,57,62,62	0
32	5MC	2a	1404	21/22	0.96	0.09	63,68,70,73	0
32	UR3	1a	1498	21/22	0.96	0.09	49,55,59,65	0
32	M2G	1a	966	25/26	0.96	0.09	54,65,71,77	0
32	MA6	2a	1518	24/25	0.96	0.10	63,70,73,75	0
32	5MC	1a	1400	21/22	0.96	0.10	43,56,64,66	0
1	5MC	2A	1942	21/22	0.96	0.08	43,57,62,67	0
1	5MU	2A	1939	21/22	0.97	0.08	39,48,50,53	0
32	5MC	1a	1404	21/22	0.97	0.07	49,54,59,61	0
1	5MC	2A	1962	21/22	0.97	0.08	44,53,56,59	0
1	OMG	2A	2251	24/25	0.97	0.09	42,46,51,51	0
1	2MA	2A	2503	23/24	0.97	0.09	31,37,43,44	0
1	2MU	2A	2552	21/23	0.97	0.08	40,46,51,53	0
1	4OC	1A	1920	21/23	0.97	0.08	47,62,69,73	0
1	PSU	1A	2605	20/21	0.97	0.08	30,33,38,39	0
32	MA6	1a	1518	24/25	0.97	0.09	44,53,57,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	4OC	1a	1402	22/23	0.97	0.07	50,55,61,64	0
1	5MC	1A	1962	21/22	0.98	0.06	30,39,45,47	0
1	OMG	1A	2251	24/25	0.98	0.06	24,29,33,33	0
1	2MA	1A	2503	23/24	0.98	0.06	20,25,30,32	0
1	2MU	1A	2552	21/23	0.98	0.08	30,35,38,43	0
1	5MU	1A	1939	21/22	0.98	0.07	29,34,38,40	0
1	5MC	1A	1942	21/22	0.98	0.06	35,42,48,56	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	3630	1/1	0.61	0.21	61,61,61,61	0
54	MG	2A	3366	1/1	0.67	0.13	79,79,79,79	0
54	MG	2A	3301	1/1	0.69	0.17	71,71,71,71	0
54	MG	1A	3693	1/1	0.72	0.15	63,63,63,63	0
54	MG	1A	3285	1/1	0.72	0.24	79,79,79,79	0
54	MG	2a	3062	1/1	0.72	0.22	79,79,79,79	0
54	MG	2A	3660	1/1	0.73	0.16	81,81,81,81	0
54	MG	2A	3634	1/1	0.73	0.21	75,75,75,75	0
54	MG	1A	3997	1/1	0.74	0.14	74,74,74,74	0
54	MG	1a	1756	1/1	0.74	0.15	59,59,59,59	0
54	MG	2A	3044	1/1	0.74	0.21	79,79,79,79	0
54	MG	2a	3108	1/1	0.74	0.37	79,79,79,79	0
54	MG	2a	3115	1/1	0.74	0.58	82,82,82,82	0
54	MG	2a	3129	1/1	0.75	0.16	77,77,77,77	0
54	MG	1A	3406	1/1	0.76	0.15	64,64,64,64	0
54	MG	1t	202	1/1	0.76	0.13	62,62,62,62	0
54	MG	1A	3678	1/1	0.76	0.13	76,76,76,76	0
54	MG	2a	3170	1/1	0.76	0.29	70,70,70,70	0
54	MG	2j	201	1/1	0.76	0.16	73,73,73,73	0
56	MPD	1T	204	8/8	0.76	0.17	61,65,73,74	0
54	MG	2a	3070	1/1	0.77	0.20	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	3580	1/1	0.78	0.22	70,70,70,70	0
54	MG	2a	3119	1/1	0.78	0.16	72,72,72,72	0
54	MG	1a	1732	1/1	0.78	0.18	79,79,79,79	0
54	MG	2A	3429	1/1	0.78	0.21	63,63,63,63	0
54	MG	2A	3528	1/1	0.78	0.26	80,80,80,80	0
54	MG	1a	1753	1/1	0.78	0.11	73,73,73,73	0
54	MG	2A	3278	1/1	0.79	0.14	44,44,44,44	0
54	MG	2a	3087	1/1	0.79	0.27	76,76,76,76	0
54	MG	2a	3094	1/1	0.79	0.16	82,82,82,82	0
54	MG	1a	1844	1/1	0.79	0.27	69,69,69,69	0
54	MG	1G	202	1/1	0.79	0.12	55,55,55,55	0
54	MG	2A	3393	1/1	0.79	0.30	69,69,69,69	0
54	MG	2A	3722	1/1	0.79	0.17	73,73,73,73	0
54	MG	2B	201	1/1	0.79	0.23	75,75,75,75	0
54	MG	2a	3058	1/1	0.79	0.28	74,74,74,74	0
54	MG	1A	3923	1/1	0.79	0.18	51,51,51,51	0
56	MPD	2B	219	8/8	0.79	0.24	61,71,72,75	0
57	ARG	1F	319	12/12	0.79	0.16	55,65,74,77	0
54	MG	2A	3582	1/1	0.80	0.14	83,83,83,83	0
54	MG	2A	3625	1/1	0.80	0.09	82,82,82,82	0
54	MG	1A	3616	1/1	0.80	0.14	34,34,34,34	0
54	MG	1A	3412	1/1	0.80	0.12	73,73,73,73	0
54	MG	1A	3220	1/1	0.80	0.16	66,66,66,66	0
54	MG	2A	3244	1/1	0.80	0.20	69,69,69,69	0
54	MG	2A	3435	1/1	0.80	0.13	59,59,59,59	0
54	MG	2A	3444	1/1	0.80	0.28	73,73,73,73	0
54	MG	2a	3060	1/1	0.80	0.31	77,77,77,77	0
54	MG	2A	3473	1/1	0.80	0.14	75,75,75,75	0
54	MG	1a	1784	1/1	0.80	0.17	69,69,69,69	0
54	MG	2G	203	1/1	0.81	0.16	70,70,70,70	0
54	MG	1a	1774	1/1	0.81	0.17	70,70,70,70	0
54	MG	2A	3475	1/1	0.81	0.12	46,46,46,46	0
54	MG	2A	3491	1/1	0.81	0.12	64,64,64,64	0
54	MG	1A	3569	1/1	0.81	0.18	70,70,70,70	0
54	MG	2A	3577	1/1	0.81	0.13	58,58,58,58	0
54	MG	1a	1800	1/1	0.81	0.14	74,74,74,74	0
54	MG	2A	3331	1/1	0.81	0.18	59,59,59,59	0
54	MG	1a	1740	1/1	0.81	0.26	76,76,76,76	0
54	MG	2A	3633	1/1	0.81	0.15	66,66,66,66	0
54	MG	1a	1867	1/1	0.81	0.14	80,80,80,80	0
54	MG	1h	202	1/1	0.81	0.12	79,79,79,79	0
54	MG	2a	3177	1/1	0.81	0.13	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1D	309	1/1	0.81	0.35	55,55,55,55	0
54	MG	1A	3589	1/1	0.81	0.16	63,63,63,63	0
54	MG	2B	203	1/1	0.81	0.20	83,83,83,83	0
54	MG	2G	201	1/1	0.81	0.12	78,78,78,78	0
54	MG	2A	3161	1/1	0.82	0.13	70,70,70,70	0
54	MG	2A	3172	1/1	0.82	0.11	63,63,63,63	0
54	MG	1A	3473	1/1	0.82	0.12	33,33,33,33	0
54	MG	2A	3253	1/1	0.82	0.12	73,73,73,73	0
54	MG	1a	1810	1/1	0.82	0.23	76,76,76,76	0
54	MG	2A	3519	1/1	0.82	0.21	64,64,64,64	0
54	MG	2a	3144	1/1	0.82	0.14	66,66,66,66	0
54	MG	1A	3633	1/1	0.82	0.40	45,45,45,45	0
54	MG	2A	3566	1/1	0.82	0.12	40,40,40,40	0
54	MG	2a	3178	1/1	0.82	0.15	65,65,65,65	0
54	MG	1A	3425	1/1	0.82	0.13	40,40,40,40	0
54	MG	1A	3602	1/1	0.82	0.12	67,67,67,67	0
54	MG	1A	3909	1/1	0.82	0.22	48,48,48,48	0
54	MG	1a	1786	1/1	0.82	0.16	62,62,62,62	0
54	MG	2O	202	1/1	0.83	0.11	80,80,80,80	0
54	MG	2a	3008	1/1	0.83	0.43	78,78,78,78	0
54	MG	2A	3494	1/1	0.83	0.11	63,63,63,63	0
54	MG	2A	3512	1/1	0.83	0.14	62,62,62,62	0
54	MG	1b	301	1/1	0.83	0.16	80,80,80,80	0
54	MG	1a	1787	1/1	0.83	0.09	70,70,70,70	0
54	MG	2A	3295	1/1	0.83	0.12	56,56,56,56	0
54	MG	1a	1682	1/1	0.83	0.29	75,75,75,75	0
54	MG	2a	3106	1/1	0.83	0.14	70,70,70,70	0
54	MG	1A	3707	1/1	0.83	0.13	70,70,70,70	0
54	MG	2A	3047	1/1	0.83	0.14	60,60,60,60	0
54	MG	2A	3055	1/1	0.83	0.23	72,72,72,72	0
54	MG	2A	3090	1/1	0.83	0.22	68,68,68,68	0
54	MG	2A	3094	1/1	0.83	0.18	76,76,76,76	0
54	MG	1a	1825	1/1	0.83	0.11	71,71,71,71	0
54	MG	2A	3704	1/1	0.83	0.17	52,52,52,52	0
54	MG	2A	3445	1/1	0.83	0.14	64,64,64,64	0
54	MG	2A	3461	1/1	0.83	0.18	56,56,56,56	0
54	MG	2A	3171	1/1	0.83	0.18	70,70,70,70	0
54	MG	1A	3965	1/1	0.83	0.18	59,59,59,59	0
54	MG	1A	3986	1/1	0.83	0.19	70,70,70,70	0
54	MG	1a	1826	1/1	0.84	0.19	72,72,72,72	0
54	MG	1A	3853	1/1	0.84	0.12	59,59,59,59	0
54	MG	2A	3708	1/1	0.84	0.11	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	1a	1604	1/1	0.84	0.15	69,69,69,69	0
54	MG	2A	3419	1/1	0.84	0.15	57,57,57,57	0
54	MG	2A	3420	1/1	0.84	0.09	73,73,73,73	0
54	MG	1A	3622	1/1	0.84	0.10	30,30,30,30	0
54	MG	1a	1700	1/1	0.84	0.13	54,54,54,54	0
54	MG	2A	3436	1/1	0.84	0.29	77,77,77,77	0
54	MG	1A	3917	1/1	0.84	0.12	35,35,35,35	0
54	MG	1A	3449	1/1	0.84	0.13	49,49,49,49	0
54	MG	1A	3927	1/1	0.84	0.12	56,56,56,56	0
54	MG	1A	3955	1/1	0.84	0.14	71,71,71,71	0
54	MG	2a	3064	1/1	0.84	0.18	69,69,69,69	0
54	MG	2a	3065	1/1	0.84	0.13	76,76,76,76	0
54	MG	1a	1772	1/1	0.84	0.13	62,62,62,62	0
54	MG	2A	3486	1/1	0.84	0.13	61,61,61,61	0
54	MG	1A	3457	1/1	0.84	0.10	36,36,36,36	0
54	MG	2A	3121	1/1	0.84	0.26	72,72,72,72	0
54	MG	2A	3511	1/1	0.84	0.17	38,38,38,38	0
54	MG	1A	3681	1/1	0.84	0.19	62,62,62,62	0
54	MG	1A	3994	1/1	0.84	0.25	48,48,48,48	0
54	MG	1A	3206	1/1	0.84	0.29	70,70,70,70	0
54	MG	2A	3209	1/1	0.84	0.14	66,66,66,66	0
54	MG	2a	3150	1/1	0.84	0.13	66,66,66,66	0
54	MG	2A	3222	1/1	0.84	0.18	58,58,58,58	0
54	MG	1B	222	1/1	0.84	0.16	54,54,54,54	0
54	MG	2A	3619	1/1	0.84	0.14	45,45,45,45	0
54	MG	1A	3203	1/1	0.84	0.21	72,72,72,72	0
54	MG	1a	1812	1/1	0.84	0.11	66,66,66,66	0
54	MG	1a	1821	1/1	0.84	0.20	68,68,68,68	0
54	MG	1D	312	1/1	0.84	0.20	66,66,66,66	0
54	MG	1A	3353	1/1	0.85	0.13	49,49,49,49	0
54	MG	1a	1811	1/1	0.85	0.13	66,66,66,66	0
54	MG	2a	3069	1/1	0.85	0.18	77,77,77,77	0
54	MG	1a	1746	1/1	0.85	0.20	71,71,71,71	0
54	MG	1A	3431	1/1	0.85	0.16	67,67,67,67	0
54	MG	1A	3776	1/1	0.85	0.11	30,30,30,30	0
54	MG	2a	3105	1/1	0.85	0.15	71,71,71,71	0
54	MG	1A	3591	1/1	0.85	0.13	51,51,51,51	0
54	MG	2A	3129	1/1	0.85	0.19	70,70,70,70	0
54	MG	2A	3518	1/1	0.85	0.16	65,65,65,65	0
54	MG	1a	1828	1/1	0.85	0.14	65,65,65,65	0
54	MG	2E	304	1/1	0.85	0.14	40,40,40,40	0
54	MG	2A	3523	1/1	0.85	0.17	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	1617	1/1	0.85	0.19	73,73,73,73	0
54	MG	2a	3167	1/1	0.85	0.38	76,76,76,76	0
54	MG	1B	207	1/1	0.85	0.10	50,50,50,50	0
54	MG	1A	3885	1/1	0.85	0.15	56,56,56,56	0
54	MG	2a	3056	1/1	0.85	0.18	74,74,74,74	0
54	MG	2a	3057	1/1	0.85	0.24	64,64,64,64	0
54	MG	1g	202	1/1	0.85	0.08	59,59,59,59	0
54	MG	1a	1701	1/1	0.85	0.20	72,72,72,72	0
54	MG	1B	231	1/1	0.85	0.14	71,71,71,71	0
54	MG	1A	3755	1/1	0.86	0.18	77,77,77,77	0
54	MG	1A	3187	1/1	0.86	0.14	54,54,54,54	0
54	MG	2A	3089	1/1	0.86	0.20	72,72,72,72	0
54	MG	10	105	1/1	0.86	0.12	60,60,60,60	0
54	MG	1A	3971	1/1	0.86	0.16	45,45,45,45	0
54	MG	2l	101	1/1	0.86	0.17	75,75,75,75	0
54	MG	2a	3004	1/1	0.86	0.28	72,72,72,72	0
54	MG	1A	3979	1/1	0.86	0.17	65,65,65,65	0
54	MG	2a	3012	1/1	0.86	0.15	62,62,62,62	0
54	MG	2a	3020	1/1	0.86	0.18	63,63,63,63	0
54	MG	1a	1675	1/1	0.86	0.24	64,64,64,64	0
54	MG	1A	3586	1/1	0.86	0.18	67,67,67,67	0
54	MG	1a	1819	1/1	0.86	0.23	75,75,75,75	0
54	MG	1a	1696	1/1	0.86	0.17	71,71,71,71	0
54	MG	2A	3177	1/1	0.86	0.15	48,48,48,48	0
54	MG	2A	3187	1/1	0.86	0.14	66,66,66,66	0
54	MG	2A	3196	1/1	0.86	0.17	67,67,67,67	0
54	MG	1A	3989	1/1	0.86	0.33	47,47,47,47	0
54	MG	2A	3219	1/1	0.86	0.14	70,70,70,70	0
54	MG	1A	3639	1/1	0.86	0.25	69,69,69,69	0
54	MG	2A	3558	1/1	0.86	0.10	65,65,65,65	0
54	MG	2A	3563	1/1	0.86	0.10	44,44,44,44	0
54	MG	1A	3893	1/1	0.86	0.10	46,46,46,46	0
54	MG	2A	3570	1/1	0.86	0.15	53,53,53,53	0
54	MG	1a	1829	1/1	0.86	0.14	82,82,82,82	0
54	MG	1A	4002	1/1	0.86	0.11	50,50,50,50	0
54	MG	1a	1848	1/1	0.86	0.10	70,70,70,70	0
54	MG	1a	1850	1/1	0.86	0.09	64,64,64,64	0
54	MG	1A	3287	1/1	0.86	0.18	69,69,69,69	0
54	MG	1A	3304	1/1	0.86	0.10	84,84,84,84	0
54	MG	2A	3390	1/1	0.86	0.23	69,69,69,69	0
54	MG	1B	230	1/1	0.86	0.10	55,55,55,55	0
54	MG	2A	3679	1/1	0.86	0.09	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	3418	1/1	0.86	0.14	47,47,47,47	0
54	MG	1a	1761	1/1	0.86	0.22	84,84,84,84	0
54	MG	1A	3487	1/1	0.86	0.16	41,41,41,41	0
54	MG	1A	3150	1/1	0.86	0.10	70,70,70,70	0
54	MG	2G	202	1/1	0.87	0.10	76,76,76,76	0
54	MG	1A	3714	1/1	0.87	0.28	53,53,53,53	0
54	MG	2A	3220	1/1	0.87	0.21	64,64,64,64	0
54	MG	2A	3495	1/1	0.87	0.13	59,59,59,59	0
54	MG	1a	1693	1/1	0.87	0.15	70,70,70,70	0
54	MG	1a	1794	1/1	0.87	0.22	86,86,86,86	0
54	MG	2A	3245	1/1	0.87	0.24	68,68,68,68	0
54	MG	1A	3527	1/1	0.87	0.16	49,49,49,49	0
54	MG	2a	3028	1/1	0.87	0.21	81,81,81,81	0
54	MG	2a	3040	1/1	0.87	0.23	75,75,75,75	0
54	MG	2a	3042	1/1	0.87	0.18	76,76,76,76	0
54	MG	2A	3254	1/1	0.87	0.15	64,64,64,64	0
54	MG	2A	3012	1/1	0.87	0.27	66,66,66,66	0
54	MG	2A	3042	1/1	0.87	0.13	48,48,48,48	0
54	MG	1A	3388	1/1	0.87	0.14	31,31,31,31	0
54	MG	1A	3789	1/1	0.87	0.16	66,66,66,66	0
54	MG	1a	1706	1/1	0.87	0.15	57,57,57,57	0
54	MG	2A	3378	1/1	0.87	0.10	39,39,39,39	0
54	MG	1A	3944	1/1	0.87	0.12	49,49,49,49	0
54	MG	2A	3588	1/1	0.87	0.17	54,54,54,54	0
54	MG	1H	201	1/1	0.87	0.16	56,56,56,56	0
54	MG	2a	3090	1/1	0.87	0.11	76,76,76,76	0
54	MG	2A	3093	1/1	0.87	0.14	67,67,67,67	0
54	MG	1a	1824	1/1	0.87	0.10	64,64,64,64	0
54	MG	1R	205	1/1	0.87	0.13	47,47,47,47	0
54	MG	2A	3423	1/1	0.87	0.14	77,77,77,77	0
54	MG	2A	3638	1/1	0.87	0.11	79,79,79,79	0
54	MG	2A	3639	1/1	0.87	0.14	73,73,73,73	0
54	MG	1A	3215	1/1	0.87	0.08	64,64,64,64	0
54	MG	2A	3671	1/1	0.87	0.18	67,67,67,67	0
54	MG	2A	3133	1/1	0.87	0.11	59,59,59,59	0
54	MG	1B	203	1/1	0.87	0.15	61,61,61,61	0
54	MG	1a	1760	1/1	0.87	0.14	66,66,66,66	0
54	MG	2A	3721	1/1	0.87	0.10	73,73,73,73	0
54	MG	1a	1837	1/1	0.87	0.12	57,57,57,57	0
54	MG	1A	3274	1/1	0.87	0.18	61,61,61,61	0
54	MG	1a	1662	1/1	0.87	0.24	74,74,74,74	0
54	MG	1a	1665	1/1	0.87	0.15	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	3521	1/1	0.87	0.14	56,56,56,56	0
54	MG	1A	3582	1/1	0.88	0.11	46,46,46,46	0
54	MG	2A	3276	1/1	0.88	0.22	56,56,56,56	0
54	MG	1a	1748	1/1	0.88	0.17	67,67,67,67	0
54	MG	1a	1872	1/1	0.88	0.10	65,65,65,65	0
54	MG	1A	3655	1/1	0.88	0.08	31,31,31,31	0
54	MG	1d	303	1/1	0.88	0.11	56,56,56,56	0
54	MG	2A	3356	1/1	0.88	0.17	73,73,73,73	0
54	MG	2A	3675	1/1	0.88	0.10	74,74,74,74	0
54	MG	1A	3903	1/1	0.88	0.11	28,28,28,28	0
54	MG	2A	3687	1/1	0.88	0.15	69,69,69,69	0
54	MG	1A	3479	1/1	0.88	0.08	22,22,22,22	0
54	MG	2A	3386	1/1	0.88	0.13	56,56,56,56	0
54	MG	2A	3715	1/1	0.88	0.13	64,64,64,64	0
54	MG	1A	3679	1/1	0.88	0.13	76,76,76,76	0
54	MG	1A	3322	1/1	0.88	0.08	29,29,29,29	0
54	MG	2A	3732	1/1	0.88	0.12	66,66,66,66	0
54	MG	1A	3433	1/1	0.88	0.16	62,62,62,62	0
54	MG	1a	1776	1/1	0.88	0.20	68,68,68,68	0
54	MG	2B	204	1/1	0.88	0.18	66,66,66,66	0
54	MG	2B	212	1/1	0.88	0.30	80,80,80,80	0
54	MG	2B	217	1/1	0.88	0.07	72,72,72,72	0
54	MG	2D	308	1/1	0.88	0.15	46,46,46,46	0
54	MG	1a	1782	1/1	0.88	0.08	82,82,82,82	0
54	MG	2F	303	1/1	0.88	0.16	67,67,67,67	0
54	MG	2A	3050	1/1	0.88	0.18	71,71,71,71	0
54	MG	2A	3424	1/1	0.88	0.10	57,57,57,57	0
54	MG	1A	3696	1/1	0.88	0.14	44,44,44,44	0
54	MG	2A	3062	1/1	0.88	0.16	57,57,57,57	0
54	MG	1A	3702	1/1	0.88	0.22	41,41,41,41	0
54	MG	2A	3440	1/1	0.88	0.13	71,71,71,71	0
54	MG	1A	3601	1/1	0.88	0.19	32,32,32,32	0
54	MG	1a	1639	1/1	0.88	0.18	75,75,75,75	0
54	MG	2A	3451	1/1	0.88	0.09	68,68,68,68	0
54	MG	2a	3025	1/1	0.88	0.17	79,79,79,79	0
54	MG	2A	3452	1/1	0.88	0.15	69,69,69,69	0
54	MG	2a	3037	1/1	0.88	0.19	65,65,65,65	0
54	MG	1a	1798	1/1	0.88	0.10	60,60,60,60	0
54	MG	2A	3462	1/1	0.88	0.12	70,70,70,70	0
54	MG	1a	1652	1/1	0.88	0.11	69,69,69,69	0
54	MG	1a	1802	1/1	0.88	0.26	72,72,72,72	0
54	MG	2A	3484	1/1	0.88	0.11	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	2A	3130	1/1	0.88	0.28	75,75,75,75	0
54	MG	1a	1807	1/1	0.88	0.12	68,68,68,68	0
54	MG	1A	3712	1/1	0.88	0.26	36,36,36,36	0
54	MG	1A	3266	1/1	0.88	0.18	66,66,66,66	0
54	MG	1A	3735	1/1	0.88	0.10	37,37,37,37	0
54	MG	1A	3354	1/1	0.88	0.09	36,36,36,36	0
54	MG	2a	3072	1/1	0.88	0.25	72,72,72,72	0
54	MG	2A	3179	1/1	0.88	0.13	60,60,60,60	0
54	MG	2A	3185	1/1	0.88	0.16	67,67,67,67	0
54	MG	1A	3992	1/1	0.88	0.15	52,52,52,52	0
54	MG	1A	3576	1/1	0.88	0.30	44,44,44,44	0
54	MG	2A	3541	1/1	0.88	0.10	63,63,63,63	0
54	MG	1A	3370	1/1	0.88	0.11	61,61,61,61	0
54	MG	2A	3562	1/1	0.88	0.12	37,37,37,37	0
54	MG	2A	3210	1/1	0.88	0.08	56,56,56,56	0
54	MG	1A	3810	1/1	0.88	0.13	46,46,46,46	0
54	MG	2a	3135	1/1	0.88	0.11	67,67,67,67	0
54	MG	1A	3817	1/1	0.88	0.17	41,41,41,41	0
54	MG	2A	3572	1/1	0.88	0.15	75,75,75,75	0
54	MG	1A	3638	1/1	0.88	0.14	60,60,60,60	0
54	MG	2A	3223	1/1	0.88	0.26	70,70,70,70	0
54	MG	1a	1738	1/1	0.88	0.10	52,52,52,52	0
54	MG	2A	3598	1/1	0.88	0.09	42,42,42,42	0
54	MG	2a	3181	1/1	0.88	0.17	72,72,72,72	0
54	MG	2A	3603	1/1	0.88	0.10	60,60,60,60	0
54	MG	1A	3857	1/1	0.88	0.12	51,51,51,51	0
54	MG	1a	1742	1/1	0.88	0.11	59,59,59,59	0
54	MG	2A	3626	1/1	0.88	0.12	57,57,57,57	0
54	MG	2B	202	1/1	0.89	0.13	71,71,71,71	0
54	MG	1a	1778	1/1	0.89	0.12	71,71,71,71	0
54	MG	1A	3883	1/1	0.89	0.08	49,49,49,49	0
54	MG	2A	3478	1/1	0.89	0.12	56,56,56,56	0
54	MG	2B	214	1/1	0.89	0.08	74,74,74,74	0
54	MG	1A	3366	1/1	0.89	0.13	39,39,39,39	0
54	MG	1A	3288	1/1	0.89	0.11	60,60,60,60	0
54	MG	2A	3489	1/1	0.89	0.16	68,68,68,68	0
54	MG	2A	3212	1/1	0.89	0.11	55,55,55,55	0
54	MG	1a	1683	1/1	0.89	0.18	79,79,79,79	0
54	MG	1B	204	1/1	0.89	0.19	52,52,52,52	0
54	MG	1l	202	1/1	0.89	0.11	70,70,70,70	0
54	MG	1n	102	1/1	0.89	0.09	58,58,58,58	0
54	MG	20	102	1/1	0.89	0.19	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	2A	3514	1/1	0.89	0.08	34,34,34,34	0
54	MG	1A	3040	1/1	0.89	0.10	52,52,52,52	0
54	MG	2A	3001	1/1	0.89	0.29	64,64,64,64	0
54	MG	1A	3086	1/1	0.89	0.12	56,56,56,56	0
54	MG	2A	3524	1/1	0.89	0.15	59,59,59,59	0
54	MG	2A	3038	1/1	0.89	0.20	68,68,68,68	0
54	MG	1A	3674	1/1	0.89	0.12	76,76,76,76	0
54	MG	2a	3035	1/1	0.89	0.14	74,74,74,74	0
54	MG	2a	3036	1/1	0.89	0.12	61,61,61,61	0
54	MG	2A	3550	1/1	0.89	0.14	63,63,63,63	0
54	MG	1A	3572	1/1	0.89	0.08	44,44,44,44	0
54	MG	2A	3287	1/1	0.89	0.12	60,60,60,60	0
54	MG	2a	3044	1/1	0.89	0.20	69,69,69,69	0
54	MG	1a	1809	1/1	0.89	0.24	71,71,71,71	0
54	MG	1a	1726	1/1	0.89	0.17	56,56,56,56	0
54	MG	2A	3330	1/1	0.89	0.10	56,56,56,56	0
54	MG	1A	3778	1/1	0.89	0.15	45,45,45,45	0
54	MG	1A	3785	1/1	0.89	0.14	45,45,45,45	0
54	MG	2A	3063	1/1	0.89	0.22	54,54,54,54	0
54	MG	1a	1814	1/1	0.89	0.09	72,72,72,72	0
54	MG	2A	3383	1/1	0.89	0.11	46,46,46,46	0
54	MG	2A	3601	1/1	0.89	0.08	63,63,63,63	0
54	MG	1A	3145	1/1	0.89	0.17	68,68,68,68	0
54	MG	1A	3614	1/1	0.89	0.19	64,64,64,64	0
54	MG	1A	3578	1/1	0.89	0.11	51,51,51,51	0
54	MG	2A	3412	1/1	0.89	0.19	72,72,72,72	0
54	MG	2A	3414	1/1	0.89	0.27	52,52,52,52	0
54	MG	2A	3105	1/1	0.89	0.14	69,69,69,69	0
54	MG	2A	3112	1/1	0.89	0.08	71,71,71,71	0
54	MG	1A	3241	1/1	0.89	0.15	67,67,67,67	0
54	MG	2a	3118	1/1	0.89	0.11	68,68,68,68	0
54	MG	18	102	1/1	0.89	0.10	58,58,58,58	0
54	MG	2a	3121	1/1	0.89	0.17	68,68,68,68	0
54	MG	1A	3628	1/1	0.89	0.13	68,68,68,68	0
54	MG	1A	3865	1/1	0.89	0.17	65,65,65,65	0
54	MG	2A	3145	1/1	0.89	0.14	49,49,49,49	0
54	MG	1a	1835	1/1	0.89	0.11	75,75,75,75	0
54	MG	2A	3682	1/1	0.89	0.13	67,67,67,67	0
54	MG	2A	3167	1/1	0.89	0.13	67,67,67,67	0
54	MG	2A	3168	1/1	0.89	0.22	58,58,58,58	0
54	MG	1A	3879	1/1	0.89	0.09	27,27,27,27	0
54	MG	2A	3447	1/1	0.89	0.23	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	1644	1/1	0.89	0.26	64,64,64,64	0
56	MPD	1A	4022	8/8	0.89	0.20	46,53,56,59	0
54	MG	1a	1847	1/1	0.89	0.09	68,68,68,68	0
56	MPD	2A	3735	8/8	0.89	0.21	50,57,60,64	0
54	MG	1A	3993	1/1	0.89	0.17	65,65,65,65	0
54	MG	1A	3881	1/1	0.89	0.06	29,29,29,29	0
54	MG	2A	3672	1/1	0.90	0.11	62,62,62,62	0
54	MG	1V	205	1/1	0.90	0.18	60,60,60,60	0
54	MG	2A	3417	1/1	0.90	0.09	72,72,72,72	0
54	MG	1A	3565	1/1	0.90	0.08	62,62,62,62	0
54	MG	1a	1779	1/1	0.90	0.20	57,57,57,57	0
54	MG	2A	3700	1/1	0.90	0.10	62,62,62,62	0
54	MG	1A	3303	1/1	0.90	0.15	67,67,67,67	0
54	MG	1A	3723	1/1	0.90	0.09	42,42,42,42	0
54	MG	2A	3714	1/1	0.90	0.09	78,78,78,78	0
54	MG	1a	1610	1/1	0.90	0.12	65,65,65,65	0
54	MG	1A	3038	1/1	0.90	0.07	38,38,38,38	0
54	MG	2A	3431	1/1	0.90	0.30	51,51,51,51	0
54	MG	2A	3727	1/1	0.90	0.16	65,65,65,65	0
54	MG	1a	1625	1/1	0.90	0.12	53,53,53,53	0
54	MG	2A	3114	1/1	0.90	0.15	69,69,69,69	0
54	MG	1a	1635	1/1	0.90	0.14	50,50,50,50	0
54	MG	2A	3442	1/1	0.90	0.10	64,64,64,64	0
54	MG	2A	3443	1/1	0.90	0.10	60,60,60,60	0
54	MG	2B	208	1/1	0.90	0.12	63,63,63,63	0
54	MG	2B	209	1/1	0.90	0.25	72,72,72,72	0
54	MG	2A	3125	1/1	0.90	0.17	54,54,54,54	0
54	MG	1A	3750	1/1	0.90	0.10	56,56,56,56	0
54	MG	1A	3435	1/1	0.90	0.10	49,49,49,49	0
54	MG	1A	3385	1/1	0.90	0.08	33,33,33,33	0
54	MG	2D	310	1/1	0.90	0.14	60,60,60,60	0
54	MG	1a	1653	1/1	0.90	0.13	62,62,62,62	0
54	MG	1a	1661	1/1	0.90	0.20	74,74,74,74	0
54	MG	1A	3640	1/1	0.90	0.14	61,61,61,61	0
54	MG	1a	1663	1/1	0.90	0.12	66,66,66,66	0
54	MG	1A	3642	1/1	0.90	0.16	70,70,70,70	0
54	MG	1a	1671	1/1	0.90	0.15	79,79,79,79	0
54	MG	2P	201	1/1	0.90	0.19	45,45,45,45	0
54	MG	1A	3646	1/1	0.90	0.14	73,73,73,73	0
54	MG	1A	3125	1/1	0.90	0.21	56,56,56,56	0
54	MG	1A	3816	1/1	0.90	0.07	27,27,27,27	0
54	MG	1a	1689	1/1	0.90	0.14	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	2a	3010	1/1	0.90	0.19	56,56,56,56	0
54	MG	1A	3657	1/1	0.90	0.07	16,16,16,16	0
54	MG	2a	3018	1/1	0.90	0.17	73,73,73,73	0
54	MG	2A	3197	1/1	0.90	0.23	58,58,58,58	0
54	MG	2a	3022	1/1	0.90	0.20	64,64,64,64	0
54	MG	2A	3498	1/1	0.90	0.12	66,66,66,66	0
54	MG	2A	3200	1/1	0.90	0.09	68,68,68,68	0
54	MG	2A	3203	1/1	0.90	0.24	53,53,53,53	0
54	MG	1A	3852	1/1	0.90	0.11	27,27,27,27	0
54	MG	2A	3516	1/1	0.90	0.16	56,56,56,56	0
54	MG	2a	3038	1/1	0.90	0.25	66,66,66,66	0
54	MG	1A	3669	1/1	0.90	0.14	61,61,61,61	0
54	MG	1A	4007	1/1	0.90	0.13	50,50,50,50	0
54	MG	1a	1702	1/1	0.90	0.12	63,63,63,63	0
54	MG	2a	3046	1/1	0.90	0.21	67,67,67,67	0
54	MG	2a	3048	1/1	0.90	0.30	69,69,69,69	0
54	MG	1A	3461	1/1	0.90	0.10	53,53,53,53	0
54	MG	2A	3525	1/1	0.90	0.12	68,68,68,68	0
54	MG	1a	1715	1/1	0.90	0.20	69,69,69,69	0
54	MG	2A	3533	1/1	0.90	0.09	37,37,37,37	0
54	MG	1a	1719	1/1	0.90	0.19	76,76,76,76	0
54	MG	1A	3401	1/1	0.90	0.14	68,68,68,68	0
54	MG	1A	3866	1/1	0.90	0.10	45,45,45,45	0
54	MG	2a	3066	1/1	0.90	0.26	63,63,63,63	0
54	MG	1B	212	1/1	0.90	0.25	61,61,61,61	0
54	MG	1A	3404	1/1	0.90	0.22	55,55,55,55	0
54	MG	1B	226	1/1	0.90	0.13	54,54,54,54	0
54	MG	2a	3077	1/1	0.90	0.11	72,72,72,72	0
54	MG	2A	3277	1/1	0.90	0.16	73,73,73,73	0
54	MG	2a	3089	1/1	0.90	0.09	71,71,71,71	0
54	MG	1A	3131	1/1	0.90	0.10	51,51,51,51	0
54	MG	1l	201	1/1	0.90	0.10	70,70,70,70	0
54	MG	2a	3099	1/1	0.90	0.18	69,69,69,69	0
54	MG	2a	3103	1/1	0.90	0.11	85,85,85,85	0
54	MG	1A	3882	1/1	0.90	0.12	52,52,52,52	0
54	MG	2A	3585	1/1	0.90	0.13	60,60,60,60	0
54	MG	1a	1750	1/1	0.90	0.16	67,67,67,67	0
54	MG	2A	3309	1/1	0.90	0.12	54,54,54,54	0
54	MG	2a	3116	1/1	0.90	0.11	59,59,59,59	0
54	MG	1A	3495	1/1	0.90	0.08	61,61,61,61	0
54	MG	1A	3067	1/1	0.90	0.12	50,50,50,50	0
54	MG	2A	3613	1/1	0.90	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3123	1/1	0.90	0.18	58,58,58,58	0
54	MG	2A	3618	1/1	0.90	0.11	39,39,39,39	0
54	MG	2A	3344	1/1	0.90	0.13	75,75,75,75	0
54	MG	2a	3136	1/1	0.90	0.19	84,84,84,84	0
54	MG	2a	3141	1/1	0.90	0.13	57,57,57,57	0
54	MG	2A	3624	1/1	0.90	0.07	68,68,68,68	0
54	MG	2A	3345	1/1	0.90	0.09	41,41,41,41	0
54	MG	2a	3151	1/1	0.90	0.29	68,68,68,68	0
54	MG	1a	1757	1/1	0.90	0.16	64,64,64,64	0
54	MG	1a	1758	1/1	0.90	0.19	68,68,68,68	0
54	MG	1A	3357	1/1	0.90	0.10	21,21,21,21	0
54	MG	1A	3705	1/1	0.90	0.10	55,55,55,55	0
54	MG	1P	204	1/1	0.90	0.27	57,57,57,57	0
54	MG	1A	3543	1/1	0.90	0.07	55,55,55,55	0
54	MG	2n	101	1/1	0.90	0.17	69,69,69,69	0
54	MG	2A	3641	1/1	0.90	0.15	65,65,65,65	0
54	MG	2A	3651	1/1	0.90	0.11	81,81,81,81	0
54	MG	2A	3054	1/1	0.90	0.23	70,70,70,70	0
54	MG	2A	3667	1/1	0.90	0.10	79,79,79,79	0
54	MG	1a	1775	1/1	0.90	0.32	79,79,79,79	0
54	MG	1B	217	1/1	0.91	0.17	50,50,50,50	0
54	MG	1B	219	1/1	0.91	0.10	52,52,52,52	0
54	MG	1d	302	1/1	0.91	0.22	71,71,71,71	0
54	MG	2A	3313	1/1	0.91	0.14	55,55,55,55	0
54	MG	1A	3312	1/1	0.91	0.16	58,58,58,58	0
54	MG	2A	3674	1/1	0.91	0.12	51,51,51,51	0
54	MG	1d	305	1/1	0.91	0.07	79,79,79,79	0
54	MG	2A	3335	1/1	0.91	0.24	61,61,61,61	0
54	MG	2A	3342	1/1	0.91	0.14	48,48,48,48	0
54	MG	2A	3683	1/1	0.91	0.10	65,65,65,65	0
54	MG	1A	3414	1/1	0.91	0.09	63,63,63,63	0
54	MG	2A	3688	1/1	0.91	0.16	71,71,71,71	0
54	MG	2A	3695	1/1	0.91	0.09	66,66,66,66	0
54	MG	1B	228	1/1	0.91	0.12	65,65,65,65	0
54	MG	1A	3571	1/1	0.91	0.08	23,23,23,23	0
54	MG	2A	3363	1/1	0.91	0.10	61,61,61,61	0
54	MG	2A	3711	1/1	0.91	0.12	64,64,64,64	0
54	MG	1A	3313	1/1	0.91	0.10	51,51,51,51	0
54	MG	2A	3368	1/1	0.91	0.08	37,37,37,37	0
54	MG	1a	1745	1/1	0.91	0.11	57,57,57,57	0
54	MG	2A	3380	1/1	0.91	0.11	68,68,68,68	0
54	MG	2A	3724	1/1	0.91	0.21	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	3671	1/1	0.91	0.07	64,64,64,64	0
54	MG	1A	3168	1/1	0.91	0.10	58,58,58,58	0
54	MG	1E	306	1/1	0.91	0.12	45,45,45,45	0
54	MG	2A	3024	1/1	0.91	0.13	67,67,67,67	0
54	MG	2A	3399	1/1	0.91	0.09	59,59,59,59	0
54	MG	1A	3324	1/1	0.91	0.14	49,49,49,49	0
54	MG	1G	203	1/1	0.91	0.13	74,74,74,74	0
54	MG	1A	3342	1/1	0.91	0.10	57,57,57,57	0
54	MG	1A	3246	1/1	0.91	0.11	48,48,48,48	0
54	MG	2A	3048	1/1	0.91	0.10	63,63,63,63	0
54	MG	1A	3584	1/1	0.91	0.09	56,56,56,56	0
54	MG	2A	3053	1/1	0.91	0.16	49,49,49,49	0
54	MG	1U	207	1/1	0.91	0.26	40,40,40,40	0
54	MG	1a	1763	1/1	0.91	0.13	64,64,64,64	0
54	MG	1a	1771	1/1	0.91	0.08	80,80,80,80	0
54	MG	1A	3454	1/1	0.91	0.07	39,39,39,39	0
54	MG	2A	3080	1/1	0.91	0.07	73,73,73,73	0
54	MG	2A	3083	1/1	0.91	0.21	71,71,71,71	0
54	MG	1A	3697	1/1	0.91	0.15	48,48,48,48	0
54	MG	15	101	1/1	0.91	0.17	42,42,42,42	0
54	MG	1A	3906	1/1	0.91	0.08	30,30,30,30	0
54	MG	1A	3455	1/1	0.91	0.16	59,59,59,59	0
54	MG	2a	3001	1/1	0.91	0.12	56,56,56,56	0
54	MG	1A	3910	1/1	0.91	0.12	31,31,31,31	0
54	MG	1A	3260	1/1	0.91	0.14	75,75,75,75	0
54	MG	1a	1783	1/1	0.91	0.11	63,63,63,63	0
54	MG	1A	3593	1/1	0.91	0.10	57,57,57,57	0
54	MG	2a	3014	1/1	0.91	0.17	64,64,64,64	0
54	MG	1A	3594	1/1	0.91	0.08	41,41,41,41	0
54	MG	2A	3463	1/1	0.91	0.11	64,64,64,64	0
54	MG	1a	1636	1/1	0.91	0.19	58,58,58,58	0
54	MG	1A	3597	1/1	0.91	0.08	36,36,36,36	0
54	MG	1a	1797	1/1	0.91	0.10	65,65,65,65	0
54	MG	2a	3030	1/1	0.91	0.24	59,59,59,59	0
54	MG	2A	3134	1/1	0.91	0.10	62,62,62,62	0
54	MG	2A	3143	1/1	0.91	0.17	71,71,71,71	0
54	MG	1a	1641	1/1	0.91	0.12	65,65,65,65	0
54	MG	2A	3152	1/1	0.91	0.26	67,67,67,67	0
54	MG	2A	3156	1/1	0.91	0.28	58,58,58,58	0
54	MG	1a	1799	1/1	0.91	0.14	71,71,71,71	0
54	MG	1A	3183	1/1	0.91	0.09	52,52,52,52	0
54	MG	2A	3500	1/1	0.91	0.20	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3733	1/1	0.91	0.10	49,49,49,49	0
54	MG	2a	3051	1/1	0.91	0.14	55,55,55,55	0
54	MG	1A	3072	1/1	0.91	0.14	47,47,47,47	0
54	MG	1a	1808	1/1	0.91	0.15	56,56,56,56	0
54	MG	1A	3127	1/1	0.91	0.13	56,56,56,56	0
54	MG	1A	3982	1/1	0.91	0.08	32,32,32,32	0
54	MG	2A	3180	1/1	0.91	0.13	66,66,66,66	0
54	MG	1A	3057	1/1	0.91	0.17	53,53,53,53	0
54	MG	1a	1664	1/1	0.91	0.12	67,67,67,67	0
54	MG	1A	3209	1/1	0.91	0.18	64,64,64,64	0
54	MG	1a	1817	1/1	0.91	0.07	67,67,67,67	0
54	MG	1a	1668	1/1	0.91	0.16	64,64,64,64	0
54	MG	2A	3540	1/1	0.91	0.10	60,60,60,60	0
54	MG	1A	3990	1/1	0.91	0.15	43,43,43,43	0
54	MG	2A	3545	1/1	0.91	0.09	71,71,71,71	0
54	MG	2A	3207	1/1	0.91	0.14	60,60,60,60	0
54	MG	1A	3505	1/1	0.91	0.08	26,26,26,26	0
54	MG	1A	3510	1/1	0.91	0.09	55,55,55,55	0
54	MG	2a	3095	1/1	0.91	0.19	65,65,65,65	0
54	MG	1A	3786	1/1	0.91	0.09	26,26,26,26	0
54	MG	2a	3100	1/1	0.91	0.12	69,69,69,69	0
54	MG	1A	3109	1/1	0.91	0.14	61,61,61,61	0
54	MG	2A	3569	1/1	0.91	0.08	61,61,61,61	0
54	MG	1A	3804	1/1	0.91	0.08	51,51,51,51	0
54	MG	2A	3571	1/1	0.91	0.09	67,67,67,67	0
54	MG	1a	1833	1/1	0.91	0.12	45,45,45,45	0
54	MG	1A	3124	1/1	0.91	0.21	60,60,60,60	0
54	MG	2A	3225	1/1	0.91	0.12	60,60,60,60	0
54	MG	2A	3227	1/1	0.91	0.13	67,67,67,67	0
54	MG	2A	3587	1/1	0.91	0.09	48,48,48,48	0
54	MG	2A	3238	1/1	0.91	0.09	61,61,61,61	0
54	MG	2a	3128	1/1	0.91	0.15	67,67,67,67	0
54	MG	2A	3240	1/1	0.91	0.32	64,64,64,64	0
54	MG	2a	3134	1/1	0.91	0.10	65,65,65,65	0
54	MG	1a	1697	1/1	0.91	0.14	71,71,71,71	0
54	MG	1a	1843	1/1	0.91	0.14	79,79,79,79	0
54	MG	2A	3247	1/1	0.91	0.27	61,61,61,61	0
54	MG	2A	3617	1/1	0.91	0.08	77,77,77,77	0
54	MG	2a	3149	1/1	0.91	0.21	71,71,71,71	0
54	MG	2A	3248	1/1	0.91	0.08	65,65,65,65	0
54	MG	1A	3538	1/1	0.91	0.08	34,34,34,34	0
54	MG	2a	3153	1/1	0.91	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	2a	3164	1/1	0.91	0.11	74,74,74,74	0
54	MG	1A	3307	1/1	0.91	0.10	38,38,38,38	0
54	MG	2A	3255	1/1	0.91	0.10	64,64,64,64	0
54	MG	2A	3261	1/1	0.91	0.08	55,55,55,55	0
54	MG	2A	3271	1/1	0.91	0.10	64,64,64,64	0
54	MG	2A	3273	1/1	0.91	0.13	63,63,63,63	0
54	MG	2e	202	1/1	0.91	0.14	64,64,64,64	0
54	MG	1A	3821	1/1	0.91	0.13	71,71,71,71	0
54	MG	2A	3635	1/1	0.91	0.18	72,72,72,72	0
54	MG	2A	3637	1/1	0.91	0.13	72,72,72,72	0
54	MG	1A	3832	1/1	0.91	0.09	59,59,59,59	0
56	MPD	1a	1875	8/8	0.91	0.12	60,64,68,69	0
54	MG	1a	1866	1/1	0.91	0.08	44,44,44,44	0
54	MG	1a	1714	1/1	0.91	0.19	77,77,77,77	0
54	MG	2A	3643	1/1	0.91	0.17	56,56,56,56	0
54	MG	1A	3010	1/1	0.92	0.17	60,60,60,60	0
54	MG	1a	1624	1/1	0.92	0.17	59,59,59,59	0
54	MG	1A	3694	1/1	0.92	0.11	52,52,52,52	0
54	MG	1a	1633	1/1	0.92	0.15	66,66,66,66	0
54	MG	2A	3622	1/1	0.92	0.17	66,66,66,66	0
54	MG	1a	1634	1/1	0.92	0.08	44,44,44,44	0
54	MG	1a	1813	1/1	0.92	0.10	56,56,56,56	0
54	MG	1A	3500	1/1	0.92	0.11	59,59,59,59	0
54	MG	1A	3063	1/1	0.92	0.08	45,45,45,45	0
54	MG	2A	3233	1/1	0.92	0.08	54,54,54,54	0
54	MG	1a	1637	1/1	0.92	0.25	60,60,60,60	0
54	MG	1A	3699	1/1	0.92	0.14	48,48,48,48	0
54	MG	1a	1640	1/1	0.92	0.19	72,72,72,72	0
54	MG	1A	3302	1/1	0.92	0.27	64,64,64,64	0
54	MG	1A	3517	1/1	0.92	0.09	53,53,53,53	0
54	MG	1A	3932	1/1	0.92	0.07	61,61,61,61	0
54	MG	1A	3934	1/1	0.92	0.08	48,48,48,48	0
54	MG	1A	3935	1/1	0.92	0.08	50,50,50,50	0
54	MG	2A	3655	1/1	0.92	0.14	73,73,73,73	0
54	MG	2A	3659	1/1	0.92	0.12	56,56,56,56	0
54	MG	1A	3936	1/1	0.92	0.13	59,59,59,59	0
54	MG	2A	3258	1/1	0.92	0.21	60,60,60,60	0
54	MG	2A	3669	1/1	0.92	0.23	71,71,71,71	0
54	MG	2A	3670	1/1	0.92	0.13	68,68,68,68	0
54	MG	1A	3102	1/1	0.92	0.09	54,54,54,54	0
54	MG	1a	1838	1/1	0.92	0.14	67,67,67,67	0
54	MG	1a	1841	1/1	0.92	0.12	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	3952	1/1	0.92	0.12	47,47,47,47	0
54	MG	1A	3368	1/1	0.92	0.11	39,39,39,39	0
54	MG	2A	3680	1/1	0.92	0.17	60,60,60,60	0
54	MG	1a	1666	1/1	0.92	0.18	56,56,56,56	0
54	MG	2A	3281	1/1	0.92	0.11	51,51,51,51	0
54	MG	2A	3684	1/1	0.92	0.08	55,55,55,55	0
54	MG	1A	3962	1/1	0.92	0.10	68,68,68,68	0
54	MG	1a	1849	1/1	0.92	0.19	85,85,85,85	0
54	MG	2A	3299	1/1	0.92	0.14	68,68,68,68	0
54	MG	2A	3698	1/1	0.92	0.09	50,50,50,50	0
54	MG	2A	3300	1/1	0.92	0.13	59,59,59,59	0
54	MG	1a	1669	1/1	0.92	0.21	61,61,61,61	0
54	MG	2A	3307	1/1	0.92	0.15	57,57,57,57	0
54	MG	1a	1857	1/1	0.92	0.10	65,65,65,65	0
54	MG	1a	1858	1/1	0.92	0.10	62,62,62,62	0
54	MG	1a	1859	1/1	0.92	0.14	68,68,68,68	0
54	MG	2A	3720	1/1	0.92	0.07	69,69,69,69	0
54	MG	1A	3609	1/1	0.92	0.23	42,42,42,42	0
54	MG	1A	3968	1/1	0.92	0.11	40,40,40,40	0
54	MG	2A	3341	1/1	0.92	0.11	47,47,47,47	0
54	MG	1a	1678	1/1	0.92	0.13	59,59,59,59	0
54	MG	1a	1679	1/1	0.92	0.11	56,56,56,56	0
54	MG	1A	3611	1/1	0.92	0.21	58,58,58,58	0
54	MG	2A	3346	1/1	0.92	0.09	66,66,66,66	0
54	MG	2A	3349	1/1	0.92	0.09	39,39,39,39	0
54	MG	2A	3352	1/1	0.92	0.09	69,69,69,69	0
54	MG	1A	3529	1/1	0.92	0.09	51,51,51,51	0
54	MG	1A	3981	1/1	0.92	0.08	46,46,46,46	0
54	MG	1e	203	1/1	0.92	0.15	70,70,70,70	0
54	MG	1f	202	1/1	0.92	0.09	39,39,39,39	0
54	MG	2A	3373	1/1	0.92	0.14	59,59,59,59	0
54	MG	2D	302	1/1	0.92	0.41	43,43,43,43	0
54	MG	1A	3195	1/1	0.92	0.10	55,55,55,55	0
54	MG	1a	1695	1/1	0.92	0.09	54,54,54,54	0
54	MG	2A	3382	1/1	0.92	0.11	54,54,54,54	0
54	MG	1A	3748	1/1	0.92	0.07	21,21,21,21	0
54	MG	1A	3619	1/1	0.92	0.10	38,38,38,38	0
54	MG	1n	101	1/1	0.92	0.25	72,72,72,72	0
54	MG	1A	3453	1/1	0.92	0.07	23,23,23,23	0
54	MG	2N	201	1/1	0.92	0.09	76,76,76,76	0
54	MG	1A	3763	1/1	0.92	0.10	56,56,56,56	0
54	MG	2A	3408	1/1	0.92	0.18	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	2A	3410	1/1	0.92	0.17	58,58,58,58	0
54	MG	1A	3765	1/1	0.92	0.20	62,62,62,62	0
54	MG	2A	3007	1/1	0.92	0.19	50,50,50,50	0
54	MG	1A	3766	1/1	0.92	0.11	47,47,47,47	0
54	MG	2A	3016	1/1	0.92	0.34	69,69,69,69	0
54	MG	2a	3009	1/1	0.92	0.10	68,68,68,68	0
54	MG	1a	1707	1/1	0.92	0.11	62,62,62,62	0
54	MG	2A	3025	1/1	0.92	0.09	56,56,56,56	0
54	MG	2A	3032	1/1	0.92	0.08	56,56,56,56	0
54	MG	2a	3017	1/1	0.92	0.21	61,61,61,61	0
54	MG	2A	3035	1/1	0.92	0.08	59,59,59,59	0
54	MG	1A	3770	1/1	0.92	0.09	32,32,32,32	0
54	MG	2A	3040	1/1	0.92	0.23	70,70,70,70	0
54	MG	2a	3023	1/1	0.92	0.17	69,69,69,69	0
54	MG	2a	3024	1/1	0.92	0.21	63,63,63,63	0
54	MG	1A	3998	1/1	0.92	0.17	48,48,48,48	0
54	MG	1a	1716	1/1	0.92	0.12	75,75,75,75	0
54	MG	1A	3554	1/1	0.92	0.09	40,40,40,40	0
54	MG	2a	3033	1/1	0.92	0.14	68,68,68,68	0
54	MG	1a	1725	1/1	0.92	0.11	66,66,66,66	0
54	MG	1A	3632	1/1	0.92	0.10	39,39,39,39	0
54	MG	1a	1730	1/1	0.92	0.11	63,63,63,63	0
54	MG	1A	3782	1/1	0.92	0.13	46,46,46,46	0
54	MG	1a	1737	1/1	0.92	0.17	59,59,59,59	0
54	MG	1A	3556	1/1	0.92	0.14	58,58,58,58	0
54	MG	1A	3634	1/1	0.92	0.11	59,59,59,59	0
54	MG	2A	3456	1/1	0.92	0.10	61,61,61,61	0
54	MG	2A	3457	1/1	0.92	0.11	74,74,74,74	0
54	MG	2A	3068	1/1	0.92	0.21	54,54,54,54	0
54	MG	2a	3054	1/1	0.92	0.14	70,70,70,70	0
54	MG	2A	3069	1/1	0.92	0.18	63,63,63,63	0
54	MG	2A	3071	1/1	0.92	0.27	57,57,57,57	0
54	MG	2A	3464	1/1	0.92	0.12	57,57,57,57	0
54	MG	2A	3465	1/1	0.92	0.10	55,55,55,55	0
54	MG	2A	3471	1/1	0.92	0.15	67,67,67,67	0
54	MG	2A	3472	1/1	0.92	0.07	54,54,54,54	0
54	MG	1A	3635	1/1	0.92	0.23	34,34,34,34	0
54	MG	1A	3798	1/1	0.92	0.07	47,47,47,47	0
54	MG	2a	3067	1/1	0.92	0.17	61,61,61,61	0
54	MG	2A	3477	1/1	0.92	0.15	54,54,54,54	0
54	MG	1A	3557	1/1	0.92	0.07	59,59,59,59	0
54	MG	1B	220	1/1	0.92	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3076	1/1	0.92	0.32	68,68,68,68	0
54	MG	1A	3377	1/1	0.92	0.13	42,42,42,42	0
54	MG	1A	3256	1/1	0.92	0.19	64,64,64,64	0
54	MG	1A	3137	1/1	0.92	0.09	54,54,54,54	0
54	MG	1A	3645	1/1	0.92	0.11	59,59,59,59	0
54	MG	1A	3066	1/1	0.92	0.20	59,59,59,59	0
54	MG	2A	3120	1/1	0.92	0.21	54,54,54,54	0
54	MG	1A	3850	1/1	0.92	0.08	35,35,35,35	0
54	MG	2A	3503	1/1	0.92	0.14	77,77,77,77	0
54	MG	2A	3507	1/1	0.92	0.15	73,73,73,73	0
54	MG	1A	3575	1/1	0.92	0.17	59,59,59,59	0
54	MG	1a	1762	1/1	0.92	0.24	72,72,72,72	0
54	MG	1D	314	1/1	0.92	0.08	63,63,63,63	0
54	MG	1A	3468	1/1	0.92	0.08	26,26,26,26	0
54	MG	1F	304	1/1	0.92	0.13	38,38,38,38	0
54	MG	2A	3138	1/1	0.92	0.20	53,53,53,53	0
54	MG	2A	3140	1/1	0.92	0.15	46,46,46,46	0
54	MG	1A	3661	1/1	0.92	0.10	47,47,47,47	0
54	MG	1A	3665	1/1	0.92	0.11	63,63,63,63	0
54	MG	1A	3014	1/1	0.92	0.12	57,57,57,57	0
54	MG	2A	3529	1/1	0.92	0.11	64,64,64,64	0
54	MG	2a	3132	1/1	0.92	0.12	65,65,65,65	0
54	MG	2a	3133	1/1	0.92	0.09	75,75,75,75	0
54	MG	1O	201	1/1	0.92	0.17	50,50,50,50	0
54	MG	1A	3869	1/1	0.92	0.06	30,30,30,30	0
54	MG	2A	3165	1/1	0.92	0.30	52,52,52,52	0
54	MG	2A	3544	1/1	0.92	0.09	56,56,56,56	0
54	MG	1A	3475	1/1	0.92	0.09	46,46,46,46	0
54	MG	2A	3547	1/1	0.92	0.07	70,70,70,70	0
54	MG	1T	202	1/1	0.92	0.10	77,77,77,77	0
54	MG	2A	3170	1/1	0.92	0.17	76,76,76,76	0
54	MG	1A	3581	1/1	0.92	0.07	38,38,38,38	0
54	MG	2a	3162	1/1	0.92	0.12	61,61,61,61	0
54	MG	1A	3676	1/1	0.92	0.09	60,60,60,60	0
54	MG	10	102	1/1	0.92	0.14	37,37,37,37	0
54	MG	1a	1790	1/1	0.92	0.09	80,80,80,80	0
54	MG	1a	1793	1/1	0.92	0.11	52,52,52,52	0
54	MG	2A	3183	1/1	0.92	0.16	54,54,54,54	0
54	MG	1A	3476	1/1	0.92	0.09	35,35,35,35	0
54	MG	2a	3182	1/1	0.92	0.16	79,79,79,79	0
54	MG	2a	3183	1/1	0.92	0.14	86,86,86,86	0
54	MG	1a	1795	1/1	0.92	0.16	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	2f	201	1/1	0.92	0.14	61,61,61,61	0
54	MG	2A	3195	1/1	0.92	0.15	54,54,54,54	0
54	MG	1A	3884	1/1	0.92	0.15	46,46,46,46	0
54	MG	15	106	1/1	0.92	0.13	68,68,68,68	0
54	MG	1A	3282	1/1	0.92	0.28	45,45,45,45	0
54	MG	1a	1602	1/1	0.92	0.22	55,55,55,55	0
54	MG	1A	3886	1/1	0.92	0.12	51,51,51,51	0
54	MG	1A	3210	1/1	0.92	0.24	46,46,46,46	0
57	ARG	1B	233	12/12	0.92	0.11	36,52,59,62	0
54	MG	2A	3606	1/1	0.92	0.16	62,62,62,62	0
54	MG	2A	3656	1/1	0.93	0.10	51,51,51,51	0
54	MG	1A	3759	1/1	0.93	0.12	59,59,59,59	0
54	MG	1A	3762	1/1	0.93	0.13	54,54,54,54	0
54	MG	1A	3399	1/1	0.93	0.12	45,45,45,45	0
54	MG	1A	3034	1/1	0.93	0.23	69,69,69,69	0
54	MG	1a	1691	1/1	0.93	0.10	55,55,55,55	0
54	MG	2A	3314	1/1	0.93	0.17	62,62,62,62	0
54	MG	2A	3328	1/1	0.93	0.15	52,52,52,52	0
54	MG	1a	1692	1/1	0.93	0.14	63,63,63,63	0
54	MG	1A	3035	1/1	0.93	0.14	43,43,43,43	0
54	MG	2A	3676	1/1	0.93	0.10	69,69,69,69	0
54	MG	2A	3677	1/1	0.93	0.09	49,49,49,49	0
54	MG	1A	3767	1/1	0.93	0.09	28,28,28,28	0
54	MG	2A	3339	1/1	0.93	0.18	59,59,59,59	0
54	MG	1A	3528	1/1	0.93	0.10	45,45,45,45	0
54	MG	1A	3158	1/1	0.93	0.24	37,37,37,37	0
54	MG	2A	3343	1/1	0.93	0.09	42,42,42,42	0
54	MG	1A	3410	1/1	0.93	0.10	25,25,25,25	0
54	MG	1A	3779	1/1	0.93	0.08	45,45,45,45	0
54	MG	2A	3692	1/1	0.93	0.08	51,51,51,51	0
54	MG	1t	201	1/1	0.93	0.09	56,56,56,56	0
54	MG	1A	3540	1/1	0.93	0.07	34,34,34,34	0
54	MG	1y	201	1/1	0.93	0.07	56,56,56,56	0
54	MG	2A	3354	1/1	0.93	0.14	63,63,63,63	0
54	MG	2A	3707	1/1	0.93	0.09	59,59,59,59	0
54	MG	1y	203	1/1	0.93	0.12	75,75,75,75	0
54	MG	1A	3999	1/1	0.93	0.07	51,51,51,51	0
54	MG	2A	3713	1/1	0.93	0.21	47,47,47,47	0
54	MG	2A	3364	1/1	0.93	0.12	62,62,62,62	0
54	MG	1A	4001	1/1	0.93	0.14	62,62,62,62	0
54	MG	2A	3716	1/1	0.93	0.07	65,65,65,65	0
54	MG	1a	1710	1/1	0.93	0.14	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	2A	3370	1/1	0.93	0.17	51,51,51,51	0
54	MG	1A	3541	1/1	0.93	0.09	47,47,47,47	0
54	MG	2A	3017	1/1	0.93	0.10	56,56,56,56	0
54	MG	1A	4006	1/1	0.93	0.09	57,57,57,57	0
54	MG	2A	3731	1/1	0.93	0.11	62,62,62,62	0
54	MG	2A	3381	1/1	0.93	0.17	53,53,53,53	0
54	MG	1A	3221	1/1	0.93	0.11	61,61,61,61	0
54	MG	2A	3028	1/1	0.93	0.06	36,36,36,36	0
54	MG	1A	4016	1/1	0.93	0.08	60,60,60,60	0
54	MG	2A	3034	1/1	0.93	0.18	57,57,57,57	0
54	MG	2B	206	1/1	0.93	0.09	63,63,63,63	0
54	MG	2B	207	1/1	0.93	0.26	63,63,63,63	0
54	MG	1B	202	1/1	0.93	0.14	50,50,50,50	0
54	MG	1A	3547	1/1	0.93	0.12	58,58,58,58	0
54	MG	2A	3404	1/1	0.93	0.11	60,60,60,60	0
54	MG	1A	3643	1/1	0.93	0.14	46,46,46,46	0
54	MG	1A	3552	1/1	0.93	0.09	51,51,51,51	0
54	MG	1B	209	1/1	0.93	0.28	60,60,60,60	0
54	MG	2D	307	1/1	0.93	0.15	42,42,42,42	0
54	MG	1B	211	1/1	0.93	0.09	54,54,54,54	0
54	MG	2D	309	1/1	0.93	0.14	51,51,51,51	0
54	MG	1A	3808	1/1	0.93	0.18	40,40,40,40	0
54	MG	1A	3166	1/1	0.93	0.16	54,54,54,54	0
54	MG	1A	3651	1/1	0.93	0.17	56,56,56,56	0
54	MG	1A	3652	1/1	0.93	0.35	47,47,47,47	0
54	MG	1A	3819	1/1	0.93	0.27	39,39,39,39	0
54	MG	1A	3654	1/1	0.93	0.06	34,34,34,34	0
54	MG	1A	3827	1/1	0.93	0.07	42,42,42,42	0
54	MG	2O	201	1/1	0.93	0.10	58,58,58,58	0
54	MG	2A	3065	1/1	0.93	0.06	44,44,44,44	0
54	MG	1a	1754	1/1	0.93	0.10	55,55,55,55	0
54	MG	1A	3828	1/1	0.93	0.11	46,46,46,46	0
54	MG	1A	3418	1/1	0.93	0.12	43,43,43,43	0
54	MG	28	102	1/1	0.93	0.13	56,56,56,56	0
54	MG	1A	3846	1/1	0.93	0.11	36,36,36,36	0
54	MG	1a	1759	1/1	0.93	0.13	60,60,60,60	0
54	MG	2a	3006	1/1	0.93	0.15	63,63,63,63	0
54	MG	1A	3656	1/1	0.93	0.07	55,55,55,55	0
54	MG	1A	3243	1/1	0.93	0.25	56,56,56,56	0
54	MG	1E	302	1/1	0.93	0.24	38,38,38,38	0
54	MG	2A	3449	1/1	0.93	0.07	53,53,53,53	0
54	MG	1E	304	1/1	0.93	0.07	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3015	1/1	0.93	0.08	63,63,63,63	0
54	MG	2A	3095	1/1	0.93	0.17	53,53,53,53	0
54	MG	2A	3097	1/1	0.93	0.07	62,62,62,62	0
54	MG	1A	3659	1/1	0.93	0.08	22,22,22,22	0
54	MG	2A	3458	1/1	0.93	0.08	74,74,74,74	0
54	MG	2A	3109	1/1	0.93	0.12	51,51,51,51	0
54	MG	1A	3856	1/1	0.93	0.07	54,54,54,54	0
54	MG	1a	1773	1/1	0.93	0.15	68,68,68,68	0
54	MG	1A	3321	1/1	0.93	0.13	63,63,63,63	0
54	MG	1A	3861	1/1	0.93	0.09	57,57,57,57	0
54	MG	2A	3468	1/1	0.93	0.07	33,33,33,33	0
54	MG	2A	3469	1/1	0.93	0.09	63,63,63,63	0
54	MG	1A	3864	1/1	0.93	0.13	41,41,41,41	0
54	MG	1a	1777	1/1	0.93	0.08	66,66,66,66	0
54	MG	1A	3663	1/1	0.93	0.09	54,54,54,54	0
54	MG	1A	3566	1/1	0.93	0.11	38,38,38,38	0
54	MG	2a	3041	1/1	0.93	0.17	73,73,73,73	0
54	MG	1a	1780	1/1	0.93	0.14	63,63,63,63	0
54	MG	2a	3043	1/1	0.93	0.19	54,54,54,54	0
54	MG	1A	3868	1/1	0.93	0.12	45,45,45,45	0
54	MG	1A	3244	1/1	0.93	0.20	39,39,39,39	0
54	MG	2A	3141	1/1	0.93	0.18	66,66,66,66	0
54	MG	2A	3142	1/1	0.93	0.10	46,46,46,46	0
54	MG	1A	3877	1/1	0.93	0.10	71,71,71,71	0
54	MG	1A	3002	1/1	0.93	0.11	56,56,56,56	0
54	MG	1W	201	1/1	0.93	0.18	51,51,51,51	0
54	MG	1Y	202	1/1	0.93	0.08	55,55,55,55	0
54	MG	2a	3059	1/1	0.93	0.19	61,61,61,61	0
54	MG	1Z	301	1/1	0.93	0.14	54,54,54,54	0
54	MG	2a	3061	1/1	0.93	0.27	64,64,64,64	0
54	MG	2A	3501	1/1	0.93	0.09	66,66,66,66	0
54	MG	1A	3439	1/1	0.93	0.09	51,51,51,51	0
54	MG	2A	3505	1/1	0.93	0.24	61,61,61,61	0
54	MG	10	104	1/1	0.93	0.10	47,47,47,47	0
54	MG	1a	1796	1/1	0.93	0.13	71,71,71,71	0
54	MG	2a	3068	1/1	0.93	0.12	60,60,60,60	0
54	MG	1A	3337	1/1	0.93	0.10	46,46,46,46	0
54	MG	10	107	1/1	0.93	0.14	51,51,51,51	0
54	MG	1A	3452	1/1	0.93	0.10	46,46,46,46	0
54	MG	1A	3341	1/1	0.93	0.07	40,40,40,40	0
54	MG	1A	3255	1/1	0.93	0.09	51,51,51,51	0
54	MG	2a	3081	1/1	0.93	0.41	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	3084	1/1	0.93	0.07	59,59,59,59	0
54	MG	2a	3085	1/1	0.93	0.07	67,67,67,67	0
54	MG	1a	1803	1/1	0.93	0.08	62,62,62,62	0
54	MG	1a	1601	1/1	0.93	0.09	50,50,50,50	0
54	MG	1A	3345	1/1	0.93	0.11	59,59,59,59	0
54	MG	1A	3348	1/1	0.93	0.08	39,39,39,39	0
54	MG	1a	1607	1/1	0.93	0.14	51,51,51,51	0
54	MG	1A	3898	1/1	0.93	0.08	61,61,61,61	0
54	MG	1A	3068	1/1	0.93	0.08	33,33,33,33	0
54	MG	2a	3101	1/1	0.93	0.14	62,62,62,62	0
54	MG	2a	3102	1/1	0.93	0.08	70,70,70,70	0
54	MG	2A	3198	1/1	0.93	0.12	62,62,62,62	0
54	MG	1a	1619	1/1	0.93	0.14	55,55,55,55	0
54	MG	2A	3202	1/1	0.93	0.21	50,50,50,50	0
54	MG	1A	3022	1/1	0.93	0.09	49,49,49,49	0
54	MG	2A	3206	1/1	0.93	0.14	64,64,64,64	0
54	MG	1A	3698	1/1	0.93	0.34	47,47,47,47	0
54	MG	1a	1818	1/1	0.93	0.21	76,76,76,76	0
54	MG	1a	1628	1/1	0.93	0.17	58,58,58,58	0
54	MG	1A	3193	1/1	0.93	0.09	57,57,57,57	0
54	MG	2a	3122	1/1	0.93	0.12	74,74,74,74	0
54	MG	1A	3474	1/1	0.93	0.09	26,26,26,26	0
54	MG	1A	3083	1/1	0.93	0.10	35,35,35,35	0
54	MG	1A	3925	1/1	0.93	0.11	66,66,66,66	0
54	MG	1A	3275	1/1	0.93	0.13	56,56,56,56	0
54	MG	2A	3575	1/1	0.93	0.10	50,50,50,50	0
54	MG	1A	3202	1/1	0.93	0.28	52,52,52,52	0
54	MG	1A	3481	1/1	0.93	0.11	27,27,27,27	0
54	MG	1a	1834	1/1	0.93	0.11	50,50,50,50	0
54	MG	2a	3139	1/1	0.93	0.18	70,70,70,70	0
54	MG	2A	3235	1/1	0.93	0.10	62,62,62,62	0
54	MG	1A	3482	1/1	0.93	0.07	27,27,27,27	0
54	MG	1A	3729	1/1	0.93	0.09	34,34,34,34	0
54	MG	1A	3938	1/1	0.93	0.09	45,45,45,45	0
54	MG	1A	3939	1/1	0.93	0.07	30,30,30,30	0
54	MG	1A	3372	1/1	0.93	0.10	44,44,44,44	0
54	MG	2a	3156	1/1	0.93	0.11	62,62,62,62	0
54	MG	2a	3160	1/1	0.93	0.10	74,74,74,74	0
54	MG	1A	3951	1/1	0.93	0.10	44,44,44,44	0
54	MG	1A	3375	1/1	0.93	0.09	45,45,45,45	0
54	MG	1A	3744	1/1	0.93	0.12	65,65,65,65	0
54	MG	1A	3960	1/1	0.93	0.10	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	2a	3172	1/1	0.93	0.10	76,76,76,76	0
54	MG	1A	3745	1/1	0.93	0.09	54,54,54,54	0
54	MG	2A	3260	1/1	0.93	0.08	59,59,59,59	0
54	MG	1a	1856	1/1	0.93	0.08	53,53,53,53	0
54	MG	1A	3132	1/1	0.93	0.28	37,37,37,37	0
54	MG	2A	3628	1/1	0.93	0.11	64,64,64,64	0
54	MG	2e	201	1/1	0.93	0.28	68,68,68,68	0
54	MG	2A	3272	1/1	0.93	0.07	58,58,58,58	0
54	MG	1A	3966	1/1	0.93	0.08	43,43,43,43	0
54	MG	1A	3027	1/1	0.93	0.07	69,69,69,69	0
54	MG	1a	1674	1/1	0.93	0.14	56,56,56,56	0
54	MG	1A	3140	1/1	0.93	0.17	43,43,43,43	0
54	MG	1a	1871	1/1	0.93	0.11	62,62,62,62	0
54	MG	1A	3976	1/1	0.93	0.09	52,52,52,52	0
54	MG	2A	3291	1/1	0.93	0.17	57,57,57,57	0
56	MPD	2A	3736	8/8	0.93	0.15	52,56,60,62	0
54	MG	1a	1873	1/1	0.93	0.09	59,59,59,59	0
54	MG	2A	3298	1/1	0.93	0.07	44,44,44,44	0
54	MG	1a	1874	1/1	0.93	0.12	71,71,71,71	0
54	MG	1a	1822	1/1	0.94	0.25	67,67,67,67	0
54	MG	1A	3918	1/1	0.94	0.14	55,55,55,55	0
54	MG	2A	3623	1/1	0.94	0.08	52,52,52,52	0
54	MG	1A	3921	1/1	0.94	0.10	67,67,67,67	0
54	MG	1a	1621	1/1	0.94	0.10	61,61,61,61	0
54	MG	1a	1623	1/1	0.94	0.10	60,60,60,60	0
54	MG	2A	3627	1/1	0.94	0.14	68,68,68,68	0
54	MG	1A	3922	1/1	0.94	0.07	43,43,43,43	0
54	MG	2A	3243	1/1	0.94	0.10	67,67,67,67	0
54	MG	1a	1832	1/1	0.94	0.10	52,52,52,52	0
54	MG	1A	3728	1/1	0.94	0.06	28,28,28,28	0
54	MG	1a	1626	1/1	0.94	0.08	49,49,49,49	0
54	MG	2A	3636	1/1	0.94	0.12	62,62,62,62	0
54	MG	1A	3605	1/1	0.94	0.23	38,38,38,38	0
54	MG	2A	3250	1/1	0.94	0.16	52,52,52,52	0
54	MG	2A	3251	1/1	0.94	0.09	58,58,58,58	0
54	MG	2A	3252	1/1	0.94	0.24	46,46,46,46	0
54	MG	1a	1629	1/1	0.94	0.16	63,63,63,63	0
54	MG	2A	3648	1/1	0.94	0.11	67,67,67,67	0
54	MG	1A	3498	1/1	0.94	0.07	45,45,45,45	0
54	MG	2A	3653	1/1	0.94	0.07	51,51,51,51	0
54	MG	1a	1839	1/1	0.94	0.09	63,63,63,63	0
54	MG	2A	3257	1/1	0.94	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3658	1/1	0.94	0.08	53,53,53,53	0
54	MG	1A	3185	1/1	0.94	0.11	44,44,44,44	0
54	MG	2A	3259	1/1	0.94	0.20	55,55,55,55	0
54	MG	2A	3661	1/1	0.94	0.09	58,58,58,58	0
54	MG	2A	3662	1/1	0.94	0.10	38,38,38,38	0
54	MG	1A	3736	1/1	0.94	0.08	51,51,51,51	0
54	MG	1A	3314	1/1	0.94	0.24	57,57,57,57	0
54	MG	1A	3615	1/1	0.94	0.06	51,51,51,51	0
54	MG	1A	3507	1/1	0.94	0.09	43,43,43,43	0
54	MG	1A	3749	1/1	0.94	0.12	35,35,35,35	0
54	MG	1A	3130	1/1	0.94	0.12	30,30,30,30	0
54	MG	1A	3947	1/1	0.94	0.08	39,39,39,39	0
54	MG	1a	1645	1/1	0.94	0.16	57,57,57,57	0
54	MG	1a	1646	1/1	0.94	0.23	51,51,51,51	0
54	MG	2A	3285	1/1	0.94	0.07	47,47,47,47	0
54	MG	2A	3286	1/1	0.94	0.07	48,48,48,48	0
54	MG	1a	1647	1/1	0.94	0.15	63,63,63,63	0
54	MG	1a	1860	1/1	0.94	0.09	57,57,57,57	0
54	MG	2A	3292	1/1	0.94	0.09	57,57,57,57	0
54	MG	2A	3685	1/1	0.94	0.11	39,39,39,39	0
54	MG	2A	3293	1/1	0.94	0.09	62,62,62,62	0
54	MG	1a	1865	1/1	0.94	0.09	74,74,74,74	0
54	MG	2A	3297	1/1	0.94	0.07	36,36,36,36	0
54	MG	1a	1651	1/1	0.94	0.14	53,53,53,53	0
54	MG	1A	3752	1/1	0.94	0.12	40,40,40,40	0
54	MG	2A	3699	1/1	0.94	0.09	54,54,54,54	0
54	MG	1a	1870	1/1	0.94	0.12	68,68,68,68	0
54	MG	1A	3515	1/1	0.94	0.14	56,56,56,56	0
54	MG	2A	3303	1/1	0.94	0.10	51,51,51,51	0
54	MG	2A	3306	1/1	0.94	0.14	67,67,67,67	0
54	MG	1a	1657	1/1	0.94	0.07	67,67,67,67	0
54	MG	1A	3954	1/1	0.94	0.07	65,65,65,65	0
54	MG	2A	3311	1/1	0.94	0.11	58,58,58,58	0
54	MG	2A	3312	1/1	0.94	0.09	50,50,50,50	0
54	MG	1A	3758	1/1	0.94	0.08	53,53,53,53	0
54	MG	1A	3958	1/1	0.94	0.10	47,47,47,47	0
54	MG	2A	3319	1/1	0.94	0.14	51,51,51,51	0
54	MG	2A	3320	1/1	0.94	0.11	41,41,41,41	0
54	MG	2A	3723	1/1	0.94	0.07	35,35,35,35	0
54	MG	2A	3321	1/1	0.94	0.16	48,48,48,48	0
54	MG	2A	3726	1/1	0.94	0.08	57,57,57,57	0
54	MG	1d	301	1/1	0.94	0.19	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	3624	1/1	0.94	0.09	57,57,57,57	0
54	MG	1A	3761	1/1	0.94	0.05	28,28,28,28	0
54	MG	1A	3408	1/1	0.94	0.07	42,42,42,42	0
54	MG	1A	3631	1/1	0.94	0.07	42,42,42,42	0
54	MG	1A	3247	1/1	0.94	0.23	40,40,40,40	0
54	MG	1A	3524	1/1	0.94	0.06	51,51,51,51	0
54	MG	1A	3525	1/1	0.94	0.12	59,59,59,59	0
54	MG	1i	201	1/1	0.94	0.10	59,59,59,59	0
54	MG	1A	3978	1/1	0.94	0.08	60,60,60,60	0
54	MG	1A	3092	1/1	0.94	0.28	36,36,36,36	0
54	MG	1A	3980	1/1	0.94	0.06	55,55,55,55	0
54	MG	1a	1681	1/1	0.94	0.10	52,52,52,52	0
54	MG	2B	215	1/1	0.94	0.12	67,67,67,67	0
54	MG	1n	103	1/1	0.94	0.15	63,63,63,63	0
54	MG	1A	3773	1/1	0.94	0.08	21,21,21,21	0
54	MG	2A	3358	1/1	0.94	0.12	58,58,58,58	0
54	MG	2A	3361	1/1	0.94	0.07	56,56,56,56	0
54	MG	1A	3636	1/1	0.94	0.11	34,34,34,34	0
54	MG	1a	1688	1/1	0.94	0.16	60,60,60,60	0
54	MG	2A	3365	1/1	0.94	0.18	61,61,61,61	0
54	MG	2E	307	1/1	0.94	0.19	63,63,63,63	0
54	MG	1A	3984	1/1	0.94	0.06	73,73,73,73	0
54	MG	2A	3367	1/1	0.94	0.09	59,59,59,59	0
54	MG	1A	3413	1/1	0.94	0.07	31,31,31,31	0
54	MG	2A	3003	1/1	0.94	0.07	51,51,51,51	0
54	MG	2A	3372	1/1	0.94	0.19	63,63,63,63	0
54	MG	1A	3096	1/1	0.94	0.07	48,48,48,48	0
54	MG	2A	3377	1/1	0.94	0.05	34,34,34,34	0
54	MG	1A	3780	1/1	0.94	0.15	40,40,40,40	0
54	MG	2P	202	1/1	0.94	0.09	61,61,61,61	0
54	MG	2Q	202	1/1	0.94	0.14	57,57,57,57	0
54	MG	2T	3301	1/1	0.94	0.09	56,56,56,56	0
54	MG	2T	3303	1/1	0.94	0.08	65,65,65,65	0
54	MG	2V	201	1/1	0.94	0.10	62,62,62,62	0
54	MG	2V	202	1/1	0.94	0.17	53,53,53,53	0
54	MG	20	101	1/1	0.94	0.10	63,63,63,63	0
54	MG	1A	3535	1/1	0.94	0.07	43,43,43,43	0
54	MG	1A	3783	1/1	0.94	0.12	50,50,50,50	0
54	MG	1A	3199	1/1	0.94	0.09	52,52,52,52	0
54	MG	1A	3265	1/1	0.94	0.11	26,26,26,26	0
54	MG	1A	3429	1/1	0.94	0.12	52,52,52,52	0
54	MG	1A	3790	1/1	0.94	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	2a	3007	1/1	0.94	0.06	72,72,72,72	0
54	MG	1A	3792	1/1	0.94	0.15	58,58,58,58	0
54	MG	1A	3794	1/1	0.94	0.09	78,78,78,78	0
54	MG	2A	3402	1/1	0.94	0.11	37,37,37,37	0
54	MG	2A	3037	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3097	1/1	0.94	0.14	66,66,66,66	0
54	MG	1a	1711	1/1	0.94	0.14	66,66,66,66	0
54	MG	2A	3041	1/1	0.94	0.20	56,56,56,56	0
54	MG	1A	3650	1/1	0.94	0.09	55,55,55,55	0
54	MG	2a	3019	1/1	0.94	0.07	67,67,67,67	0
54	MG	1A	3805	1/1	0.94	0.12	73,73,73,73	0
54	MG	1A	4019	1/1	0.94	0.11	58,58,58,58	0
54	MG	1B	201	1/1	0.94	0.14	51,51,51,51	0
54	MG	1a	1721	1/1	0.94	0.09	80,80,80,80	0
54	MG	1A	3346	1/1	0.94	0.08	36,36,36,36	0
54	MG	2a	3026	1/1	0.94	0.17	63,63,63,63	0
54	MG	1A	3809	1/1	0.94	0.09	57,57,57,57	0
54	MG	2A	3425	1/1	0.94	0.08	48,48,48,48	0
54	MG	1a	1727	1/1	0.94	0.12	65,65,65,65	0
54	MG	2A	3057	1/1	0.94	0.12	52,52,52,52	0
54	MG	1A	3551	1/1	0.94	0.07	49,49,49,49	0
54	MG	1A	3813	1/1	0.94	0.11	48,48,48,48	0
54	MG	2A	3064	1/1	0.94	0.09	48,48,48,48	0
54	MG	2a	3039	1/1	0.94	0.17	56,56,56,56	0
54	MG	1a	1736	1/1	0.94	0.22	62,62,62,62	0
54	MG	2A	3066	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3815	1/1	0.94	0.08	53,53,53,53	0
54	MG	1A	3139	1/1	0.94	0.15	42,42,42,42	0
54	MG	1A	3099	1/1	0.94	0.07	44,44,44,44	0
54	MG	1B	216	1/1	0.94	0.08	56,56,56,56	0
54	MG	2a	3047	1/1	0.94	0.19	61,61,61,61	0
54	MG	1A	3440	1/1	0.94	0.14	74,74,74,74	0
54	MG	2a	3050	1/1	0.94	0.23	54,54,54,54	0
54	MG	2A	3087	1/1	0.94	0.10	80,80,80,80	0
54	MG	2a	3052	1/1	0.94	0.08	57,57,57,57	0
54	MG	1B	218	1/1	0.94	0.13	63,63,63,63	0
54	MG	1A	3059	1/1	0.94	0.11	45,45,45,45	0
54	MG	1a	1749	1/1	0.94	0.09	70,70,70,70	0
54	MG	2A	3459	1/1	0.94	0.08	59,59,59,59	0
54	MG	1A	3826	1/1	0.94	0.07	43,43,43,43	0
54	MG	1A	3356	1/1	0.94	0.06	45,45,45,45	0
54	MG	1A	3104	1/1	0.94	0.41	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	3102	1/1	0.94	0.12	51,51,51,51	0
54	MG	2a	3063	1/1	0.94	0.18	59,59,59,59	0
54	MG	2A	3103	1/1	0.94	0.18	66,66,66,66	0
54	MG	2A	3104	1/1	0.94	0.21	54,54,54,54	0
54	MG	1B	227	1/1	0.94	0.07	42,42,42,42	0
54	MG	1A	3830	1/1	0.94	0.07	50,50,50,50	0
54	MG	2A	3110	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3831	1/1	0.94	0.06	37,37,37,37	0
54	MG	2A	3474	1/1	0.94	0.12	59,59,59,59	0
54	MG	2A	3113	1/1	0.94	0.08	56,56,56,56	0
54	MG	1A	3359	1/1	0.94	0.12	55,55,55,55	0
54	MG	1B	232	1/1	0.94	0.08	68,68,68,68	0
54	MG	2a	3078	1/1	0.94	0.14	57,57,57,57	0
54	MG	2a	3079	1/1	0.94	0.11	59,59,59,59	0
54	MG	1A	3835	1/1	0.94	0.08	49,49,49,49	0
54	MG	2a	3083	1/1	0.94	0.18	52,52,52,52	0
54	MG	1A	3364	1/1	0.94	0.09	50,50,50,50	0
54	MG	1A	3849	1/1	0.94	0.10	42,42,42,42	0
54	MG	1A	3214	1/1	0.94	0.32	47,47,47,47	0
54	MG	2A	3132	1/1	0.94	0.12	60,60,60,60	0
54	MG	1A	3670	1/1	0.94	0.11	38,38,38,38	0
54	MG	1A	3459	1/1	0.94	0.06	55,55,55,55	0
54	MG	1A	3855	1/1	0.94	0.07	47,47,47,47	0
54	MG	2a	3096	1/1	0.94	0.06	49,49,49,49	0
54	MG	1F	312	1/1	0.94	0.12	41,41,41,41	0
54	MG	1A	3672	1/1	0.94	0.07	53,53,53,53	0
54	MG	2A	3504	1/1	0.94	0.08	67,67,67,67	0
54	MG	1A	3673	1/1	0.94	0.07	41,41,41,41	0
54	MG	1A	3036	1/1	0.94	0.12	37,37,37,37	0
54	MG	2A	3510	1/1	0.94	0.09	54,54,54,54	0
54	MG	1N	203	1/1	0.94	0.06	53,53,53,53	0
54	MG	2a	3107	1/1	0.94	0.09	66,66,66,66	0
54	MG	2A	3150	1/1	0.94	0.14	53,53,53,53	0
54	MG	2A	3513	1/1	0.94	0.08	47,47,47,47	0
54	MG	1A	3297	1/1	0.94	0.07	48,48,48,48	0
54	MG	1A	3470	1/1	0.94	0.07	23,23,23,23	0
54	MG	1A	3471	1/1	0.94	0.07	27,27,27,27	0
54	MG	2A	3163	1/1	0.94	0.12	56,56,56,56	0
54	MG	2A	3520	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3164	1/1	0.94	0.09	48,48,48,48	0
54	MG	1T	203	1/1	0.94	0.13	57,57,57,57	0
54	MG	1A	3691	1/1	0.94	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	2A	3526	1/1	0.94	0.14	47,47,47,47	0
54	MG	2A	3169	1/1	0.94	0.10	67,67,67,67	0
54	MG	1A	3871	1/1	0.94	0.12	28,28,28,28	0
54	MG	1V	206	1/1	0.94	0.12	47,47,47,47	0
54	MG	2A	3536	1/1	0.94	0.09	38,38,38,38	0
54	MG	1A	3373	1/1	0.94	0.09	54,54,54,54	0
54	MG	2a	3140	1/1	0.94	0.16	67,67,67,67	0
54	MG	1A	3076	1/1	0.94	0.15	43,43,43,43	0
54	MG	1A	3695	1/1	0.94	0.25	33,33,33,33	0
54	MG	2a	3146	1/1	0.94	0.10	67,67,67,67	0
54	MG	2a	3148	1/1	0.94	0.09	69,69,69,69	0
54	MG	1A	3587	1/1	0.94	0.06	25,25,25,25	0
54	MG	1A	3234	1/1	0.94	0.28	42,42,42,42	0
54	MG	1A	3384	1/1	0.94	0.08	32,32,32,32	0
54	MG	2A	3186	1/1	0.94	0.37	72,72,72,72	0
54	MG	10	106	1/1	0.94	0.16	63,63,63,63	0
54	MG	2a	3158	1/1	0.94	0.08	69,69,69,69	0
54	MG	2a	3159	1/1	0.94	0.11	66,66,66,66	0
54	MG	2A	3189	1/1	0.94	0.07	53,53,53,53	0
54	MG	2A	3565	1/1	0.94	0.06	41,41,41,41	0
54	MG	2A	3191	1/1	0.94	0.08	49,49,49,49	0
54	MG	2a	3165	1/1	0.94	0.07	68,68,68,68	0
54	MG	2a	3166	1/1	0.94	0.10	66,66,66,66	0
54	MG	1A	3046	1/1	0.94	0.14	50,50,50,50	0
54	MG	11	103	1/1	0.94	0.10	56,56,56,56	0
54	MG	1a	1805	1/1	0.94	0.10	56,56,56,56	0
54	MG	2a	3174	1/1	0.94	0.17	75,75,75,75	0
54	MG	1A	3310	1/1	0.94	0.21	53,53,53,53	0
54	MG	1A	3704	1/1	0.94	0.14	50,50,50,50	0
54	MG	2a	3179	1/1	0.94	0.19	62,62,62,62	0
54	MG	2A	3201	1/1	0.94	0.17	63,63,63,63	0
54	MG	2A	3581	1/1	0.94	0.11	53,53,53,53	0
54	MG	1A	3394	1/1	0.94	0.09	22,22,22,22	0
54	MG	1A	3600	1/1	0.94	0.07	32,32,32,32	0
54	MG	1A	3004	1/1	0.94	0.08	45,45,45,45	0
54	MG	1A	3496	1/1	0.94	0.09	39,39,39,39	0
54	MG	2A	3592	1/1	0.94	0.11	65,65,65,65	0
54	MG	2l	201	1/1	0.94	0.12	63,63,63,63	0
54	MG	1a	1605	1/1	0.94	0.10	73,73,73,73	0
54	MG	2o	101	1/1	0.94	0.11	65,65,65,65	0
54	MG	2A	3599	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3715	1/1	0.94	0.42	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MPD	18	103	8/8	0.94	0.12	33,41,46,48	0
54	MG	1a	1816	1/1	0.94	0.06	92,92,92,92	0
54	MG	2A	3604	1/1	0.94	0.06	52,52,52,52	0
54	MG	1a	1608	1/1	0.94	0.10	63,63,63,63	0
54	MG	1a	1609	1/1	0.94	0.09	67,67,67,67	0
54	MG	1A	3604	1/1	0.94	0.21	39,39,39,39	0
54	MG	1a	1615	1/1	0.94	0.13	60,60,60,60	0
54	MG	2A	3239	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3149	1/1	0.95	0.09	46,46,46,46	0
54	MG	2A	3241	1/1	0.95	0.10	48,48,48,48	0
54	MG	2A	3242	1/1	0.95	0.08	59,59,59,59	0
54	MG	1A	3945	1/1	0.95	0.09	65,65,65,65	0
54	MG	1A	3946	1/1	0.95	0.06	24,24,24,24	0
54	MG	1A	3623	1/1	0.95	0.06	43,43,43,43	0
54	MG	2A	3246	1/1	0.95	0.25	60,60,60,60	0
54	MG	2A	3632	1/1	0.95	0.10	58,58,58,58	0
54	MG	1a	1627	1/1	0.95	0.07	62,62,62,62	0
54	MG	1A	3949	1/1	0.95	0.09	33,33,33,33	0
54	MG	1A	3286	1/1	0.95	0.07	37,37,37,37	0
54	MG	1a	1631	1/1	0.95	0.08	51,51,51,51	0
54	MG	1A	3376	1/1	0.95	0.08	52,52,52,52	0
54	MG	1A	3079	1/1	0.95	0.09	40,40,40,40	0
54	MG	1A	3764	1/1	0.95	0.06	30,30,30,30	0
54	MG	1A	3499	1/1	0.95	0.07	25,25,25,25	0
54	MG	1A	3378	1/1	0.95	0.06	36,36,36,36	0
54	MG	1A	3379	1/1	0.95	0.08	30,30,30,30	0
54	MG	1A	3154	1/1	0.95	0.13	57,57,57,57	0
54	MG	1A	3292	1/1	0.95	0.05	44,44,44,44	0
54	MG	1a	1642	1/1	0.95	0.10	67,67,67,67	0
54	MG	2A	3263	1/1	0.95	0.07	52,52,52,52	0
54	MG	1A	3386	1/1	0.95	0.08	29,29,29,29	0
54	MG	1a	1863	1/1	0.95	0.09	61,61,61,61	0
54	MG	1A	3969	1/1	0.95	0.09	55,55,55,55	0
54	MG	2A	3274	1/1	0.95	0.10	56,56,56,56	0
54	MG	2A	3275	1/1	0.95	0.10	48,48,48,48	0
54	MG	2A	3663	1/1	0.95	0.09	33,33,33,33	0
54	MG	1A	3296	1/1	0.95	0.06	40,40,40,40	0
54	MG	1A	3389	1/1	0.95	0.08	36,36,36,36	0
54	MG	1A	3977	1/1	0.95	0.18	63,63,63,63	0
54	MG	1A	3037	1/1	0.95	0.14	43,43,43,43	0
54	MG	1A	3396	1/1	0.95	0.05	28,28,28,28	0
54	MG	1A	3301	1/1	0.95	0.08	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	1a	1659	1/1	0.95	0.21	42,42,42,42	0
54	MG	2A	3288	1/1	0.95	0.10	52,52,52,52	0
54	MG	1a	1660	1/1	0.95	0.25	56,56,56,56	0
54	MG	1A	3126	1/1	0.95	0.07	46,46,46,46	0
54	MG	1A	3100	1/1	0.95	0.33	38,38,38,38	0
54	MG	2A	3681	1/1	0.95	0.06	55,55,55,55	0
54	MG	1A	3983	1/1	0.95	0.07	46,46,46,46	0
54	MG	1A	3788	1/1	0.95	0.12	42,42,42,42	0
54	MG	1A	3530	1/1	0.95	0.08	52,52,52,52	0
54	MG	1f	201	1/1	0.95	0.15	55,55,55,55	0
54	MG	2A	3686	1/1	0.95	0.07	56,56,56,56	0
54	MG	1A	3988	1/1	0.95	0.05	21,21,21,21	0
54	MG	1g	201	1/1	0.95	0.23	62,62,62,62	0
54	MG	2A	3691	1/1	0.95	0.06	57,57,57,57	0
54	MG	1A	3533	1/1	0.95	0.08	49,49,49,49	0
54	MG	1A	3534	1/1	0.95	0.05	25,25,25,25	0
54	MG	1a	1670	1/1	0.95	0.26	58,58,58,58	0
54	MG	2A	3308	1/1	0.95	0.09	39,39,39,39	0
54	MG	1A	3224	1/1	0.95	0.16	35,35,35,35	0
54	MG	2A	3703	1/1	0.95	0.11	67,67,67,67	0
54	MG	2A	3310	1/1	0.95	0.08	43,43,43,43	0
54	MG	2A	3705	1/1	0.95	0.07	56,56,56,56	0
54	MG	1a	1672	1/1	0.95	0.09	62,62,62,62	0
54	MG	1A	3795	1/1	0.95	0.07	41,41,41,41	0
54	MG	1A	3228	1/1	0.95	0.23	42,42,42,42	0
54	MG	1A	3229	1/1	0.95	0.21	42,42,42,42	0
54	MG	2A	3317	1/1	0.95	0.10	31,31,31,31	0
54	MG	2A	3318	1/1	0.95	0.10	50,50,50,50	0
54	MG	1A	3658	1/1	0.95	0.07	51,51,51,51	0
54	MG	1A	3311	1/1	0.95	0.23	36,36,36,36	0
54	MG	1A	3542	1/1	0.95	0.12	40,40,40,40	0
54	MG	2A	3322	1/1	0.95	0.10	64,64,64,64	0
54	MG	2A	3325	1/1	0.95	0.12	39,39,39,39	0
54	MG	1y	202	1/1	0.95	0.13	53,53,53,53	0
54	MG	1A	3662	1/1	0.95	0.16	33,33,33,33	0
54	MG	1a	1685	1/1	0.95	0.13	58,58,58,58	0
54	MG	2A	3002	1/1	0.95	0.08	52,52,52,52	0
54	MG	2A	3336	1/1	0.95	0.08	41,41,41,41	0
54	MG	1a	1687	1/1	0.95	0.08	53,53,53,53	0
54	MG	1A	4003	1/1	0.95	0.09	90,90,90,90	0
54	MG	1A	4005	1/1	0.95	0.08	15,15,15,15	0
54	MG	2A	3013	1/1	0.95	0.06	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	1690	1/1	0.95	0.15	60,60,60,60	0
54	MG	1A	3008	1/1	0.95	0.09	42,42,42,42	0
54	MG	2A	3019	1/1	0.95	0.20	44,44,44,44	0
54	MG	2A	3348	1/1	0.95	0.08	53,53,53,53	0
54	MG	2A	3023	1/1	0.95	0.17	58,58,58,58	0
54	MG	2A	3351	1/1	0.95	0.11	47,47,47,47	0
54	MG	1A	3546	1/1	0.95	0.11	37,37,37,37	0
54	MG	2B	216	1/1	0.95	0.07	59,59,59,59	0
54	MG	2A	3353	1/1	0.95	0.20	65,65,65,65	0
54	MG	1A	4013	1/1	0.95	0.10	42,42,42,42	0
54	MG	1A	3668	1/1	0.95	0.06	44,44,44,44	0
54	MG	2A	3029	1/1	0.95	0.08	54,54,54,54	0
54	MG	1A	4017	1/1	0.95	0.13	43,43,43,43	0
54	MG	1A	4018	1/1	0.95	0.07	46,46,46,46	0
54	MG	1A	3235	1/1	0.95	0.23	36,36,36,36	0
54	MG	1A	3415	1/1	0.95	0.10	28,28,28,28	0
54	MG	1A	3417	1/1	0.95	0.07	46,46,46,46	0
54	MG	1A	3236	1/1	0.95	0.20	43,43,43,43	0
54	MG	1A	3419	1/1	0.95	0.12	25,25,25,25	0
54	MG	1B	206	1/1	0.95	0.24	43,43,43,43	0
54	MG	2I	201	1/1	0.95	0.12	59,59,59,59	0
54	MG	1A	3319	1/1	0.95	0.14	58,58,58,58	0
54	MG	2A	3045	1/1	0.95	0.12	52,52,52,52	0
54	MG	1B	208	1/1	0.95	0.11	47,47,47,47	0
54	MG	1A	3427	1/1	0.95	0.08	37,37,37,37	0
54	MG	1A	3238	1/1	0.95	0.16	39,39,39,39	0
54	MG	1a	1718	1/1	0.95	0.06	60,60,60,60	0
54	MG	2R	202	1/1	0.95	0.16	52,52,52,52	0
54	MG	1A	3176	1/1	0.95	0.13	48,48,48,48	0
54	MG	1a	1720	1/1	0.95	0.10	63,63,63,63	0
54	MG	1A	3834	1/1	0.95	0.07	39,39,39,39	0
54	MG	2A	3387	1/1	0.95	0.12	59,59,59,59	0
54	MG	2W	202	1/1	0.95	0.15	61,61,61,61	0
54	MG	2W	203	1/1	0.95	0.07	61,61,61,61	0
54	MG	2A	3389	1/1	0.95	0.14	70,70,70,70	0
54	MG	2A	3058	1/1	0.95	0.07	41,41,41,41	0
54	MG	2A	3059	1/1	0.95	0.15	54,54,54,54	0
54	MG	25	102	1/1	0.95	0.21	42,42,42,42	0
54	MG	2A	3398	1/1	0.95	0.14	42,42,42,42	0
54	MG	2A	3060	1/1	0.95	0.07	46,46,46,46	0
54	MG	1a	1723	1/1	0.95	0.08	63,63,63,63	0
54	MG	2a	3005	1/1	0.95	0.10	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	3178	1/1	0.95	0.13	48,48,48,48	0
54	MG	2A	3406	1/1	0.95	0.11	51,51,51,51	0
54	MG	1A	3840	1/1	0.95	0.09	54,54,54,54	0
54	MG	1A	3843	1/1	0.95	0.10	55,55,55,55	0
54	MG	2A	3411	1/1	0.95	0.08	53,53,53,53	0
54	MG	1A	3683	1/1	0.95	0.11	35,35,35,35	0
54	MG	2a	3013	1/1	0.95	0.11	73,73,73,73	0
54	MG	1A	3686	1/1	0.95	0.11	56,56,56,56	0
54	MG	1a	1733	1/1	0.95	0.09	43,43,43,43	0
54	MG	1B	223	1/1	0.95	0.13	55,55,55,55	0
54	MG	2A	3073	1/1	0.95	0.08	49,49,49,49	0
54	MG	2A	3074	1/1	0.95	0.18	65,65,65,65	0
54	MG	1A	3687	1/1	0.95	0.12	58,58,58,58	0
54	MG	2A	3082	1/1	0.95	0.12	49,49,49,49	0
54	MG	1A	3688	1/1	0.95	0.17	58,58,58,58	0
54	MG	1A	3331	1/1	0.95	0.07	47,47,47,47	0
54	MG	1A	3573	1/1	0.95	0.09	29,29,29,29	0
54	MG	1a	1744	1/1	0.95	0.10	65,65,65,65	0
54	MG	2a	3027	1/1	0.95	0.09	70,70,70,70	0
54	MG	2A	3091	1/1	0.95	0.09	54,54,54,54	0
54	MG	2A	3439	1/1	0.95	0.06	61,61,61,61	0
54	MG	1A	3436	1/1	0.95	0.09	54,54,54,54	0
54	MG	2a	3034	1/1	0.95	0.07	58,58,58,58	0
54	MG	2A	3441	1/1	0.95	0.15	57,57,57,57	0
54	MG	1A	3336	1/1	0.95	0.09	48,48,48,48	0
54	MG	1A	3860	1/1	0.95	0.11	37,37,37,37	0
54	MG	2A	3096	1/1	0.95	0.09	46,46,46,46	0
54	MG	1D	310	1/1	0.95	0.18	33,33,33,33	0
54	MG	1D	311	1/1	0.95	0.19	39,39,39,39	0
54	MG	2A	3448	1/1	0.95	0.07	49,49,49,49	0
54	MG	1A	3025	1/1	0.95	0.20	40,40,40,40	0
54	MG	2A	3450	1/1	0.95	0.13	57,57,57,57	0
54	MG	1D	313	1/1	0.95	0.09	57,57,57,57	0
54	MG	2a	3045	1/1	0.95	0.28	59,59,59,59	0
54	MG	1a	1755	1/1	0.95	0.12	61,61,61,61	0
54	MG	2A	3455	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3442	1/1	0.95	0.07	46,46,46,46	0
54	MG	2a	3049	1/1	0.95	0.23	59,59,59,59	0
54	MG	1A	3448	1/1	0.95	0.11	49,49,49,49	0
54	MG	1A	3339	1/1	0.95	0.11	61,61,61,61	0
54	MG	1A	3106	1/1	0.95	0.15	39,39,39,39	0
54	MG	2A	3460	1/1	0.95	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3055	1/1	0.95	0.09	65,65,65,65	0
54	MG	1E	310	1/1	0.95	0.08	58,58,58,58	0
54	MG	2A	3118	1/1	0.95	0.19	56,56,56,56	0
54	MG	1A	3133	1/1	0.95	0.21	37,37,37,37	0
54	MG	1A	3344	1/1	0.95	0.10	53,53,53,53	0
54	MG	1F	313	1/1	0.95	0.27	48,48,48,48	0
54	MG	2A	3127	1/1	0.95	0.14	47,47,47,47	0
54	MG	1a	1765	1/1	0.95	0.10	65,65,65,65	0
54	MG	1a	1768	1/1	0.95	0.14	60,60,60,60	0
54	MG	1a	1770	1/1	0.95	0.14	69,69,69,69	0
54	MG	1F	317	1/1	0.95	0.08	51,51,51,51	0
54	MG	1A	3874	1/1	0.95	0.10	39,39,39,39	0
54	MG	1A	3706	1/1	0.95	0.06	41,41,41,41	0
54	MG	1A	3249	1/1	0.95	0.46	43,43,43,43	0
54	MG	1A	3880	1/1	0.95	0.07	62,62,62,62	0
54	MG	2A	3480	1/1	0.95	0.09	45,45,45,45	0
54	MG	2a	3071	1/1	0.95	0.09	58,58,58,58	0
54	MG	2A	3481	1/1	0.95	0.11	59,59,59,59	0
54	MG	2a	3074	1/1	0.95	0.15	58,58,58,58	0
54	MG	1A	3708	1/1	0.95	0.06	52,52,52,52	0
54	MG	1A	3188	1/1	0.95	0.13	71,71,71,71	0
54	MG	1P	205	1/1	0.95	0.06	65,65,65,65	0
54	MG	2A	3149	1/1	0.95	0.09	60,60,60,60	0
54	MG	1R	204	1/1	0.95	0.10	44,44,44,44	0
54	MG	2A	3151	1/1	0.95	0.09	57,57,57,57	0
54	MG	2A	3496	1/1	0.95	0.11	56,56,56,56	0
54	MG	1A	3016	1/1	0.95	0.28	36,36,36,36	0
54	MG	2A	3499	1/1	0.95	0.08	46,46,46,46	0
54	MG	1T	201	1/1	0.95	0.08	64,64,64,64	0
54	MG	2A	3157	1/1	0.95	0.05	47,47,47,47	0
54	MG	2a	3092	1/1	0.95	0.16	67,67,67,67	0
54	MG	2A	3159	1/1	0.95	0.07	61,61,61,61	0
54	MG	1A	3194	1/1	0.95	0.14	43,43,43,43	0
54	MG	1A	3719	1/1	0.95	0.08	47,47,47,47	0
54	MG	2a	3098	1/1	0.95	0.20	60,60,60,60	0
54	MG	1a	1785	1/1	0.95	0.13	68,68,68,68	0
54	MG	2A	3509	1/1	0.95	0.12	63,63,63,63	0
54	MG	1U	201	1/1	0.95	0.22	36,36,36,36	0
54	MG	1A	3466	1/1	0.95	0.07	42,42,42,42	0
54	MG	1a	1788	1/1	0.95	0.07	75,75,75,75	0
54	MG	2a	3104	1/1	0.95	0.08	68,68,68,68	0
54	MG	1A	3887	1/1	0.95	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3889	1/1	0.95	0.08	40,40,40,40	0
54	MG	1A	3891	1/1	0.95	0.06	52,52,52,52	0
54	MG	1A	3725	1/1	0.95	0.10	49,49,49,49	0
54	MG	2a	3114	1/1	0.95	0.14	70,70,70,70	0
54	MG	1A	3467	1/1	0.95	0.12	56,56,56,56	0
54	MG	1A	3900	1/1	0.95	0.09	54,54,54,54	0
54	MG	2a	3117	1/1	0.95	0.08	66,66,66,66	0
54	MG	2A	3521	1/1	0.95	0.09	64,64,64,64	0
54	MG	2A	3181	1/1	0.95	0.10	55,55,55,55	0
54	MG	1A	3262	1/1	0.95	0.10	55,55,55,55	0
54	MG	2A	3184	1/1	0.95	0.14	60,60,60,60	0
54	MG	1A	3905	1/1	0.95	0.06	54,54,54,54	0
54	MG	2a	3124	1/1	0.95	0.07	56,56,56,56	0
54	MG	2a	3127	1/1	0.95	0.09	63,63,63,63	0
54	MG	2A	3527	1/1	0.95	0.12	45,45,45,45	0
54	MG	1A	3730	1/1	0.95	0.09	57,57,57,57	0
54	MG	1A	3138	1/1	0.95	0.06	45,45,45,45	0
54	MG	2A	3530	1/1	0.95	0.10	51,51,51,51	0
54	MG	2A	3188	1/1	0.95	0.12	54,54,54,54	0
54	MG	1A	3734	1/1	0.95	0.10	40,40,40,40	0
54	MG	1l	104	1/1	0.95	0.08	45,45,45,45	0
54	MG	2a	3137	1/1	0.95	0.11	59,59,59,59	0
54	MG	2A	3192	1/1	0.95	0.12	60,60,60,60	0
54	MG	2A	3543	1/1	0.95	0.08	69,69,69,69	0
54	MG	2A	3193	1/1	0.95	0.09	57,57,57,57	0
54	MG	1A	3911	1/1	0.95	0.11	49,49,49,49	0
54	MG	1A	3112	1/1	0.95	0.09	39,39,39,39	0
54	MG	2a	3147	1/1	0.95	0.09	62,62,62,62	0
54	MG	2A	3548	1/1	0.95	0.10	45,45,45,45	0
54	MG	2A	3549	1/1	0.95	0.06	59,59,59,59	0
54	MG	18	101	1/1	0.95	0.15	34,34,34,34	0
54	MG	2A	3552	1/1	0.95	0.06	39,39,39,39	0
54	MG	2A	3553	1/1	0.95	0.07	63,63,63,63	0
54	MG	2a	3154	1/1	0.95	0.12	57,57,57,57	0
54	MG	2a	3155	1/1	0.95	0.09	70,70,70,70	0
54	MG	2A	3555	1/1	0.95	0.14	48,48,48,48	0
54	MG	2a	3157	1/1	0.95	0.07	73,73,73,73	0
54	MG	1A	3269	1/1	0.95	0.27	35,35,35,35	0
54	MG	2A	3559	1/1	0.95	0.08	69,69,69,69	0
54	MG	19	101	1/1	0.95	0.09	69,69,69,69	0
54	MG	1A	3738	1/1	0.95	0.05	39,39,39,39	0
54	MG	1A	3740	1/1	0.95	0.16	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1603	1/1	0.95	0.14	75,75,75,75	0
54	MG	2A	3204	1/1	0.95	0.07	57,57,57,57	0
54	MG	1A	3741	1/1	0.95	0.17	44,44,44,44	0
54	MG	1A	3270	1/1	0.95	0.06	53,53,53,53	0
54	MG	1A	3610	1/1	0.95	0.09	49,49,49,49	0
54	MG	1A	3746	1/1	0.95	0.07	34,34,34,34	0
54	MG	2a	3175	1/1	0.95	0.10	71,71,71,71	0
54	MG	2a	3176	1/1	0.95	0.10	60,60,60,60	0
54	MG	1A	3933	1/1	0.95	0.12	55,55,55,55	0
54	MG	2A	3579	1/1	0.95	0.12	54,54,54,54	0
54	MG	2A	3580	1/1	0.95	0.12	60,60,60,60	0
54	MG	2A	3213	1/1	0.95	0.19	55,55,55,55	0
54	MG	2A	3215	1/1	0.95	0.09	56,56,56,56	0
54	MG	1A	3113	1/1	0.95	0.22	40,40,40,40	0
54	MG	2A	3586	1/1	0.95	0.08	53,53,53,53	0
54	MG	1a	1612	1/1	0.95	0.12	43,43,43,43	0
54	MG	2A	3221	1/1	0.95	0.13	52,52,52,52	0
54	MG	2A	3590	1/1	0.95	0.07	59,59,59,59	0
54	MG	1a	1613	1/1	0.95	0.10	74,74,74,74	0
54	MG	1A	3144	1/1	0.95	0.06	30,30,30,30	0
54	MG	2A	3224	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3369	1/1	0.95	0.09	70,70,70,70	0
54	MG	1A	3122	1/1	0.95	0.10	37,37,37,37	0
54	MG	2A	3228	1/1	0.95	0.13	47,47,47,47	0
54	MG	2A	3232	1/1	0.95	0.07	54,54,54,54	0
54	MG	2A	3608	1/1	0.95	0.08	45,45,45,45	0
54	MG	1a	1830	1/1	0.95	0.09	66,66,66,66	0
54	MG	2A	3234	1/1	0.95	0.17	39,39,39,39	0
54	MG	1a	1831	1/1	0.95	0.08	69,69,69,69	0
54	MG	1A	3283	1/1	0.95	0.15	58,58,58,58	0
54	MG	2A	3305	1/1	0.96	0.12	60,60,60,60	0
54	MG	1A	3875	1/1	0.96	0.10	39,39,39,39	0
54	MG	2A	3033	1/1	0.96	0.14	57,57,57,57	0
54	MG	1D	305	1/1	0.96	0.04	40,40,40,40	0
54	MG	1A	3489	1/1	0.96	0.07	46,46,46,46	0
54	MG	1a	1717	1/1	0.96	0.06	54,54,54,54	0
54	MG	1A	3878	1/1	0.96	0.12	49,49,49,49	0
54	MG	1A	3119	1/1	0.96	0.19	33,33,33,33	0
54	MG	1A	3724	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3305	1/1	0.96	0.10	48,48,48,48	0
54	MG	2A	3043	1/1	0.96	0.05	30,30,30,30	0
54	MG	2A	3664	1/1	0.96	0.05	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	3665	1/1	0.96	0.08	40,40,40,40	0
54	MG	1A	3091	1/1	0.96	0.10	28,28,28,28	0
54	MG	1D	316	1/1	0.96	0.20	32,32,32,32	0
54	MG	1E	301	1/1	0.96	0.18	40,40,40,40	0
54	MG	1A	3189	1/1	0.96	0.07	36,36,36,36	0
54	MG	2A	3049	1/1	0.96	0.07	64,64,64,64	0
54	MG	2A	3324	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3015	1/1	0.96	0.05	33,33,33,33	0
54	MG	1A	3612	1/1	0.96	0.20	39,39,39,39	0
54	MG	1A	3613	1/1	0.96	0.07	34,34,34,34	0
54	MG	2A	3678	1/1	0.96	0.08	39,39,39,39	0
54	MG	1A	3503	1/1	0.96	0.05	19,19,19,19	0
54	MG	2A	3333	1/1	0.96	0.06	51,51,51,51	0
54	MG	2A	3056	1/1	0.96	0.26	62,62,62,62	0
54	MG	1F	308	1/1	0.96	0.10	24,24,24,24	0
54	MG	1F	310	1/1	0.96	0.20	56,56,56,56	0
54	MG	1A	3242	1/1	0.96	0.22	55,55,55,55	0
54	MG	1A	3506	1/1	0.96	0.07	20,20,20,20	0
54	MG	1F	314	1/1	0.96	0.29	43,43,43,43	0
54	MG	1A	3892	1/1	0.96	0.10	42,42,42,42	0
54	MG	1F	318	1/1	0.96	0.07	60,60,60,60	0
54	MG	2A	3689	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3147	1/1	0.96	0.20	32,32,32,32	0
54	MG	1A	3896	1/1	0.96	0.07	46,46,46,46	0
54	MG	2A	3693	1/1	0.96	0.07	54,54,54,54	0
54	MG	1G	204	1/1	0.96	0.15	58,58,58,58	0
54	MG	2A	3696	1/1	0.96	0.07	55,55,55,55	0
54	MG	1a	1751	1/1	0.96	0.10	58,58,58,58	0
54	MG	1A	3508	1/1	0.96	0.05	50,50,50,50	0
54	MG	1H	202	1/1	0.96	0.05	46,46,46,46	0
54	MG	1N	202	1/1	0.96	0.15	41,41,41,41	0
54	MG	2A	3076	1/1	0.96	0.11	54,54,54,54	0
54	MG	2A	3077	1/1	0.96	0.11	44,44,44,44	0
54	MG	1A	3011	1/1	0.96	0.05	43,43,43,43	0
54	MG	2A	3362	1/1	0.96	0.08	53,53,53,53	0
54	MG	2A	3081	1/1	0.96	0.07	57,57,57,57	0
54	MG	2A	3712	1/1	0.96	0.10	57,57,57,57	0
54	MG	1A	3902	1/1	0.96	0.09	31,31,31,31	0
54	MG	1A	3513	1/1	0.96	0.06	21,21,21,21	0
54	MG	2A	3084	1/1	0.96	0.08	45,45,45,45	0
54	MG	2A	3086	1/1	0.96	0.07	48,48,48,48	0
54	MG	1A	3625	1/1	0.96	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	2A	3369	1/1	0.96	0.09	68,68,68,68	0
54	MG	1A	3626	1/1	0.96	0.07	34,34,34,34	0
54	MG	1A	3907	1/1	0.96	0.06	37,37,37,37	0
54	MG	1A	3908	1/1	0.96	0.06	21,21,21,21	0
54	MG	2A	3725	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3514	1/1	0.96	0.13	39,39,39,39	0
54	MG	1A	3629	1/1	0.96	0.06	39,39,39,39	0
54	MG	2A	3729	1/1	0.96	0.08	54,54,54,54	0
54	MG	2A	3730	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3751	1/1	0.96	0.10	51,51,51,51	0
54	MG	1A	3630	1/1	0.96	0.07	40,40,40,40	0
54	MG	2A	3733	1/1	0.96	0.05	52,52,52,52	0
54	MG	1A	3317	1/1	0.96	0.10	34,34,34,34	0
54	MG	1A	3516	1/1	0.96	0.06	22,22,22,22	0
54	MG	1V	207	1/1	0.96	0.09	67,67,67,67	0
54	MG	1A	3196	1/1	0.96	0.24	62,62,62,62	0
54	MG	2B	205	1/1	0.96	0.10	51,51,51,51	0
54	MG	1W	204	1/1	0.96	0.08	54,54,54,54	0
54	MG	2A	3106	1/1	0.96	0.12	56,56,56,56	0
54	MG	1A	3411	1/1	0.96	0.10	25,25,25,25	0
54	MG	2A	3394	1/1	0.96	0.14	59,59,59,59	0
54	MG	2B	210	1/1	0.96	0.05	64,64,64,64	0
54	MG	1A	3197	1/1	0.96	0.16	44,44,44,44	0
54	MG	1A	3048	1/1	0.96	0.15	47,47,47,47	0
54	MG	2A	3400	1/1	0.96	0.06	47,47,47,47	0
54	MG	1A	3250	1/1	0.96	0.19	34,34,34,34	0
54	MG	1A	3326	1/1	0.96	0.06	31,31,31,31	0
54	MG	2A	3405	1/1	0.96	0.06	41,41,41,41	0
54	MG	2D	303	1/1	0.96	0.13	51,51,51,51	0
54	MG	2A	3115	1/1	0.96	0.20	48,48,48,48	0
54	MG	2A	3407	1/1	0.96	0.09	61,61,61,61	0
54	MG	1a	1781	1/1	0.96	0.06	74,74,74,74	0
54	MG	2A	3409	1/1	0.96	0.11	47,47,47,47	0
54	MG	1A	3330	1/1	0.96	0.10	34,34,34,34	0
54	MG	2E	306	1/1	0.96	0.07	30,30,30,30	0
54	MG	1A	3641	1/1	0.96	0.14	41,41,41,41	0
54	MG	2F	301	1/1	0.96	0.18	47,47,47,47	0
54	MG	2A	3124	1/1	0.96	0.06	39,39,39,39	0
54	MG	2A	3413	1/1	0.96	0.11	62,62,62,62	0
54	MG	1A	3251	1/1	0.96	0.19	42,42,42,42	0
54	MG	2A	3415	1/1	0.96	0.09	50,50,50,50	0
54	MG	2A	3416	1/1	0.96	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3126	1/1	0.96	0.08	65,65,65,65	0
54	MG	1A	3937	1/1	0.96	0.07	69,69,69,69	0
54	MG	13	101	1/1	0.96	0.09	39,39,39,39	0
54	MG	13	102	1/1	0.96	0.09	41,41,41,41	0
54	MG	2A	3421	1/1	0.96	0.06	36,36,36,36	0
54	MG	2Q	201	1/1	0.96	0.14	63,63,63,63	0
54	MG	2A	3422	1/1	0.96	0.13	60,60,60,60	0
54	MG	2A	3131	1/1	0.96	0.16	51,51,51,51	0
54	MG	13	104	1/1	0.96	0.06	40,40,40,40	0
54	MG	1A	3772	1/1	0.96	0.05	34,34,34,34	0
54	MG	2A	3428	1/1	0.96	0.10	69,69,69,69	0
54	MG	1a	1791	1/1	0.96	0.08	68,68,68,68	0
54	MG	1a	1792	1/1	0.96	0.07	57,57,57,57	0
54	MG	2A	3434	1/1	0.96	0.08	60,60,60,60	0
54	MG	2X	101	1/1	0.96	0.08	57,57,57,57	0
54	MG	1A	3201	1/1	0.96	0.06	40,40,40,40	0
54	MG	1A	3941	1/1	0.96	0.12	55,55,55,55	0
54	MG	2A	3437	1/1	0.96	0.07	58,58,58,58	0
54	MG	25	101	1/1	0.96	0.26	44,44,44,44	0
54	MG	1A	3942	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3422	1/1	0.96	0.05	20,20,20,20	0
54	MG	2A	3144	1/1	0.96	0.13	41,41,41,41	0
54	MG	2a	3003	1/1	0.96	0.21	64,64,64,64	0
54	MG	1A	3070	1/1	0.96	0.17	27,27,27,27	0
54	MG	2A	3146	1/1	0.96	0.12	34,34,34,34	0
54	MG	2A	3147	1/1	0.96	0.25	60,60,60,60	0
54	MG	1A	3647	1/1	0.96	0.07	33,33,33,33	0
54	MG	1A	3648	1/1	0.96	0.07	49,49,49,49	0
54	MG	1A	3259	1/1	0.96	0.06	41,41,41,41	0
54	MG	1A	3539	1/1	0.96	0.08	41,41,41,41	0
54	MG	2A	3154	1/1	0.96	0.06	65,65,65,65	0
54	MG	1A	3129	1/1	0.96	0.04	34,34,34,34	0
54	MG	1A	3160	1/1	0.96	0.34	36,36,36,36	0
54	MG	1A	3787	1/1	0.96	0.08	43,43,43,43	0
54	MG	1A	3956	1/1	0.96	0.08	50,50,50,50	0
54	MG	1A	3163	1/1	0.96	0.12	52,52,52,52	0
54	MG	1A	3959	1/1	0.96	0.12	54,54,54,54	0
54	MG	1A	3049	1/1	0.96	0.12	39,39,39,39	0
54	MG	1a	1616	1/1	0.96	0.05	56,56,56,56	0
54	MG	1A	3213	1/1	0.96	0.09	43,43,43,43	0
54	MG	1a	1618	1/1	0.96	0.08	62,62,62,62	0
54	MG	1a	1815	1/1	0.96	0.06	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3075	1/1	0.96	0.06	44,44,44,44	0
54	MG	2A	3173	1/1	0.96	0.07	45,45,45,45	0
54	MG	2A	3466	1/1	0.96	0.07	48,48,48,48	0
54	MG	2A	3175	1/1	0.96	0.07	57,57,57,57	0
54	MG	2a	3031	1/1	0.96	0.21	59,59,59,59	0
54	MG	2A	3176	1/1	0.96	0.06	42,42,42,42	0
54	MG	2A	3470	1/1	0.96	0.11	67,67,67,67	0
54	MG	1A	3793	1/1	0.96	0.19	61,61,61,61	0
54	MG	1a	1622	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3548	1/1	0.96	0.11	43,43,43,43	0
54	MG	1A	3349	1/1	0.96	0.05	25,25,25,25	0
54	MG	1A	3970	1/1	0.96	0.06	34,34,34,34	0
54	MG	1A	3020	1/1	0.96	0.16	39,39,39,39	0
54	MG	1A	3799	1/1	0.96	0.05	40,40,40,40	0
54	MG	2A	3479	1/1	0.96	0.11	31,31,31,31	0
54	MG	1A	3801	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3802	1/1	0.96	0.10	56,56,56,56	0
54	MG	1a	1630	1/1	0.96	0.11	57,57,57,57	0
54	MG	2A	3485	1/1	0.96	0.05	37,37,37,37	0
54	MG	1A	3803	1/1	0.96	0.07	38,38,38,38	0
54	MG	2A	3190	1/1	0.96	0.11	47,47,47,47	0
54	MG	1A	3553	1/1	0.96	0.10	54,54,54,54	0
54	MG	2A	3493	1/1	0.96	0.06	47,47,47,47	0
54	MG	1A	3664	1/1	0.96	0.08	52,52,52,52	0
54	MG	1A	3443	1/1	0.96	0.12	48,48,48,48	0
54	MG	2a	3053	1/1	0.96	0.06	66,66,66,66	0
54	MG	2A	3194	1/1	0.96	0.06	62,62,62,62	0
54	MG	1A	3555	1/1	0.96	0.11	33,33,33,33	0
54	MG	1A	3217	1/1	0.96	0.05	38,38,38,38	0
54	MG	1a	1836	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3276	1/1	0.96	0.09	48,48,48,48	0
54	MG	2A	3502	1/1	0.96	0.07	49,49,49,49	0
54	MG	2A	3199	1/1	0.96	0.23	50,50,50,50	0
54	MG	1A	3987	1/1	0.96	0.07	55,55,55,55	0
54	MG	1A	3560	1/1	0.96	0.08	49,49,49,49	0
54	MG	2A	3506	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3277	1/1	0.96	0.07	41,41,41,41	0
54	MG	2A	3508	1/1	0.96	0.09	46,46,46,46	0
54	MG	1a	1643	1/1	0.96	0.07	63,63,63,63	0
54	MG	1A	3280	1/1	0.96	0.16	49,49,49,49	0
54	MG	2A	3205	1/1	0.96	0.05	43,43,43,43	0
54	MG	1a	1846	1/1	0.96	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	1A	3361	1/1	0.96	0.05	27,27,27,27	0
54	MG	1A	3570	1/1	0.96	0.05	49,49,49,49	0
54	MG	2A	3515	1/1	0.96	0.09	49,49,49,49	0
54	MG	1A	3823	1/1	0.96	0.09	34,34,34,34	0
54	MG	2a	3075	1/1	0.96	0.12	61,61,61,61	0
54	MG	2A	3211	1/1	0.96	0.16	48,48,48,48	0
54	MG	1a	1649	1/1	0.96	0.14	50,50,50,50	0
54	MG	1A	3996	1/1	0.96	0.08	36,36,36,36	0
54	MG	2A	3214	1/1	0.96	0.14	57,57,57,57	0
54	MG	2a	3080	1/1	0.96	0.08	57,57,57,57	0
54	MG	1A	3825	1/1	0.96	0.04	18,18,18,18	0
54	MG	2a	3082	1/1	0.96	0.21	61,61,61,61	0
54	MG	2A	3216	1/1	0.96	0.09	59,59,59,59	0
54	MG	2A	3217	1/1	0.96	0.09	54,54,54,54	0
54	MG	2A	3218	1/1	0.96	0.15	45,45,45,45	0
54	MG	2a	3086	1/1	0.96	0.09	60,60,60,60	0
54	MG	1A	3281	1/1	0.96	0.14	36,36,36,36	0
54	MG	1a	1654	1/1	0.96	0.06	50,50,50,50	0
54	MG	1a	1656	1/1	0.96	0.16	51,51,51,51	0
54	MG	2a	3091	1/1	0.96	0.06	71,71,71,71	0
54	MG	1A	3218	1/1	0.96	0.13	30,30,30,30	0
54	MG	2a	3093	1/1	0.96	0.11	49,49,49,49	0
54	MG	1a	1658	1/1	0.96	0.08	64,64,64,64	0
54	MG	2A	3534	1/1	0.96	0.06	43,43,43,43	0
54	MG	1A	4000	1/1	0.96	0.05	60,60,60,60	0
54	MG	2a	3097	1/1	0.96	0.25	61,61,61,61	0
54	MG	2A	3537	1/1	0.96	0.10	47,47,47,47	0
54	MG	2A	3538	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3170	1/1	0.96	0.07	48,48,48,48	0
54	MG	2A	3226	1/1	0.96	0.06	43,43,43,43	0
54	MG	1a	1868	1/1	0.96	0.15	63,63,63,63	0
54	MG	1a	1869	1/1	0.96	0.09	64,64,64,64	0
54	MG	2A	3230	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3682	1/1	0.96	0.09	49,49,49,49	0
54	MG	1A	3029	1/1	0.96	0.08	39,39,39,39	0
54	MG	1A	3465	1/1	0.96	0.07	47,47,47,47	0
54	MG	1A	3222	1/1	0.96	0.20	37,37,37,37	0
54	MG	2a	3109	1/1	0.96	0.10	81,81,81,81	0
54	MG	2a	3110	1/1	0.96	0.07	61,61,61,61	0
54	MG	2a	3112	1/1	0.96	0.08	64,64,64,64	0
54	MG	2A	3237	1/1	0.96	0.11	52,52,52,52	0
54	MG	1A	3081	1/1	0.96	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	4009	1/1	0.96	0.10	47,47,47,47	0
54	MG	1A	4010	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3838	1/1	0.96	0.06	44,44,44,44	0
54	MG	2A	3560	1/1	0.96	0.08	65,65,65,65	0
54	MG	2a	3120	1/1	0.96	0.17	68,68,68,68	0
54	MG	1A	3839	1/1	0.96	0.17	41,41,41,41	0
54	MG	1d	304	1/1	0.96	0.07	60,60,60,60	0
54	MG	2A	3564	1/1	0.96	0.08	58,58,58,58	0
54	MG	1A	3689	1/1	0.96	0.08	39,39,39,39	0
54	MG	2a	3126	1/1	0.96	0.13	66,66,66,66	0
54	MG	1A	3226	1/1	0.96	0.14	42,42,42,42	0
54	MG	1A	3291	1/1	0.96	0.18	44,44,44,44	0
54	MG	1A	3847	1/1	0.96	0.09	39,39,39,39	0
54	MG	1a	1676	1/1	0.96	0.10	68,68,68,68	0
54	MG	2A	3249	1/1	0.96	0.22	44,44,44,44	0
54	MG	1A	3848	1/1	0.96	0.09	45,45,45,45	0
54	MG	2A	3576	1/1	0.96	0.24	65,65,65,65	0
54	MG	1h	201	1/1	0.96	0.15	57,57,57,57	0
54	MG	2A	3578	1/1	0.96	0.07	54,54,54,54	0
54	MG	1A	3227	1/1	0.96	0.05	31,31,31,31	0
54	MG	1a	1680	1/1	0.96	0.08	52,52,52,52	0
54	MG	1A	3585	1/1	0.96	0.08	55,55,55,55	0
54	MG	1A	3295	1/1	0.96	0.08	45,45,45,45	0
54	MG	2a	3145	1/1	0.96	0.09	60,60,60,60	0
54	MG	2A	3584	1/1	0.96	0.06	46,46,46,46	0
54	MG	2A	3256	1/1	0.96	0.08	59,59,59,59	0
54	MG	1A	3182	1/1	0.96	0.27	42,42,42,42	0
54	MG	1a	1684	1/1	0.96	0.14	53,53,53,53	0
54	MG	1A	3588	1/1	0.96	0.14	50,50,50,50	0
54	MG	1A	3060	1/1	0.96	0.10	49,49,49,49	0
54	MG	2a	3152	1/1	0.96	0.09	71,71,71,71	0
54	MG	2A	3591	1/1	0.96	0.06	59,59,59,59	0
54	MG	1A	3380	1/1	0.96	0.05	19,19,19,19	0
54	MG	2A	3593	1/1	0.96	0.06	50,50,50,50	0
54	MG	2A	3596	1/1	0.96	0.06	34,34,34,34	0
54	MG	1A	3858	1/1	0.96	0.08	52,52,52,52	0
54	MG	2A	3264	1/1	0.96	0.08	55,55,55,55	0
54	MG	2A	3267	1/1	0.96	0.09	53,53,53,53	0
54	MG	2A	3270	1/1	0.96	0.27	51,51,51,51	0
54	MG	2a	3161	1/1	0.96	0.09	69,69,69,69	0
54	MG	1A	3859	1/1	0.96	0.09	48,48,48,48	0
54	MG	2a	3163	1/1	0.96	0.14	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	3605	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3592	1/1	0.96	0.09	51,51,51,51	0
54	MG	2A	3607	1/1	0.96	0.05	57,57,57,57	0
54	MG	1A	3477	1/1	0.96	0.12	33,33,33,33	0
54	MG	2a	3169	1/1	0.96	0.19	64,64,64,64	0
54	MG	1A	3230	1/1	0.96	0.07	36,36,36,36	0
54	MG	2A	3614	1/1	0.96	0.10	51,51,51,51	0
54	MG	2A	3616	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3595	1/1	0.96	0.07	44,44,44,44	0
54	MG	2A	3005	1/1	0.96	0.07	56,56,56,56	0
54	MG	2A	3006	1/1	0.96	0.12	54,54,54,54	0
54	MG	2A	3620	1/1	0.96	0.07	50,50,50,50	0
54	MG	2A	3621	1/1	0.96	0.09	52,52,52,52	0
54	MG	2a	3180	1/1	0.96	0.06	57,57,57,57	0
54	MG	1B	221	1/1	0.96	0.07	31,31,31,31	0
54	MG	2A	3279	1/1	0.96	0.11	53,53,53,53	0
54	MG	1A	3231	1/1	0.96	0.10	49,49,49,49	0
54	MG	2A	3284	1/1	0.96	0.07	41,41,41,41	0
54	MG	1a	1699	1/1	0.96	0.14	60,60,60,60	0
54	MG	2A	3014	1/1	0.96	0.08	55,55,55,55	0
54	MG	2A	3015	1/1	0.96	0.10	38,38,38,38	0
54	MG	1A	3867	1/1	0.96	0.05	37,37,37,37	0
54	MG	2A	3631	1/1	0.96	0.14	51,51,51,51	0
54	MG	1B	224	1/1	0.96	0.05	53,53,53,53	0
55	ERY	1A	4021	51/51	0.96	0.09	23,35,44,46	0
55	ERY	2A	3734	51/51	0.96	0.10	32,46,59,66	0
54	MG	1A	3598	1/1	0.96	0.09	41,41,41,41	0
54	MG	2A	3020	1/1	0.96	0.09	45,45,45,45	0
54	MG	2A	3022	1/1	0.96	0.23	54,54,54,54	0
54	MG	1a	1703	1/1	0.96	0.16	52,52,52,52	0
54	MG	1A	3033	1/1	0.96	0.12	37,37,37,37	0
54	MG	1A	3387	1/1	0.96	0.09	24,24,24,24	0
54	MG	2A	3027	1/1	0.96	0.08	59,59,59,59	0
54	MG	1A	3873	1/1	0.96	0.09	50,50,50,50	0
54	MG	1A	3717	1/1	0.96	0.09	34,34,34,34	0
58	ZN	2Y	501	1/1	0.96	0.06	84,84,84,84	0
54	MG	1A	3458	1/1	0.97	0.07	52,52,52,52	0
54	MG	1a	1632	1/1	0.97	0.07	55,55,55,55	0
54	MG	1A	3760	1/1	0.97	0.10	33,33,33,33	0
54	MG	2A	3642	1/1	0.97	0.06	48,48,48,48	0
54	MG	2A	3289	1/1	0.97	0.06	33,33,33,33	0
54	MG	2A	3645	1/1	0.97	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3012	1/1	0.97	0.17	39,39,39,39	0
54	MG	1m	201	1/1	0.97	0.05	68,68,68,68	0
54	MG	2A	3652	1/1	0.97	0.10	51,51,51,51	0
54	MG	1A	3599	1/1	0.97	0.06	55,55,55,55	0
54	MG	2A	3654	1/1	0.97	0.06	54,54,54,54	0
54	MG	1A	3343	1/1	0.97	0.06	29,29,29,29	0
54	MG	2A	3296	1/1	0.97	0.05	46,46,46,46	0
54	MG	1A	3462	1/1	0.97	0.12	47,47,47,47	0
54	MG	1o	101	1/1	0.97	0.06	53,53,53,53	0
54	MG	1A	3464	1/1	0.97	0.09	46,46,46,46	0
54	MG	1A	3603	1/1	0.97	0.06	51,51,51,51	0
54	MG	1A	3252	1/1	0.97	0.06	36,36,36,36	0
54	MG	2A	3302	1/1	0.97	0.12	57,57,57,57	0
54	MG	1A	3080	1/1	0.97	0.11	42,42,42,42	0
54	MG	1A	3606	1/1	0.97	0.22	35,35,35,35	0
54	MG	1A	3052	1/1	0.97	0.14	43,43,43,43	0
54	MG	1A	3775	1/1	0.97	0.11	34,34,34,34	0
54	MG	1A	3974	1/1	0.97	0.06	52,52,52,52	0
54	MG	1A	3975	1/1	0.97	0.08	52,52,52,52	0
54	MG	1A	3192	1/1	0.97	0.18	64,64,64,64	0
54	MG	1A	3777	1/1	0.97	0.09	44,44,44,44	0
54	MG	2A	3008	1/1	0.97	0.19	49,49,49,49	0
54	MG	2A	3010	1/1	0.97	0.05	60,60,60,60	0
54	MG	1A	3082	1/1	0.97	0.19	34,34,34,34	0
54	MG	2A	3316	1/1	0.97	0.05	39,39,39,39	0
54	MG	1A	3350	1/1	0.97	0.08	32,32,32,32	0
54	MG	1A	3351	1/1	0.97	0.04	22,22,22,22	0
54	MG	1A	3261	1/1	0.97	0.07	40,40,40,40	0
54	MG	1A	3128	1/1	0.97	0.04	62,62,62,62	0
54	MG	1A	3263	1/1	0.97	0.11	40,40,40,40	0
54	MG	2A	3018	1/1	0.97	0.12	41,41,41,41	0
54	MG	2A	3323	1/1	0.97	0.05	46,46,46,46	0
54	MG	1A	3617	1/1	0.97	0.07	23,23,23,23	0
54	MG	1A	3985	1/1	0.97	0.11	39,39,39,39	0
54	MG	2A	3327	1/1	0.97	0.09	42,42,42,42	0
54	MG	1A	3021	1/1	0.97	0.24	43,43,43,43	0
54	MG	1A	3621	1/1	0.97	0.11	54,54,54,54	0
54	MG	1A	3009	1/1	0.97	0.06	26,26,26,26	0
54	MG	2A	3332	1/1	0.97	0.05	33,33,33,33	0
54	MG	2A	3694	1/1	0.97	0.04	66,66,66,66	0
54	MG	1A	3267	1/1	0.97	0.13	33,33,33,33	0
54	MG	2A	3334	1/1	0.97	0.11	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3697	1/1	0.97	0.05	40,40,40,40	0
54	MG	1A	3268	1/1	0.97	0.29	34,34,34,34	0
54	MG	1A	3991	1/1	0.97	0.06	43,43,43,43	0
54	MG	1a	1667	1/1	0.97	0.09	63,63,63,63	0
54	MG	2A	3702	1/1	0.97	0.06	48,48,48,48	0
54	MG	2A	3340	1/1	0.97	0.07	44,44,44,44	0
54	MG	2A	3030	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3483	1/1	0.97	0.06	35,35,35,35	0
54	MG	2A	3706	1/1	0.97	0.06	52,52,52,52	0
54	MG	1A	3088	1/1	0.97	0.06	35,35,35,35	0
54	MG	1A	3367	1/1	0.97	0.08	26,26,26,26	0
54	MG	2A	3710	1/1	0.97	0.07	48,48,48,48	0
54	MG	1A	3797	1/1	0.97	0.11	41,41,41,41	0
54	MG	2A	3036	1/1	0.97	0.06	48,48,48,48	0
54	MG	2A	3347	1/1	0.97	0.08	35,35,35,35	0
54	MG	1A	3492	1/1	0.97	0.07	44,44,44,44	0
54	MG	1a	1673	1/1	0.97	0.27	66,66,66,66	0
54	MG	2A	3350	1/1	0.97	0.06	32,32,32,32	0
54	MG	2A	3717	1/1	0.97	0.07	64,64,64,64	0
54	MG	2A	3718	1/1	0.97	0.08	56,56,56,56	0
54	MG	1A	3494	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3090	1/1	0.97	0.08	37,37,37,37	0
54	MG	1A	3271	1/1	0.97	0.17	51,51,51,51	0
54	MG	1a	1677	1/1	0.97	0.22	58,58,58,58	0
54	MG	1A	3272	1/1	0.97	0.13	43,43,43,43	0
54	MG	1A	3371	1/1	0.97	0.04	31,31,31,31	0
54	MG	2A	3046	1/1	0.97	0.12	51,51,51,51	0
54	MG	1A	3017	1/1	0.97	0.18	36,36,36,36	0
54	MG	1A	4004	1/1	0.97	0.25	41,41,41,41	0
54	MG	1A	3806	1/1	0.97	0.10	30,30,30,30	0
54	MG	1A	3807	1/1	0.97	0.17	44,44,44,44	0
54	MG	2A	3052	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3501	1/1	0.97	0.10	53,53,53,53	0
54	MG	1A	3135	1/1	0.97	0.06	49,49,49,49	0
54	MG	1a	1686	1/1	0.97	0.18	59,59,59,59	0
54	MG	1A	3374	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	4011	1/1	0.97	0.08	58,58,58,58	0
54	MG	1A	4012	1/1	0.97	0.10	43,43,43,43	0
54	MG	2A	3376	1/1	0.97	0.04	53,53,53,53	0
54	MG	1A	3811	1/1	0.97	0.04	30,30,30,30	0
54	MG	1A	4014	1/1	0.97	0.07	39,39,39,39	0
54	MG	2A	3379	1/1	0.97	0.07	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	4015	1/1	0.97	0.13	40,40,40,40	0
54	MG	2B	211	1/1	0.97	0.11	59,59,59,59	0
54	MG	1A	3061	1/1	0.97	0.12	38,38,38,38	0
54	MG	1a	1694	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3814	1/1	0.97	0.04	43,43,43,43	0
54	MG	2A	3385	1/1	0.97	0.11	53,53,53,53	0
54	MG	1A	3205	1/1	0.97	0.08	49,49,49,49	0
54	MG	2B	218	1/1	0.97	0.12	68,68,68,68	0
54	MG	2A	3067	1/1	0.97	0.05	48,48,48,48	0
54	MG	1A	3093	1/1	0.97	0.09	41,41,41,41	0
54	MG	2D	304	1/1	0.97	0.23	44,44,44,44	0
54	MG	2D	305	1/1	0.97	0.15	38,38,38,38	0
54	MG	2D	306	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3509	1/1	0.97	0.12	23,23,23,23	0
54	MG	1A	3644	1/1	0.97	0.07	41,41,41,41	0
54	MG	2A	3072	1/1	0.97	0.06	30,30,30,30	0
54	MG	2A	3395	1/1	0.97	0.04	36,36,36,36	0
54	MG	1A	3820	1/1	0.97	0.22	27,27,27,27	0
54	MG	2E	305	1/1	0.97	0.05	50,50,50,50	0
54	MG	1A	3208	1/1	0.97	0.21	45,45,45,45	0
54	MG	1B	205	1/1	0.97	0.05	41,41,41,41	0
54	MG	2A	3401	1/1	0.97	0.14	59,59,59,59	0
54	MG	2F	302	1/1	0.97	0.05	39,39,39,39	0
54	MG	1a	1705	1/1	0.97	0.06	59,59,59,59	0
54	MG	2A	3403	1/1	0.97	0.10	69,69,69,69	0
54	MG	2A	3079	1/1	0.97	0.14	54,54,54,54	0
54	MG	1A	3822	1/1	0.97	0.06	19,19,19,19	0
54	MG	1A	3511	1/1	0.97	0.05	52,52,52,52	0
54	MG	1a	1708	1/1	0.97	0.06	47,47,47,47	0
54	MG	1a	1709	1/1	0.97	0.06	35,35,35,35	0
54	MG	1A	3512	1/1	0.97	0.06	46,46,46,46	0
54	MG	2A	3085	1/1	0.97	0.29	50,50,50,50	0
54	MG	1A	3095	1/1	0.97	0.06	18,18,18,18	0
54	MG	1a	1713	1/1	0.97	0.05	48,48,48,48	0
54	MG	2A	3088	1/1	0.97	0.16	39,39,39,39	0
54	MG	2R	201	1/1	0.97	0.08	46,46,46,46	0
54	MG	1B	210	1/1	0.97	0.05	46,46,46,46	0
54	MG	1A	3062	1/1	0.97	0.06	32,32,32,32	0
54	MG	2T	3302	1/1	0.97	0.06	53,53,53,53	0
54	MG	1A	3381	1/1	0.97	0.04	31,31,31,31	0
54	MG	2A	3092	1/1	0.97	0.06	46,46,46,46	0
54	MG	1B	213	1/1	0.97	0.03	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	2W	201	1/1	0.97	0.16	45,45,45,45	0
54	MG	1A	3212	1/1	0.97	0.12	39,39,39,39	0
54	MG	1A	3018	1/1	0.97	0.12	27,27,27,27	0
54	MG	1A	3064	1/1	0.97	0.07	31,31,31,31	0
54	MG	1A	3833	1/1	0.97	0.12	34,34,34,34	0
54	MG	2A	3098	1/1	0.97	0.04	57,57,57,57	0
54	MG	2A	3099	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3522	1/1	0.97	0.09	41,41,41,41	0
54	MG	1A	3028	1/1	0.97	0.20	25,25,25,25	0
54	MG	27	101	1/1	0.97	0.12	39,39,39,39	0
54	MG	28	101	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3837	1/1	0.97	0.07	35,35,35,35	0
54	MG	1A	3216	1/1	0.97	0.18	37,37,37,37	0
54	MG	1a	1729	1/1	0.97	0.04	62,62,62,62	0
54	MG	2A	3108	1/1	0.97	0.07	60,60,60,60	0
54	MG	1A	3039	1/1	0.97	0.05	41,41,41,41	0
54	MG	1a	1731	1/1	0.97	0.05	56,56,56,56	0
54	MG	2A	3111	1/1	0.97	0.05	51,51,51,51	0
54	MG	1A	3393	1/1	0.97	0.06	20,20,20,20	0
54	MG	1A	3293	1/1	0.97	0.11	48,48,48,48	0
54	MG	1a	1734	1/1	0.97	0.07	60,60,60,60	0
54	MG	1A	3844	1/1	0.97	0.05	35,35,35,35	0
54	MG	2A	3117	1/1	0.97	0.11	43,43,43,43	0
54	MG	1A	3845	1/1	0.97	0.06	52,52,52,52	0
54	MG	2A	3446	1/1	0.97	0.06	60,60,60,60	0
54	MG	2a	3016	1/1	0.97	0.04	52,52,52,52	0
54	MG	2A	3119	1/1	0.97	0.07	52,52,52,52	0
54	MG	1A	3019	1/1	0.97	0.21	28,28,28,28	0
54	MG	1a	1739	1/1	0.97	0.15	53,53,53,53	0
54	MG	2A	3123	1/1	0.97	0.08	44,44,44,44	0
54	MG	1A	3531	1/1	0.97	0.05	47,47,47,47	0
54	MG	1a	1741	1/1	0.97	0.07	52,52,52,52	0
54	MG	2A	3454	1/1	0.97	0.05	59,59,59,59	0
54	MG	1D	301	1/1	0.97	0.26	40,40,40,40	0
54	MG	1D	303	1/1	0.97	0.08	33,33,33,33	0
54	MG	2A	3128	1/1	0.97	0.19	43,43,43,43	0
54	MG	1A	3532	1/1	0.97	0.32	35,35,35,35	0
54	MG	2a	3029	1/1	0.97	0.15	59,59,59,59	0
54	MG	1A	3152	1/1	0.97	0.25	36,36,36,36	0
54	MG	1A	3400	1/1	0.97	0.06	32,32,32,32	0
54	MG	1A	3153	1/1	0.97	0.09	30,30,30,30	0
54	MG	1A	3300	1/1	0.97	0.19	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3854	1/1	0.97	0.06	39,39,39,39	0
54	MG	2A	3135	1/1	0.97	0.08	54,54,54,54	0
54	MG	1a	1752	1/1	0.97	0.07	61,61,61,61	0
54	MG	1A	3105	1/1	0.97	0.07	38,38,38,38	0
54	MG	1A	3407	1/1	0.97	0.06	35,35,35,35	0
54	MG	1A	3156	1/1	0.97	0.20	39,39,39,39	0
54	MG	1A	3675	1/1	0.97	0.17	57,57,57,57	0
54	MG	1A	3157	1/1	0.97	0.07	48,48,48,48	0
54	MG	1E	305	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	3677	1/1	0.97	0.08	55,55,55,55	0
54	MG	1E	307	1/1	0.97	0.06	23,23,23,23	0
54	MG	1E	308	1/1	0.97	0.04	25,25,25,25	0
54	MG	1E	309	1/1	0.97	0.05	52,52,52,52	0
54	MG	1A	3069	1/1	0.97	0.18	36,36,36,36	0
54	MG	1F	302	1/1	0.97	0.29	33,33,33,33	0
54	MG	1a	1767	1/1	0.97	0.08	66,66,66,66	0
54	MG	1A	3863	1/1	0.97	0.09	35,35,35,35	0
54	MG	1F	306	1/1	0.97	0.17	34,34,34,34	0
54	MG	2A	3158	1/1	0.97	0.15	59,59,59,59	0
54	MG	1F	307	1/1	0.97	0.08	39,39,39,39	0
54	MG	2A	3487	1/1	0.97	0.05	56,56,56,56	0
54	MG	2A	3488	1/1	0.97	0.06	54,54,54,54	0
54	MG	2A	3160	1/1	0.97	0.09	50,50,50,50	0
54	MG	1A	3544	1/1	0.97	0.20	45,45,45,45	0
54	MG	2A	3492	1/1	0.97	0.05	40,40,40,40	0
54	MG	2A	3162	1/1	0.97	0.07	56,56,56,56	0
54	MG	1F	309	1/1	0.97	0.12	34,34,34,34	0
54	MG	1A	3680	1/1	0.97	0.10	28,28,28,28	0
54	MG	1A	3545	1/1	0.97	0.14	32,32,32,32	0
54	MG	2A	3497	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3107	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	3043	1/1	0.97	0.06	28,28,28,28	0
54	MG	1F	316	1/1	0.97	0.06	42,42,42,42	0
54	MG	1A	3684	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3870	1/1	0.97	0.05	51,51,51,51	0
54	MG	1G	201	1/1	0.97	0.06	61,61,61,61	0
54	MG	2A	3174	1/1	0.97	0.21	45,45,45,45	0
54	MG	1A	3111	1/1	0.97	0.16	36,36,36,36	0
54	MG	2a	3073	1/1	0.97	0.20	55,55,55,55	0
54	MG	1A	3549	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	3045	1/1	0.97	0.08	14,14,14,14	0
54	MG	2A	3178	1/1	0.97	0.06	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	1A	3232	1/1	0.97	0.19	30,30,30,30	0
54	MG	1A	3876	1/1	0.97	0.06	30,30,30,30	0
54	MG	1A	3690	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3030	1/1	0.97	0.07	34,34,34,34	0
54	MG	1a	1789	1/1	0.97	0.05	56,56,56,56	0
54	MG	1N	204	1/1	0.97	0.05	65,65,65,65	0
54	MG	1A	3692	1/1	0.97	0.09	43,43,43,43	0
54	MG	1A	3115	1/1	0.97	0.20	36,36,36,36	0
54	MG	1A	3420	1/1	0.97	0.09	28,28,28,28	0
54	MG	1P	206	1/1	0.97	0.05	30,30,30,30	0
54	MG	1Q	203	1/1	0.97	0.09	41,41,41,41	0
54	MG	2a	3088	1/1	0.97	0.11	68,68,68,68	0
54	MG	1Q	204	1/1	0.97	0.06	47,47,47,47	0
54	MG	2A	3522	1/1	0.97	0.13	63,63,63,63	0
54	MG	1R	203	1/1	0.97	0.07	38,38,38,38	0
54	MG	1A	3421	1/1	0.97	0.08	30,30,30,30	0
54	MG	1A	3315	1/1	0.97	0.05	27,27,27,27	0
54	MG	1A	3558	1/1	0.97	0.06	56,56,56,56	0
54	MG	1A	3559	1/1	0.97	0.04	40,40,40,40	0
54	MG	1A	3423	1/1	0.97	0.07	41,41,41,41	0
54	MG	1a	1804	1/1	0.97	0.06	47,47,47,47	0
54	MG	1A	3700	1/1	0.97	0.16	35,35,35,35	0
54	MG	2A	3531	1/1	0.97	0.06	65,65,65,65	0
54	MG	1a	1806	1/1	0.97	0.05	69,69,69,69	0
54	MG	1U	204	1/1	0.97	0.24	33,33,33,33	0
54	MG	1U	205	1/1	0.97	0.12	36,36,36,36	0
54	MG	1A	3888	1/1	0.97	0.31	38,38,38,38	0
54	MG	1U	208	1/1	0.97	0.20	41,41,41,41	0
54	MG	2A	3539	1/1	0.97	0.06	76,76,76,76	0
54	MG	1V	203	1/1	0.97	0.08	45,45,45,45	0
54	MG	1A	3701	1/1	0.97	0.10	53,53,53,53	0
54	MG	2A	3542	1/1	0.97	0.05	56,56,56,56	0
54	MG	1A	3561	1/1	0.97	0.06	43,43,43,43	0
54	MG	2A	3208	1/1	0.97	0.09	59,59,59,59	0
54	MG	2a	3111	1/1	0.97	0.04	57,57,57,57	0
54	MG	1A	3562	1/1	0.97	0.15	43,43,43,43	0
54	MG	2a	3113	1/1	0.97	0.09	55,55,55,55	0
54	MG	2A	3546	1/1	0.97	0.16	44,44,44,44	0
54	MG	1A	3563	1/1	0.97	0.06	21,21,21,21	0
54	MG	1A	3564	1/1	0.97	0.10	39,39,39,39	0
54	MG	1Y	201	1/1	0.97	0.09	57,57,57,57	0
54	MG	1A	3424	1/1	0.97	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3899	1/1	0.97	0.06	42,42,42,42	0
54	MG	1a	1820	1/1	0.97	0.08	64,64,64,64	0
54	MG	10	101	1/1	0.97	0.06	42,42,42,42	0
54	MG	2A	3556	1/1	0.97	0.07	58,58,58,58	0
54	MG	2A	3557	1/1	0.97	0.05	69,69,69,69	0
54	MG	1A	3316	1/1	0.97	0.07	35,35,35,35	0
54	MG	1a	1823	1/1	0.97	0.07	52,52,52,52	0
54	MG	10	103	1/1	0.97	0.04	40,40,40,40	0
54	MG	1A	3567	1/1	0.97	0.06	45,45,45,45	0
54	MG	1A	3568	1/1	0.97	0.06	31,31,31,31	0
54	MG	2a	3130	1/1	0.97	0.04	64,64,64,64	0
54	MG	1A	3904	1/1	0.97	0.06	37,37,37,37	0
54	MG	1A	3172	1/1	0.97	0.04	30,30,30,30	0
54	MG	11	101	1/1	0.97	0.10	38,38,38,38	0
54	MG	2A	3567	1/1	0.97	0.09	53,53,53,53	0
54	MG	1A	3716	1/1	0.97	0.13	38,38,38,38	0
54	MG	1A	3173	1/1	0.97	0.06	49,49,49,49	0
54	MG	2a	3138	1/1	0.97	0.09	65,65,65,65	0
54	MG	1A	3430	1/1	0.97	0.06	51,51,51,51	0
54	MG	1A	3721	1/1	0.97	0.05	42,42,42,42	0
54	MG	1A	3320	1/1	0.97	0.08	29,29,29,29	0
54	MG	2A	3231	1/1	0.97	0.09	55,55,55,55	0
54	MG	1A	3239	1/1	0.97	0.22	32,32,32,32	0
54	MG	15	102	1/1	0.97	0.18	25,25,25,25	0
54	MG	15	103	1/1	0.97	0.24	36,36,36,36	0
54	MG	15	105	1/1	0.97	0.06	49,49,49,49	0
54	MG	1A	3915	1/1	0.97	0.07	50,50,50,50	0
54	MG	1a	1842	1/1	0.97	0.06	63,63,63,63	0
54	MG	17	101	1/1	0.97	0.10	28,28,28,28	0
54	MG	17	103	1/1	0.97	0.18	40,40,40,40	0
54	MG	1a	1845	1/1	0.97	0.16	64,64,64,64	0
54	MG	17	104	1/1	0.97	0.14	35,35,35,35	0
54	MG	17	105	1/1	0.97	0.06	42,42,42,42	0
54	MG	1A	3574	1/1	0.97	0.08	33,33,33,33	0
54	MG	1A	3434	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3919	1/1	0.97	0.12	62,62,62,62	0
54	MG	1a	1855	1/1	0.97	0.10	63,63,63,63	0
54	MG	2A	3594	1/1	0.97	0.17	54,54,54,54	0
54	MG	2A	3595	1/1	0.97	0.07	47,47,47,47	0
54	MG	1A	3920	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3116	1/1	0.97	0.08	41,41,41,41	0
54	MG	1A	3577	1/1	0.97	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3732	1/1	0.97	0.06	32,32,32,32	0
54	MG	2A	3602	1/1	0.97	0.04	70,70,70,70	0
54	MG	1A	3323	1/1	0.97	0.10	30,30,30,30	0
54	MG	2a	3168	1/1	0.97	0.08	50,50,50,50	0
54	MG	1a	1606	1/1	0.97	0.06	49,49,49,49	0
54	MG	1A	3579	1/1	0.97	0.06	36,36,36,36	0
54	MG	2a	3171	1/1	0.97	0.11	63,63,63,63	0
54	MG	1A	3931	1/1	0.97	0.09	56,56,56,56	0
54	MG	2a	3173	1/1	0.97	0.12	65,65,65,65	0
54	MG	1A	3437	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3438	1/1	0.97	0.07	44,44,44,44	0
54	MG	2A	3610	1/1	0.97	0.10	38,38,38,38	0
54	MG	2A	3612	1/1	0.97	0.05	62,62,62,62	0
54	MG	1A	3177	1/1	0.97	0.17	37,37,37,37	0
54	MG	1A	3739	1/1	0.97	0.11	42,42,42,42	0
54	MG	2A	3615	1/1	0.97	0.07	68,68,68,68	0
54	MG	1a	1614	1/1	0.97	0.17	38,38,38,38	0
54	MG	1A	3117	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3441	1/1	0.97	0.06	43,43,43,43	0
54	MG	1A	3743	1/1	0.97	0.10	53,53,53,53	0
54	MG	2A	3266	1/1	0.97	0.34	42,42,42,42	0
54	MG	1A	3179	1/1	0.97	0.18	35,35,35,35	0
54	MG	2A	3268	1/1	0.97	0.12	29,29,29,29	0
54	MG	2A	3269	1/1	0.97	0.16	48,48,48,48	0
54	MG	1A	3031	1/1	0.97	0.08	19,19,19,19	0
54	MG	1A	3333	1/1	0.97	0.07	48,48,48,48	0
54	MG	2t	201	1/1	0.97	0.09	42,42,42,42	0
54	MG	1A	3334	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3335	1/1	0.97	0.08	35,35,35,35	0
54	MG	1A	3077	1/1	0.97	0.17	30,30,30,30	0
54	MG	2A	3629	1/1	0.97	0.07	46,46,46,46	0
54	MG	1e	201	1/1	0.97	0.15	48,48,48,48	0
54	MG	1A	3248	1/1	0.97	0.08	39,39,39,39	0
54	MG	1A	3184	1/1	0.97	0.09	41,41,41,41	0
54	MG	1A	3950	1/1	0.97	0.07	48,48,48,48	0
54	MG	1A	3123	1/1	0.97	0.17	32,32,32,32	0
54	MG	1A	3596	1/1	0.97	0.05	53,53,53,53	0
54	MG	1g	203	1/1	0.97	0.13	51,51,51,51	0
54	MG	1A	3953	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3121	1/1	0.98	0.09	35,35,35,35	0
54	MG	2A	3719	1/1	0.98	0.08	48,48,48,48	0
54	MG	1A	4020	1/1	0.98	0.04	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1853	1/1	0.98	0.03	55,55,55,55	0
54	MG	2A	3182	1/1	0.98	0.09	43,43,43,43	0
54	MG	1a	1854	1/1	0.98	0.07	61,61,61,61	0
54	MG	1A	3456	1/1	0.98	0.07	45,45,45,45	0
54	MG	1A	3161	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3162	1/1	0.98	0.15	35,35,35,35	0
54	MG	1A	3006	1/1	0.98	0.05	25,25,25,25	0
54	MG	2A	3728	1/1	0.98	0.04	46,46,46,46	0
54	MG	1a	1648	1/1	0.98	0.23	61,61,61,61	0
54	MG	1A	3460	1/1	0.98	0.04	41,41,41,41	0
54	MG	1a	1861	1/1	0.98	0.10	54,54,54,54	0
54	MG	1a	1650	1/1	0.98	0.12	55,55,55,55	0
54	MG	1a	1864	1/1	0.98	0.08	47,47,47,47	0
54	MG	1A	3278	1/1	0.98	0.11	42,42,42,42	0
54	MG	2A	3453	1/1	0.98	0.04	36,36,36,36	0
54	MG	1A	3279	1/1	0.98	0.06	42,42,42,42	0
54	MG	1A	3362	1/1	0.98	0.07	27,27,27,27	0
54	MG	1A	3583	1/1	0.98	0.06	42,42,42,42	0
54	MG	1a	1655	1/1	0.98	0.13	58,58,58,58	0
54	MG	1A	3862	1/1	0.98	0.04	28,28,28,28	0
54	MG	1A	3053	1/1	0.98	0.18	37,37,37,37	0
54	MG	1A	3710	1/1	0.98	0.03	33,33,33,33	0
54	MG	1A	3365	1/1	0.98	0.09	44,44,44,44	0
54	MG	1B	214	1/1	0.98	0.06	45,45,45,45	0
54	MG	1A	3165	1/1	0.98	0.11	35,35,35,35	0
54	MG	2B	213	1/1	0.98	0.08	60,60,60,60	0
54	MG	1A	3219	1/1	0.98	0.05	27,27,27,27	0
54	MG	1A	3055	1/1	0.98	0.12	41,41,41,41	0
54	MG	1A	3284	1/1	0.98	0.11	49,49,49,49	0
54	MG	2A	3467	1/1	0.98	0.06	60,60,60,60	0
54	MG	1A	3167	1/1	0.98	0.03	27,27,27,27	0
54	MG	1A	3720	1/1	0.98	0.07	32,32,32,32	0
54	MG	1A	3872	1/1	0.98	0.06	35,35,35,35	0
54	MG	1e	202	1/1	0.98	0.06	55,55,55,55	0
54	MG	1A	3094	1/1	0.98	0.12	31,31,31,31	0
54	MG	1A	3223	1/1	0.98	0.08	41,41,41,41	0
54	MG	1B	225	1/1	0.98	0.04	49,49,49,49	0
54	MG	1A	3169	1/1	0.98	0.35	38,38,38,38	0
54	MG	1A	3290	1/1	0.98	0.04	21,21,21,21	0
54	MG	1A	3727	1/1	0.98	0.09	54,54,54,54	0
54	MG	2E	301	1/1	0.98	0.09	43,43,43,43	0
54	MG	2E	303	1/1	0.98	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1B	229	1/1	0.98	0.09	45,45,45,45	0
54	MG	1A	3071	1/1	0.98	0.16	30,30,30,30	0
54	MG	1A	3480	1/1	0.98	0.04	51,51,51,51	0
54	MG	2A	3483	1/1	0.98	0.08	43,43,43,43	0
54	MG	1A	3171	1/1	0.98	0.05	49,49,49,49	0
54	MG	1A	3731	1/1	0.98	0.07	49,49,49,49	0
54	MG	1D	302	1/1	0.98	0.09	50,50,50,50	0
54	MG	2F	304	1/1	0.98	0.13	42,42,42,42	0
54	MG	1A	3056	1/1	0.98	0.04	41,41,41,41	0
54	MG	1A	3294	1/1	0.98	0.07	29,29,29,29	0
54	MG	1D	307	1/1	0.98	0.06	49,49,49,49	0
54	MG	1D	308	1/1	0.98	0.15	33,33,33,33	0
54	MG	1A	3485	1/1	0.98	0.04	36,36,36,36	0
54	MG	1A	3486	1/1	0.98	0.05	30,30,30,30	0
54	MG	2A	3229	1/1	0.98	0.06	56,56,56,56	0
54	MG	1A	3074	1/1	0.98	0.08	42,42,42,42	0
54	MG	1A	3174	1/1	0.98	0.18	31,31,31,31	0
54	MG	1A	3490	1/1	0.98	0.09	30,30,30,30	0
54	MG	1A	3491	1/1	0.98	0.04	56,56,56,56	0
54	MG	1D	315	1/1	0.98	0.09	49,49,49,49	0
54	MG	1A	3607	1/1	0.98	0.12	28,28,28,28	0
54	MG	2A	3236	1/1	0.98	0.10	45,45,45,45	0
54	MG	1A	3742	1/1	0.98	0.06	58,58,58,58	0
54	MG	1A	3608	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3894	1/1	0.98	0.05	39,39,39,39	0
54	MG	1A	3895	1/1	0.98	0.04	27,27,27,27	0
54	MG	2V	203	1/1	0.98	0.06	47,47,47,47	0
54	MG	2A	3009	1/1	0.98	0.05	43,43,43,43	0
54	MG	1A	3098	1/1	0.98	0.07	31,31,31,31	0
54	MG	1A	3493	1/1	0.98	0.10	36,36,36,36	0
54	MG	1A	3382	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3747	1/1	0.98	0.12	34,34,34,34	0
54	MG	1A	3901	1/1	0.98	0.10	32,32,32,32	0
54	MG	1F	301	1/1	0.98	0.04	29,29,29,29	0
54	MG	23	101	1/1	0.98	0.18	54,54,54,54	0
54	MG	1A	3383	1/1	0.98	0.07	50,50,50,50	0
54	MG	1A	3298	1/1	0.98	0.12	49,49,49,49	0
54	MG	1F	305	1/1	0.98	0.08	35,35,35,35	0
54	MG	1A	3299	1/1	0.98	0.11	38,38,38,38	0
54	MG	2A	3517	1/1	0.98	0.13	63,63,63,63	0
54	MG	2A	3021	1/1	0.98	0.04	50,50,50,50	0
54	MG	1A	3013	1/1	0.98	0.04	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3233	1/1	0.98	0.26	34,34,34,34	0
54	MG	1A	3753	1/1	0.98	0.04	51,51,51,51	0
54	MG	1A	3754	1/1	0.98	0.05	37,37,37,37	0
54	MG	2A	3026	1/1	0.98	0.05	42,42,42,42	0
54	MG	1a	1712	1/1	0.98	0.04	44,44,44,44	0
54	MG	1F	311	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3058	1/1	0.98	0.08	24,24,24,24	0
54	MG	2a	3011	1/1	0.98	0.07	59,59,59,59	0
54	MG	1A	3756	1/1	0.98	0.08	32,32,32,32	0
54	MG	2A	3031	1/1	0.98	0.07	37,37,37,37	0
54	MG	1A	3757	1/1	0.98	0.08	37,37,37,37	0
54	MG	2A	3265	1/1	0.98	0.09	32,32,32,32	0
54	MG	1F	315	1/1	0.98	0.05	41,41,41,41	0
54	MG	2A	3532	1/1	0.98	0.11	50,50,50,50	0
54	MG	1A	3914	1/1	0.98	0.19	33,33,33,33	0
54	MG	1A	3618	1/1	0.98	0.12	32,32,32,32	0
54	MG	2A	3535	1/1	0.98	0.10	34,34,34,34	0
54	MG	2a	3021	1/1	0.98	0.04	41,41,41,41	0
54	MG	1A	3916	1/1	0.98	0.03	41,41,41,41	0
54	MG	1A	3502	1/1	0.98	0.04	50,50,50,50	0
54	MG	1A	3620	1/1	0.98	0.09	52,52,52,52	0
54	MG	2A	3039	1/1	0.98	0.10	51,51,51,51	0
54	MG	1A	3044	1/1	0.98	0.09	32,32,32,32	0
54	MG	1A	3390	1/1	0.98	0.04	30,30,30,30	0
54	MG	1A	3392	1/1	0.98	0.05	24,24,24,24	0
54	MG	1A	3181	1/1	0.98	0.17	35,35,35,35	0
54	MG	1N	201	1/1	0.98	0.05	36,36,36,36	0
54	MG	1A	3103	1/1	0.98	0.08	31,31,31,31	0
54	MG	2a	3032	1/1	0.98	0.04	49,49,49,49	0
54	MG	1A	3924	1/1	0.98	0.05	51,51,51,51	0
54	MG	2A	3280	1/1	0.98	0.07	32,32,32,32	0
54	MG	1A	3395	1/1	0.98	0.05	24,24,24,24	0
54	MG	2A	3283	1/1	0.98	0.05	66,66,66,66	0
54	MG	1A	3926	1/1	0.98	0.06	32,32,32,32	0
54	MG	2A	3551	1/1	0.98	0.05	44,44,44,44	0
54	MG	1a	1735	1/1	0.98	0.04	54,54,54,54	0
54	MG	1P	202	1/1	0.98	0.10	29,29,29,29	0
54	MG	2A	3554	1/1	0.98	0.05	28,28,28,28	0
54	MG	1P	203	1/1	0.98	0.19	36,36,36,36	0
54	MG	1A	3627	1/1	0.98	0.10	23,23,23,23	0
54	MG	1A	3928	1/1	0.98	0.09	54,54,54,54	0
54	MG	2A	3290	1/1	0.98	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3929	1/1	0.98	0.11	38,38,38,38	0
54	MG	1Q	201	1/1	0.98	0.04	40,40,40,40	0
54	MG	2A	3561	1/1	0.98	0.05	54,54,54,54	0
54	MG	1Q	202	1/1	0.98	0.04	29,29,29,29	0
54	MG	2A	3294	1/1	0.98	0.03	33,33,33,33	0
54	MG	1A	3768	1/1	0.98	0.05	46,46,46,46	0
54	MG	1A	3769	1/1	0.98	0.04	40,40,40,40	0
54	MG	1R	201	1/1	0.98	0.07	29,29,29,29	0
54	MG	2A	3061	1/1	0.98	0.06	48,48,48,48	0
54	MG	2A	3568	1/1	0.98	0.04	33,33,33,33	0
54	MG	1a	1747	1/1	0.98	0.16	50,50,50,50	0
54	MG	1R	202	1/1	0.98	0.08	41,41,41,41	0
54	MG	1A	3306	1/1	0.98	0.07	28,28,28,28	0
54	MG	1A	3397	1/1	0.98	0.07	22,22,22,22	0
54	MG	2A	3573	1/1	0.98	0.07	67,67,67,67	0
54	MG	2A	3574	1/1	0.98	0.14	53,53,53,53	0
54	MG	1A	3398	1/1	0.98	0.11	48,48,48,48	0
54	MG	2A	3304	1/1	0.98	0.04	32,32,32,32	0
54	MG	1A	3774	1/1	0.98	0.06	38,38,38,38	0
54	MG	1A	3134	1/1	0.98	0.14	36,36,36,36	0
54	MG	1A	3308	1/1	0.98	0.03	23,23,23,23	0
54	MG	2A	3070	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3309	1/1	0.98	0.21	35,35,35,35	0
54	MG	1U	202	1/1	0.98	0.15	32,32,32,32	0
54	MG	1A	3940	1/1	0.98	0.04	36,36,36,36	0
54	MG	1A	3402	1/1	0.98	0.06	17,17,17,17	0
54	MG	2A	3075	1/1	0.98	0.07	37,37,37,37	0
54	MG	1U	206	1/1	0.98	0.21	33,33,33,33	0
54	MG	1A	3403	1/1	0.98	0.05	33,33,33,33	0
54	MG	2A	3589	1/1	0.98	0.07	42,42,42,42	0
54	MG	2A	3078	1/1	0.98	0.04	42,42,42,42	0
54	MG	1A	3943	1/1	0.98	0.07	41,41,41,41	0
54	MG	1V	201	1/1	0.98	0.20	29,29,29,29	0
54	MG	1V	202	1/1	0.98	0.15	32,32,32,32	0
54	MG	1a	1764	1/1	0.98	0.09	39,39,39,39	0
54	MG	1A	3518	1/1	0.98	0.04	44,44,44,44	0
54	MG	1a	1766	1/1	0.98	0.04	69,69,69,69	0
54	MG	2A	3597	1/1	0.98	0.07	50,50,50,50	0
54	MG	1V	204	1/1	0.98	0.06	52,52,52,52	0
54	MG	1A	3781	1/1	0.98	0.05	33,33,33,33	0
54	MG	2A	3600	1/1	0.98	0.04	40,40,40,40	0
54	MG	2A	3326	1/1	0.98	0.10	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	1769	1/1	0.98	0.06	63,63,63,63	0
54	MG	1A	3637	1/1	0.98	0.15	27,27,27,27	0
54	MG	2A	3329	1/1	0.98	0.09	36,36,36,36	0
54	MG	1A	3520	1/1	0.98	0.23	32,32,32,32	0
54	MG	1A	3948	1/1	0.98	0.13	27,27,27,27	0
54	MG	1A	3240	1/1	0.98	0.09	25,25,25,25	0
54	MG	1A	3405	1/1	0.98	0.03	29,29,29,29	0
54	MG	2A	3609	1/1	0.98	0.05	39,39,39,39	0
54	MG	1A	3523	1/1	0.98	0.04	25,25,25,25	0
54	MG	2A	3611	1/1	0.98	0.05	33,33,33,33	0
54	MG	1A	3023	1/1	0.98	0.07	26,26,26,26	0
54	MG	1A	3024	1/1	0.98	0.03	19,19,19,19	0
54	MG	1A	3526	1/1	0.98	0.07	31,31,31,31	0
54	MG	1A	3186	1/1	0.98	0.07	46,46,46,46	0
54	MG	1A	3409	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3957	1/1	0.98	0.04	59,59,59,59	0
54	MG	2A	3101	1/1	0.98	0.09	61,61,61,61	0
54	MG	1A	3047	1/1	0.98	0.07	29,29,29,29	0
54	MG	1A	3007	1/1	0.98	0.05	38,38,38,38	0
54	MG	1A	3649	1/1	0.98	0.15	40,40,40,40	0
54	MG	1A	3961	1/1	0.98	0.06	57,57,57,57	0
54	MG	1A	3108	1/1	0.98	0.07	34,34,34,34	0
54	MG	2A	3107	1/1	0.98	0.06	38,38,38,38	0
54	MG	1A	3963	1/1	0.98	0.11	51,51,51,51	0
54	MG	1A	3190	1/1	0.98	0.14	39,39,39,39	0
54	MG	13	103	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3318	1/1	0.98	0.05	40,40,40,40	0
54	MG	1A	3967	1/1	0.98	0.04	27,27,27,27	0
54	MG	1A	3653	1/1	0.98	0.07	31,31,31,31	0
54	MG	1A	3191	1/1	0.98	0.11	40,40,40,40	0
54	MG	2A	3360	1/1	0.98	0.05	44,44,44,44	0
54	MG	15	104	1/1	0.98	0.15	25,25,25,25	0
54	MG	2A	3116	1/1	0.98	0.05	50,50,50,50	0
54	MG	1A	3416	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3536	1/1	0.98	0.05	28,28,28,28	0
54	MG	1A	3142	1/1	0.98	0.08	37,37,37,37	0
54	MG	17	102	1/1	0.98	0.10	33,33,33,33	0
54	MG	2a	3125	1/1	0.98	0.09	64,64,64,64	0
54	MG	1A	3143	1/1	0.98	0.05	36,36,36,36	0
54	MG	2A	3640	1/1	0.98	0.06	47,47,47,47	0
54	MG	2A	3122	1/1	0.98	0.11	43,43,43,43	0
54	MG	1A	3026	1/1	0.98	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3253	1/1	0.98	0.07	37,37,37,37	0
54	MG	2A	3644	1/1	0.98	0.10	38,38,38,38	0
54	MG	2A	3371	1/1	0.98	0.06	53,53,53,53	0
54	MG	2A	3646	1/1	0.98	0.04	69,69,69,69	0
54	MG	1A	3254	1/1	0.98	0.07	53,53,53,53	0
54	MG	1A	3110	1/1	0.98	0.19	31,31,31,31	0
54	MG	2A	3374	1/1	0.98	0.10	56,56,56,56	0
54	MG	1A	3327	1/1	0.98	0.05	39,39,39,39	0
54	MG	1A	3328	1/1	0.98	0.09	15,15,15,15	0
54	MG	1A	3666	1/1	0.98	0.05	47,47,47,47	0
54	MG	1A	3667	1/1	0.98	0.14	37,37,37,37	0
54	MG	2a	3142	1/1	0.98	0.07	57,57,57,57	0
54	MG	2A	3657	1/1	0.98	0.04	44,44,44,44	0
54	MG	1A	3084	1/1	0.98	0.09	43,43,43,43	0
54	MG	1A	3818	1/1	0.98	0.09	39,39,39,39	0
54	MG	1A	3257	1/1	0.98	0.09	46,46,46,46	0
54	MG	1A	3428	1/1	0.98	0.05	50,50,50,50	0
54	MG	2A	3384	1/1	0.98	0.10	47,47,47,47	0
54	MG	1A	3258	1/1	0.98	0.18	32,32,32,32	0
54	MG	1A	3550	1/1	0.98	0.07	43,43,43,43	0
54	MG	2A	3139	1/1	0.98	0.09	46,46,46,46	0
54	MG	2A	3666	1/1	0.98	0.07	33,33,33,33	0
54	MG	2A	3388	1/1	0.98	0.11	46,46,46,46	0
54	MG	2A	3668	1/1	0.98	0.10	44,44,44,44	0
54	MG	1A	3148	1/1	0.98	0.05	51,51,51,51	0
54	MG	1a	1611	1/1	0.98	0.20	48,48,48,48	0
54	MG	2A	3391	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3085	1/1	0.98	0.25	41,41,41,41	0
54	MG	1A	3432	1/1	0.98	0.04	18,18,18,18	0
54	MG	1A	3200	1/1	0.98	0.07	53,53,53,53	0
54	MG	2A	3396	1/1	0.98	0.11	47,47,47,47	0
54	MG	2A	3397	1/1	0.98	0.04	55,55,55,55	0
54	MG	1A	3065	1/1	0.98	0.08	55,55,55,55	0
54	MG	1A	3995	1/1	0.98	0.06	52,52,52,52	0
54	MG	1A	3829	1/1	0.98	0.05	45,45,45,45	0
54	MG	2A	3148	1/1	0.98	0.09	64,64,64,64	0
54	MG	1A	3151	1/1	0.98	0.08	46,46,46,46	0
54	MG	1A	3340	1/1	0.98	0.06	28,28,28,28	0
54	MG	1a	1620	1/1	0.98	0.05	48,48,48,48	0
54	MG	1A	3264	1/1	0.98	0.21	27,27,27,27	0
54	MG	2A	3153	1/1	0.98	0.06	45,45,45,45	0
54	MG	1a	1827	1/1	0.98	0.04	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3155	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3087	1/1	0.98	0.11	32,32,32,32	0
54	MG	2A	3690	1/1	0.98	0.04	38,38,38,38	0
54	MG	1A	3050	1/1	0.98	0.25	46,46,46,46	0
54	MG	1A	3089	1/1	0.98	0.13	38,38,38,38	0
54	MG	1A	3207	1/1	0.98	0.21	41,41,41,41	0
54	MG	1A	3155	1/1	0.98	0.15	43,43,43,43	0
54	MG	1A	3347	1/1	0.98	0.07	31,31,31,31	0
54	MG	1A	3445	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3841	1/1	0.98	0.03	23,23,23,23	0
54	MG	2A	3164	1/1	0.98	0.17	48,48,48,48	0
54	MG	1A	4008	1/1	0.98	0.06	38,38,38,38	0
54	MG	2A	3166	1/1	0.98	0.14	38,38,38,38	0
54	MG	2A	3701	1/1	0.98	0.06	50,50,50,50	0
54	MG	1A	3842	1/1	0.98	0.09	44,44,44,44	0
54	MG	1A	3446	1/1	0.98	0.08	57,57,57,57	0
54	MG	1A	3447	1/1	0.98	0.06	55,55,55,55	0
54	MG	1a	1840	1/1	0.98	0.10	42,42,42,42	0
54	MG	1A	3118	1/1	0.98	0.13	35,35,35,35	0
54	MG	1A	3051	1/1	0.98	0.20	42,42,42,42	0
54	MG	2A	3426	1/1	0.98	0.10	49,49,49,49	0
54	MG	2A	3709	1/1	0.98	0.04	57,57,57,57	0
54	MG	2A	3427	1/1	0.98	0.04	38,38,38,38	0
54	MG	1A	3450	1/1	0.98	0.09	45,45,45,45	0
54	MG	1A	3120	1/1	0.98	0.10	26,26,26,26	0
54	MG	1a	1638	1/1	0.98	0.07	49,49,49,49	0
54	MG	2A	3432	1/1	0.98	0.05	48,48,48,48	0
54	MG	1A	3273	1/1	0.98	0.08	26,26,26,26	0
54	MG	1A	3352	1/1	0.98	0.05	46,46,46,46	0
58	ZN	14	501	1/1	0.98	0.08	110,110,110,110	0
54	MG	1A	3851	1/1	0.98	0.07	46,46,46,46	0
58	ZN	24	501	1/1	0.98	0.12	122,122,122,122	0
54	MG	1a	1851	1/1	0.99	0.03	53,53,53,53	0
54	MG	1a	1852	1/1	0.99	0.04	57,57,57,57	0
54	MG	2A	3433	1/1	0.99	0.04	47,47,47,47	0
54	MG	1A	3472	1/1	0.99	0.02	25,25,25,25	0
54	MG	1A	3338	1/1	0.99	0.05	49,49,49,49	0
54	MG	2A	3136	1/1	0.99	0.03	42,42,42,42	0
54	MG	2A	3137	1/1	0.99	0.10	60,60,60,60	0
54	MG	2A	3438	1/1	0.99	0.02	54,54,54,54	0
54	MG	1A	3041	1/1	0.99	0.08	30,30,30,30	0
54	MG	1A	3136	1/1	0.99	0.17	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3519	1/1	0.99	0.03	26,26,26,26	0
54	MG	1A	3289	1/1	0.99	0.11	25,25,25,25	0
54	MG	1A	3114	1/1	0.99	0.11	28,28,28,28	0
54	MG	1A	3824	1/1	0.99	0.07	33,33,33,33	0
54	MG	2A	3337	1/1	0.99	0.03	36,36,36,36	0
54	MG	2A	3338	1/1	0.99	0.03	37,37,37,37	0
54	MG	1A	3478	1/1	0.99	0.07	28,28,28,28	0
54	MG	1a	1862	1/1	0.99	0.03	35,35,35,35	0
54	MG	2A	3051	1/1	0.99	0.08	56,56,56,56	0
54	MG	1A	3709	1/1	0.99	0.04	37,37,37,37	0
54	MG	1A	3890	1/1	0.99	0.02	32,32,32,32	0
54	MG	1A	3660	1/1	0.99	0.04	54,54,54,54	0
54	MG	1A	3711	1/1	0.99	0.06	20,20,20,20	0
54	MG	1P	201	1/1	0.99	0.31	36,36,36,36	0
54	MG	1A	3054	1/1	0.99	0.15	24,24,24,24	0
54	MG	1A	3713	1/1	0.99	0.05	32,32,32,32	0
54	MG	1A	3245	1/1	0.99	0.25	36,36,36,36	0
54	MG	1A	3964	1/1	0.99	0.08	51,51,51,51	0
54	MG	1A	3042	1/1	0.99	0.07	24,24,24,24	0
54	MG	1a	1698	1/1	0.99	0.04	54,54,54,54	0
54	MG	1A	3897	1/1	0.99	0.03	47,47,47,47	0
54	MG	1A	3771	1/1	0.99	0.04	44,44,44,44	0
54	MG	2a	3002	1/1	0.99	0.04	56,56,56,56	0
54	MG	2A	3355	1/1	0.99	0.06	47,47,47,47	0
54	MG	1A	3204	1/1	0.99	0.05	38,38,38,38	0
54	MG	2A	3357	1/1	0.99	0.05	47,47,47,47	0
54	MG	1A	3444	1/1	0.99	0.05	29,29,29,29	0
54	MG	2A	3359	1/1	0.99	0.06	38,38,38,38	0
54	MG	1A	3836	1/1	0.99	0.05	30,30,30,30	0
54	MG	1a	1704	1/1	0.99	0.06	42,42,42,42	0
54	MG	1A	3718	1/1	0.99	0.03	30,30,30,30	0
54	MG	1A	3972	1/1	0.99	0.05	19,19,19,19	0
54	MG	2A	3583	1/1	0.99	0.04	55,55,55,55	0
54	MG	1A	3973	1/1	0.99	0.03	26,26,26,26	0
54	MG	2A	3262	1/1	0.99	0.20	41,41,41,41	0
54	MG	1A	3484	1/1	0.99	0.04	56,56,56,56	0
54	MG	1A	3225	1/1	0.99	0.04	36,36,36,36	0
54	MG	2A	3476	1/1	0.99	0.03	42,42,42,42	0
54	MG	1A	3078	1/1	0.99	0.05	34,34,34,34	0
54	MG	1A	3722	1/1	0.99	0.03	65,65,65,65	0
54	MG	1A	3141	1/1	0.99	0.11	31,31,31,31	0
54	MG	1A	3488	1/1	0.99	0.04	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	1U	203	1/1	0.99	0.09	34,34,34,34	0
54	MG	2A	3482	1/1	0.99	0.03	48,48,48,48	0
54	MG	1a	1801	1/1	0.99	0.04	65,65,65,65	0
54	MG	2a	3143	1/1	0.99	0.07	64,64,64,64	0
54	MG	1A	3005	1/1	0.99	0.11	22,22,22,22	0
54	MG	2A	3375	1/1	0.99	0.05	57,57,57,57	0
54	MG	1A	3726	1/1	0.99	0.05	24,24,24,24	0
54	MG	1A	3003	1/1	0.99	0.07	36,36,36,36	0
54	MG	1A	3912	1/1	0.99	0.04	20,20,20,20	0
54	MG	1D	304	1/1	0.99	0.03	36,36,36,36	0
54	MG	2A	3490	1/1	0.99	0.03	29,29,29,29	0
54	MG	1A	3913	1/1	0.99	0.08	36,36,36,36	0
54	MG	1D	306	1/1	0.99	0.04	16,16,16,16	0
54	MG	1A	3784	1/1	0.99	0.04	29,29,29,29	0
54	MG	1a	1724	1/1	0.99	0.04	40,40,40,40	0
54	MG	1A	3001	1/1	0.99	0.04	33,33,33,33	0
54	MG	1A	3451	1/1	0.99	0.04	61,61,61,61	0
54	MG	2A	3282	1/1	0.99	0.05	21,21,21,21	0
54	MG	1A	3537	1/1	0.99	0.05	40,40,40,40	0
54	MG	1a	1728	1/1	0.99	0.06	54,54,54,54	0
54	MG	1A	3325	1/1	0.99	0.05	25,25,25,25	0
54	MG	1A	3159	1/1	0.99	0.08	29,29,29,29	0
54	MG	1W	202	1/1	0.99	0.15	52,52,52,52	0
54	MG	2A	3392	1/1	0.99	0.08	37,37,37,37	0
54	MG	2A	3004	1/1	0.99	0.02	40,40,40,40	0
54	MG	1W	203	1/1	0.99	0.04	28,28,28,28	0
54	MG	1A	3355	1/1	0.99	0.03	18,18,18,18	0
54	MG	1A	3791	1/1	0.99	0.02	53,53,53,53	0
54	MG	2A	3100	1/1	0.99	0.06	39,39,39,39	0
54	MG	1A	3211	1/1	0.99	0.05	46,46,46,46	0
54	MG	1A	3497	1/1	0.99	0.04	40,40,40,40	0
54	MG	1A	3175	1/1	0.99	0.16	22,22,22,22	0
54	MG	2A	3011	1/1	0.99	0.02	35,35,35,35	0
54	MG	1A	3737	1/1	0.99	0.06	28,28,28,28	0
54	MG	1E	303	1/1	0.99	0.07	36,36,36,36	0
54	MG	1A	3796	1/1	0.99	0.07	32,32,32,32	0
54	MG	1A	3329	1/1	0.99	0.04	38,38,38,38	0
54	MG	1A	3590	1/1	0.99	0.03	39,39,39,39	0
54	MG	1a	1743	1/1	0.99	0.03	52,52,52,52	0
54	MG	1A	3391	1/1	0.99	0.07	18,18,18,18	0
54	MG	1A	3930	1/1	0.99	0.08	39,39,39,39	0
54	MG	1I	102	1/1	0.99	0.03	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3800	1/1	0.99	0.13	41,41,41,41	0
54	MG	1A	3685	1/1	0.99	0.03	45,45,45,45	0
54	MG	2D	301	1/1	0.99	0.17	45,45,45,45	0
54	MG	1A	3360	1/1	0.99	0.04	32,32,32,32	0
54	MG	1A	3073	1/1	0.99	0.04	29,29,29,29	0
54	MG	1F	303	1/1	0.99	0.19	28,28,28,28	0
54	MG	1A	3426	1/1	0.99	0.05	40,40,40,40	0
54	MG	1A	3504	1/1	0.99	0.03	22,22,22,22	0
54	MG	1A	3146	1/1	0.99	0.06	30,30,30,30	0
54	MG	1A	3463	1/1	0.99	0.03	38,38,38,38	0
54	MG	2A	3315	1/1	0.99	0.04	49,49,49,49	0
54	MG	1A	3363	1/1	0.99	0.06	34,34,34,34	0
54	MG	1A	3332	1/1	0.99	0.04	33,33,33,33	0
54	MG	2E	302	1/1	0.99	0.03	45,45,45,45	0
54	MG	1A	3101	1/1	0.99	0.24	33,33,33,33	0
54	MG	1A	3237	1/1	0.99	0.06	34,34,34,34	0
54	MG	2A	3649	1/1	0.99	0.04	46,46,46,46	0
54	MG	2A	3650	1/1	0.99	0.04	53,53,53,53	0
54	MG	1A	3812	1/1	0.99	0.03	45,45,45,45	0
54	MG	1A	3032	1/1	0.99	0.07	42,42,42,42	0
54	MG	1A	3469	1/1	0.99	0.06	43,43,43,43	0
58	ZN	1Y	203	1/1	0.99	0.02	56,56,56,56	0
54	MG	1A	3180	1/1	0.99	0.07	30,30,30,30	0
58	ZN	15	107	1/1	0.99	0.02	47,47,47,47	0
58	ZN	1n	104	1/1	0.99	0.03	68,68,68,68	0
54	MG	1A	3198	1/1	0.99	0.11	34,34,34,34	0
54	MG	2A	3430	1/1	0.99	0.06	36,36,36,36	0
58	ZN	25	103	1/1	0.99	0.02	57,57,57,57	0
58	ZN	29	501	1/1	0.99	0.03	81,81,81,81	0
58	ZN	2n	102	1/1	0.99	0.04	93,93,93,93	0
59	SF4	1d	306	8/8	0.99	0.04	61,69,73,74	0
59	SF4	2d	501	8/8	0.99	0.04	70,71,85,85	0
58	ZN	19	102	1/1	1.00	0.04	49,49,49,49	0
54	MG	1A	3358	1/1	1.00	0.03	20,20,20,20	0
54	MG	1B	215	1/1	1.00	0.03	39,39,39,39	0
54	MG	2a	3131	1/1	1.00	0.11	61,61,61,61	0
54	MG	1A	3703	1/1	1.00	0.02	33,33,33,33	0
58	ZN	26	501	1/1	1.00	0.04	60,60,60,60	0
54	MG	2A	3647	1/1	1.00	0.03	53,53,53,53	0
54	MG	2A	3673	1/1	1.00	0.04	51,51,51,51	0
54	MG	1a	1722	1/1	1.00	0.03	43,43,43,43	0
58	ZN	16	501	1/1	1.00	0.06	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.