



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 03:48 AM EDT

PDB ID : 5V8I / pdb_00005v8i
Title : Thermus thermophilus 70S ribosome lacking ribosomal protein uS17
Authors : Gregory, S.T.; Jogl, G.
Deposited on : 2017-03-22
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

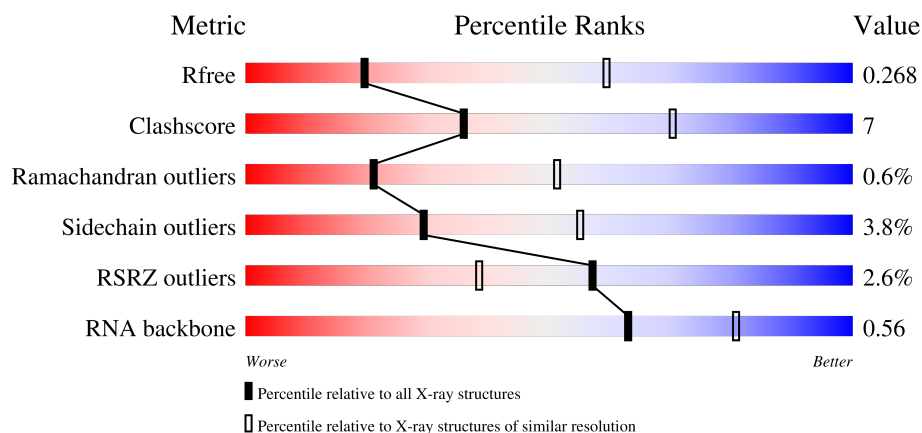
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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.



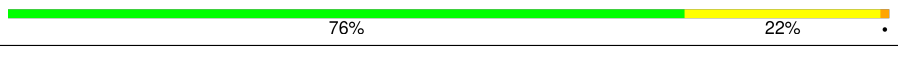
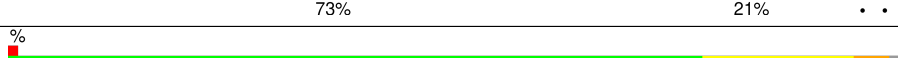
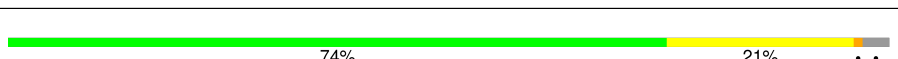
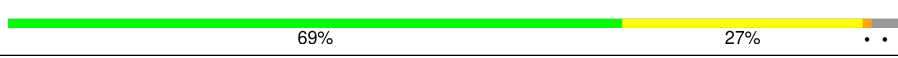
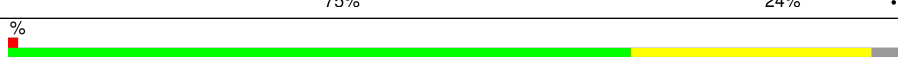
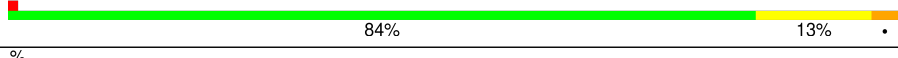
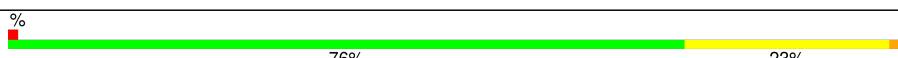
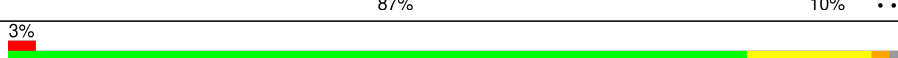
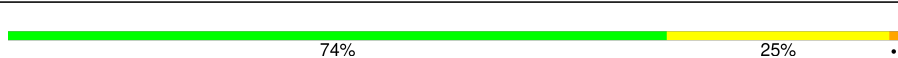
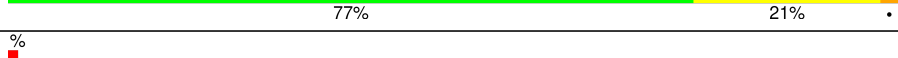
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)
RNA backbone	3983	1006 (3.54-2.98)

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	2894	% 65% 29% 5% •
1	2A	2894	% 62% 30% 6% •
2	1B	120	% 81% 16% • •
2	2B	120	% 65% 29% • •

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

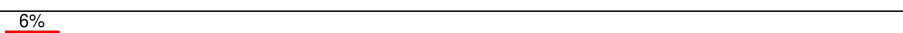
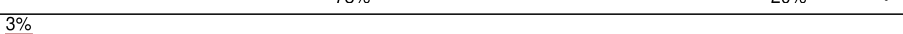
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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25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

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Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1522	
32	2a	1522	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	135	
43	2l	135	
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	1r	88	
48	2r	88	
49	1s	93	
49	2s	93	
50	1t	106	
50	2t	106	
51	1u	27	
51	2u	27	
52	1y	113	
52	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
53	MPD	2B	201	-	-	-	X
54	MG	1A	3727	-	-	-	X
54	MG	1a	1670	-	-	-	X
54	MG	1t	202	-	-	-	X
54	MG	2A	3105	-	-	-	X
54	MG	2i	201	-	-	-	X

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 290709 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	2862	Total	C	N	O	P	0	0	0
			61654	27444	11530	19819	2861			
1	2A	2858	Total	C	N	O	P	0	0	0
			61564	27404	11511	19793	2856			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	118	Total	C	N	O	P	0	0	0
			2536	1128	471	819	118			
2	2B	118	Total	C	N	O	P	0	0	0
			2536	1128	471	819	118			

- 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
			1586	1011	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1582	1009	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
			1427	917	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1425	913	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
			1095	700	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1077	688	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
			932	587	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
			932	587	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
			1121	715	212	187	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	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	681	225	184	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	676	224	182	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
			606	375	127	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			606	375	127	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
			756	475	150	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			761	478	151	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
			460	290	90	75	5			
27	25	59	Total	C	N	O	S	0	0	0
			456	287	89	75	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
			32249	14359	5977	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32334	14397	5992	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
			987	625	194	168			
40	2i	126	Total	C	N	O	0	0	0
			967	613	187	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 S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
48	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
49	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1t	96	Total	C	N	O	S	0	0	0
			731	448	157	124	2			
50	2t	98	Total	C	N	O	S	0	0	0
			732	450	154	126	2			

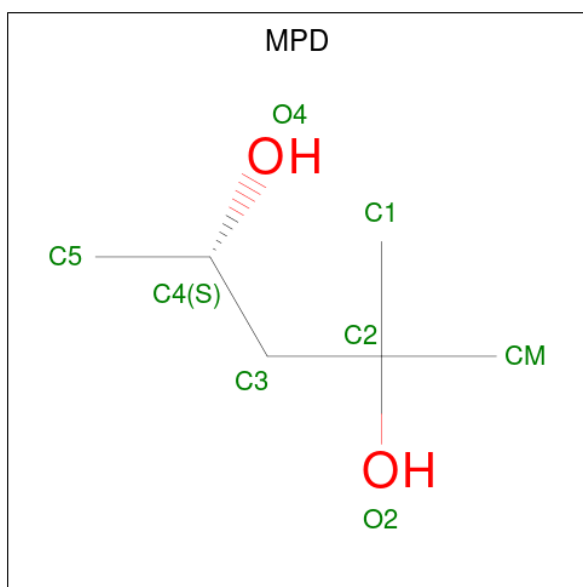
- Molecule 51 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
51	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 52 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
52	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 53 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
53	1A	1	Total 8	C 6	O 2	0	0
53	1T	1	Total 8	C 6	O 2	0	0
53	18	1	Total 8	C 6	O 2	0	0
53	1a	1	Total 8	C 6	O 2	0	0
53	2A	1	Total 8	C 6	O 2	0	0
53	2A	1	Total 8	C 6	O 2	0	0
53	2B	1	Total 8	C 6	O 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1A	900	Total Mg 900 900	0	0
54	1B	29	Total Mg 29 29	0	0
54	1D	12	Total Mg 12 12	0	0
54	1E	5	Total Mg 5 5	0	0
54	1F	12	Total Mg 12 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1G	4	Total 4	Mg 4	0	0
54	1H	2	Total 2	Mg 2	0	0
54	1N	3	Total 3	Mg 3	0	0
54	1O	1	Total 1	Mg 1	0	0
54	1P	5	Total 5	Mg 5	0	0
54	1Q	3	Total 3	Mg 3	0	0
54	1R	7	Total 7	Mg 7	0	0
54	1T	5	Total 5	Mg 5	0	0
54	1U	3	Total 3	Mg 3	0	0
54	1V	3	Total 3	Mg 3	0	0
54	1W	4	Total 4	Mg 4	0	0
54	1X	2	Total 2	Mg 2	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	10	6	Total 6	Mg 6	0	0
54	11	4	Total 4	Mg 4	0	0
54	13	2	Total 2	Mg 2	0	0
54	15	3	Total 3	Mg 3	0	0
54	16	1	Total 1	Mg 1	0	0
54	17	3	Total 3	Mg 3	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	257	Total 257	Mg 257	0	0

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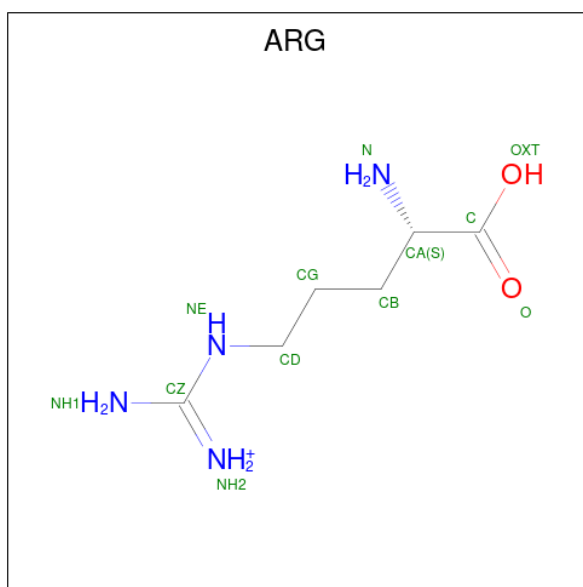
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1b	1	Total 1	Mg 1	0	0
54	1d	6	Total 6	Mg 6	0	0
54	1e	3	Total 3	Mg 3	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1n	2	Total 2	Mg 2	0	0
54	1o	1	Total 1	Mg 1	0	0
54	1t	2	Total 2	Mg 2	0	0
54	1y	4	Total 4	Mg 4	0	0
54	2A	641	Total 641	Mg 641	0	0
54	2B	16	Total 16	Mg 16	0	0
54	2D	6	Total 6	Mg 6	0	0
54	2E	2	Total 2	Mg 2	0	0
54	2F	2	Total 2	Mg 2	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2I	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2R	3	Total 3	Mg 3	0	0
54	2T	5	Total 5	Mg 5	0	0
54	2V	1	Total 1	Mg 1	0	0
54	2W	2	Total 2	Mg 2	0	0
54	2X	1	Total 1	Mg 1	0	0
54	2Y	1	Total 1	Mg 1	0	0
54	20	1	Total 1	Mg 1	0	0
54	21	4	Total 4	Mg 4	0	0
54	23	1	Total 1	Mg 1	0	0
54	28	1	Total 1	Mg 1	0	0
54	2a	164	Total 164	Mg 164	0	0
54	2e	1	Total 1	Mg 1	0	0
54	2f	1	Total 1	Mg 1	0	0
54	2i	1	Total 1	Mg 1	0	0
54	2j	1	Total 1	Mg 1	0	0
54	2k	1	Total 1	Mg 1	0	0
54	2l	2	Total 2	Mg 2	0	0
54	2p	1	Total 1	Mg 1	0	0
54	2t	1	Total 1	Mg 1	0	0

- Molecule 55 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	1B	1	Total	C	N	O	0	0
			12	6	4	2		
55	1F	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

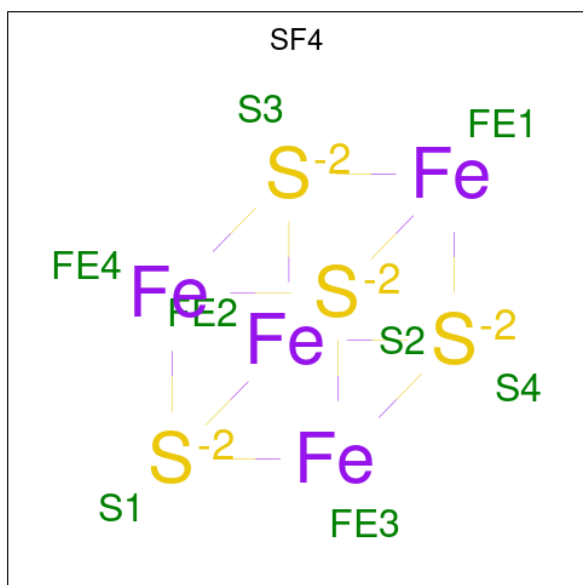
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	1	Total	Zn	0	0
			1	1		
56	14	1	Total	Zn	0	0
			1	1		
56	15	1	Total	Zn	0	0
			1	1		
56	16	1	Total	Zn	0	0
			1	1		
56	19	1	Total	Zn	0	0
			1	1		
56	1n	1	Total	Zn	0	0
			1	1		
56	2Y	1	Total	Zn	0	0
			1	1		
56	24	1	Total	Zn	0	0
			1	1		
56	25	1	Total	Zn	0	0
			1	1		
56	26	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	29	1	Total	Zn	0	0
			1	1		
56	2n	1	Total	Zn	0	0
			1	1		

- Molecule 57 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1d	1	Total	Fe	S	0	0
			8	4	4		
57	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1801	Total	O	0	0
			1801	1801		
58	1B	56	Total	O	0	0
			56	56		
58	1D	14	Total	O	0	0
			14	14		
58	1E	17	Total	O	0	0
			17	17		
58	1F	16	Total	O	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1G	5	Total	O	0	0
			5	5		
58	1H	5	Total	O	0	0
			5	5		
58	1N	7	Total	O	0	0
			7	7		
58	1O	2	Total	O	0	0
			2	2		
58	1P	17	Total	O	0	0
			17	17		
58	1Q	5	Total	O	0	0
			5	5		
58	1R	5	Total	O	0	0
			5	5		
58	1T	8	Total	O	0	0
			8	8		
58	1U	6	Total	O	0	0
			6	6		
58	1V	5	Total	O	0	0
			5	5		
58	1W	2	Total	O	0	0
			2	2		
58	1X	6	Total	O	0	0
			6	6		
58	1Y	1	Total	O	0	0
			1	1		
58	1Z	1	Total	O	0	0
			1	1		
58	10	5	Total	O	0	0
			5	5		
58	11	3	Total	O	0	0
			3	3		
58	13	6	Total	O	0	0
			6	6		
58	15	3	Total	O	0	0
			3	3		
58	16	2	Total	O	0	0
			2	2		
58	17	1	Total	O	0	0
			1	1		
58	18	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	19	3	Total 3	O 3	0	0
58	1a	424	Total 424	O 424	0	0
58	1c	1	Total 1	O 1	0	0
58	1d	8	Total 8	O 8	0	0
58	1e	4	Total 4	O 4	0	0
58	1f	1	Total 1	O 1	0	0
58	1h	1	Total 1	O 1	0	0
58	1j	1	Total 1	O 1	0	0
58	1l	3	Total 3	O 3	0	0
58	1m	1	Total 1	O 1	0	0
58	1o	3	Total 3	O 3	0	0
58	1p	1	Total 1	O 1	0	0
58	1t	2	Total 2	O 2	0	0
58	1y	3	Total 3	O 3	0	0
58	2A	1310	Total 1310	O 1310	0	0
58	2B	32	Total 32	O 32	0	0
58	2D	16	Total 16	O 16	0	0
58	2E	10	Total 10	O 10	0	0
58	2F	6	Total 6	O 6	0	0
58	2G	1	Total 1	O 1	0	0
58	2N	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2O	3	Total 3	O 3	0	0
58	2P	14	Total 14	O 14	0	0
58	2Q	5	Total 5	O 5	0	0
58	2R	1	Total 1	O 1	0	0
58	2T	4	Total 4	O 4	0	0
58	2V	2	Total 2	O 2	0	0
58	2W	3	Total 3	O 3	0	0
58	2X	4	Total 4	O 4	0	0
58	2Y	1	Total 1	O 1	0	0
58	20	2	Total 2	O 2	0	0
58	21	1	Total 1	O 1	0	0
58	23	2	Total 2	O 2	0	0
58	25	1	Total 1	O 1	0	0
58	26	1	Total 1	O 1	0	0
58	27	2	Total 2	O 2	0	0
58	28	5	Total 5	O 5	0	0
58	2a	282	Total 282	O 282	0	0
58	2e	1	Total 1	O 1	0	0
58	2j	2	Total 2	O 2	0	0
58	2l	1	Total 1	O 1	0	0
58	2t	2	Total 2	O 2	0	0

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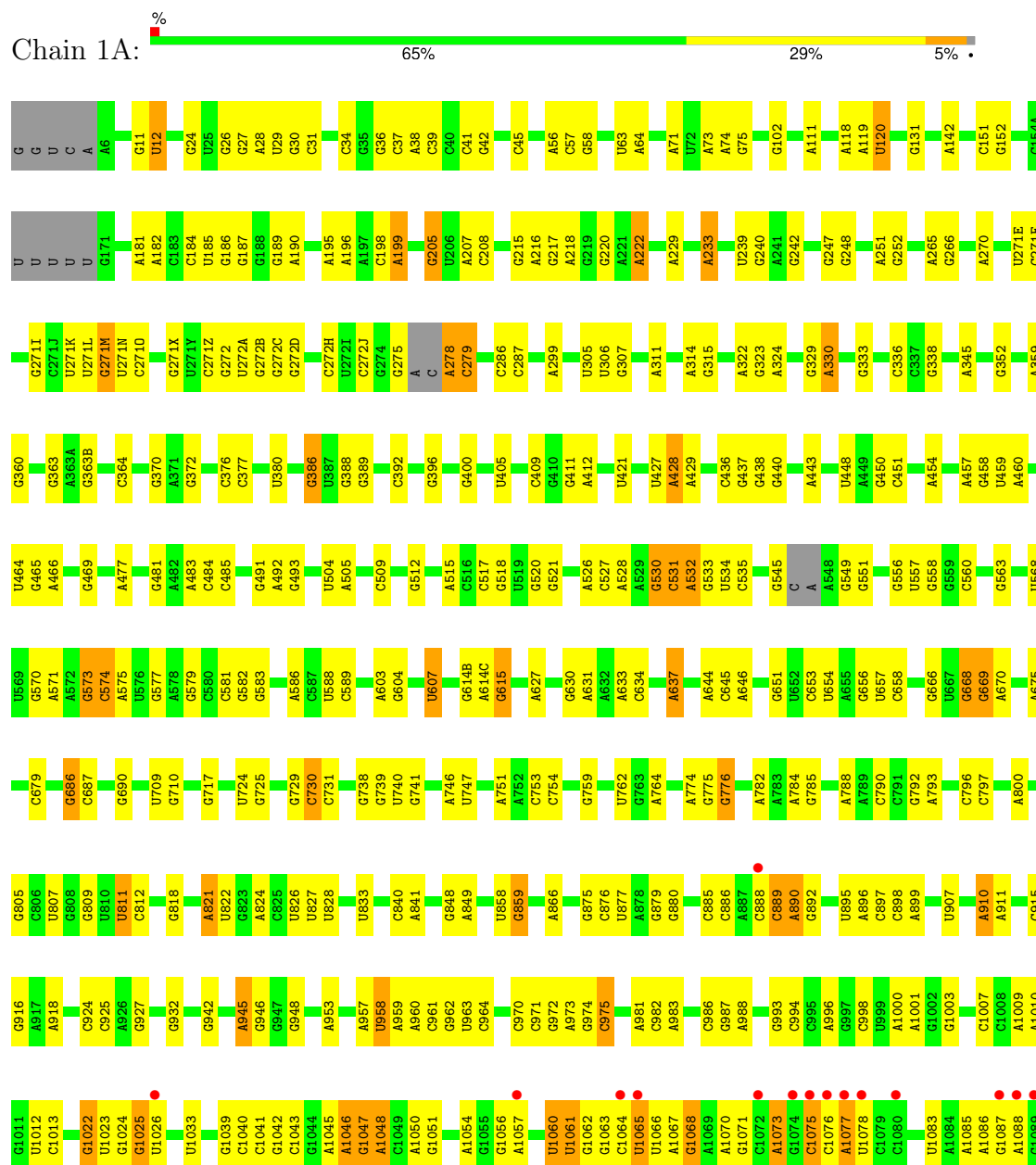
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2y	3	Total	O	0	0
			3	3		

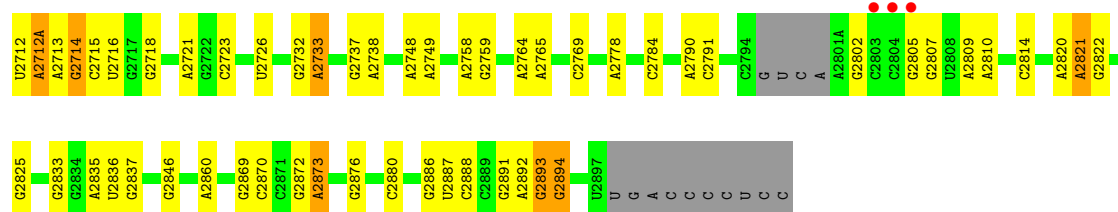
3 Residue-property plots

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.

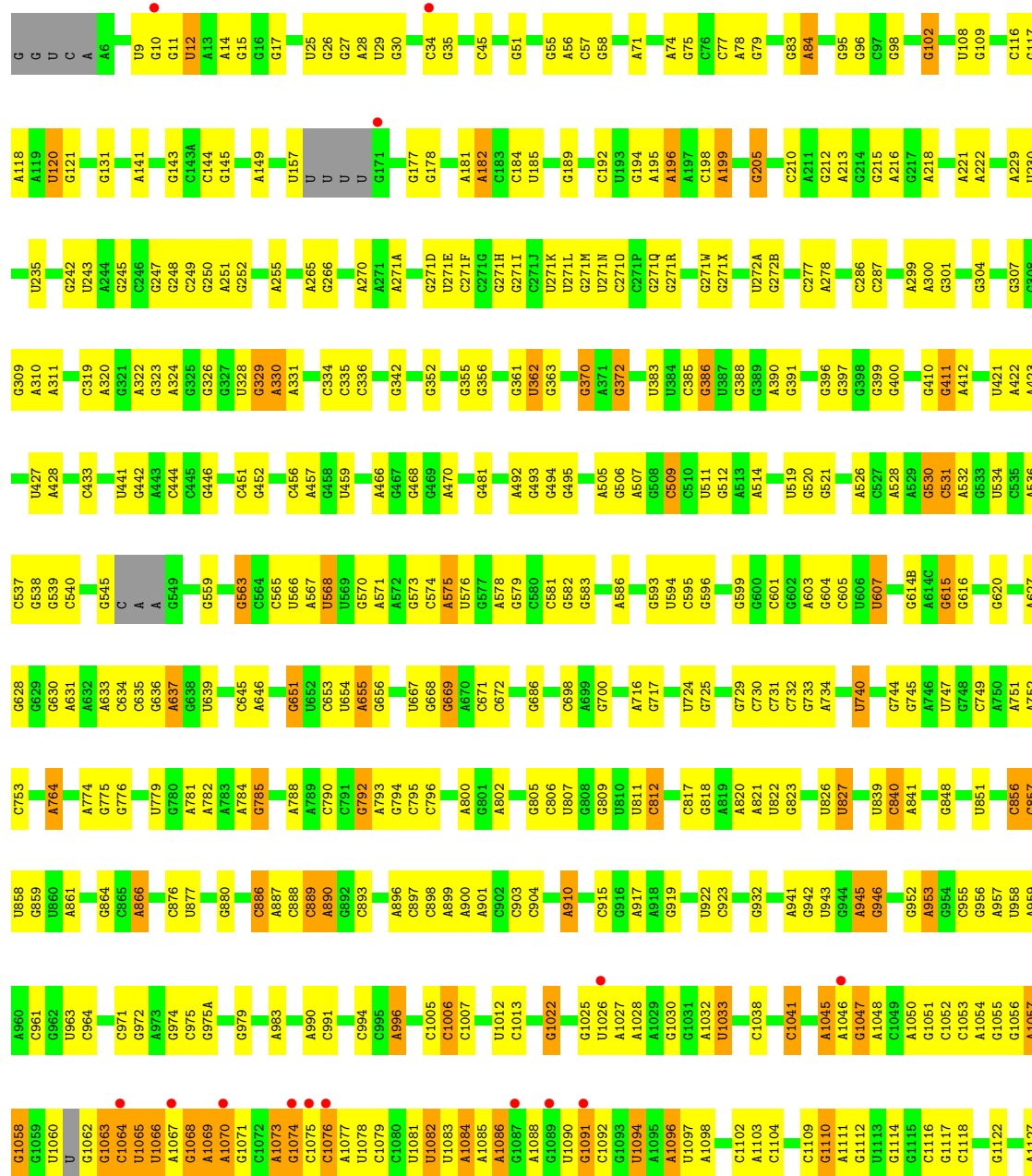
• Molecule 1: 23S Ribosomal RNA



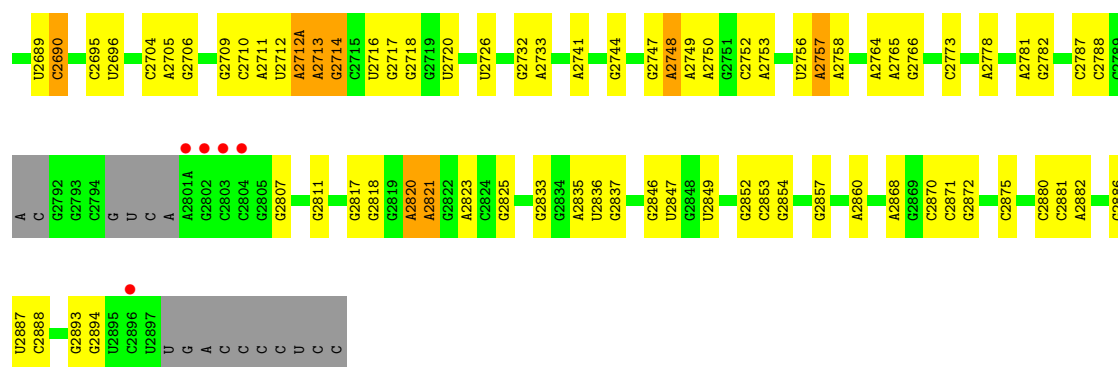
U090	G187	G1309	A1439	C1543	G1826	U1955	C2153	C2371	C2477	U2605
G1091	U188	A1309	G1440	G1552	C1827	A2278	G2154	G2372	A2478	U2608
C1092	A189	C1315	G1441	G1552	A1828	G2279	G2157	G2373	U2492	U2609
U1094	U199	U199	A1442	A1557	A1829	C1962	A2159	A2377	U2493	C2610
A1095	C1200	A1321	A1445	A1568	A1847	U1963	G2159	A2378	U2494	U2611
A1096	U1097	A1322	A1445	A1569	A1848	G1964	G2166	C2381	U2495	C2612
U1101	G1203	G1332	G1447	A1578	A1853	C1967	U2167	G2382	C2498	U2615
C1102	G1206	C1333	A1448	A1578	A1854	U1968	G2168	G2383	C2499	U2616
A1103	U1209	G1334	A1449	A1580	G1855	A1969	A2173	G2384	U2500	C2617
U1105	U1211	A1335	G1450	G1581	A1856	U1970	G2172	C2385	C2501	U2622
G1106	G1212	U1336	A1452	C1584	G1857	A1971	A1972	C2386	C2502	G2625
		G1337	U1453	A1586	G1858	U1972	G1973	U2387	A2503	A2629
		A1342	U1453	U1590	G1865	A1973	A1981	C2391	U2504	C2630
	A1220	A1345	C1464	U1591	A1877	C1981	C1990	U2392	U2506	U2637
	A1226	G1346	G1465	G1595	G1878	C1990	U1993	U2393	C2512	G2641
	G1230	G1347	G1466	C1599	A1889	C1994	C1995	G2405	G2516	U2647
	G1231	U1352	G1467	C1599	A1890	C1996	C1997	U2406	C2517	
		U1357	A1468	C1599	G1899	C1997	G1997	G2420	A2518	
	G1236	G1358	A1469	C1607	A1900	C1998	U1997	G2421	U2522	
	A1237	A1359	A1471	A1608	G1762	C1999	C1999	A2422	G2529	A2654
	G1238	A1360	G1475	A1609	G1763	C2000	C2001	U2423	A2530	A2660
	G1239	A1365	G1482	A1610	G1764	C2002	C2002	A2424	A2535	G2661
	U1240	A1365	G1482	A1616	A1773	C2003	C2003	A2425	A2535	A2662
	A1242	G1370	A1486	G1622	U1779	C2004	C2004	C2426	G2548	
	A1246	C1371	G1487	G1622	G1781	C2005	C2005	G2427	C2549	
	A1247	U1372	A1490	C1636	A1912	G2006	C2006	C2428	C2550	C2665
	G1248	A1379	A1493	C1637	A1783	C2007	C2007	A2430	C2551	C2667
		G1380	C1493	C1638	A1784	C2008	C2008	A2432	U2552	G2668
	A1253	A1254	C1499	C1640	A1785	C2009	C2009	A2435	U2553	
	U1255	G1256	G1500	C1642	A1786	C2010	C2010	A2439	U2554	A2679
	C1257	C1257	C1506	C1648	C1790	C2011	C2011	C2440	A2564	C2680
			A1507	C1648	A1791	C2012	C2012	C2441	A2565	
	A1265	A1265	A1508	C1651	U1794	C2013	C2013	G2445	A2566	
	C1152	G1266	A1509	A1652	C1795	C2014	C2014	A2448	C2572	
	C1153	U1267	A1509A	G1653	U1796	C2015	C2015	G2455	C2575	
	G1154	A1268	U1512	A1654	C1797	C2016	C2016	G2458	U2583	U2696
	U1165	C1269	C1408	C1662	U1798	C2017	C2017	C2464	U2584	C2697
	C1166	G1270	C1416	C1663	G1799	C2018	C2018	C2467	C2585	U2698
		A1272	C1417	C1664	C1800	C2019	C2019	G2470	C2586	C2699
	G1171	U1273	C1420	A1664	G1801	C2020	C2020	C2474	G2595	U2702
	G1173	A1278	G1421	C1664	A1802	C2021	C2021	C2475	A2598	C2704
	A1174	U1279	G1422	C1670	A1803	C2022	C2022	C2476	A2602	A2705
	U1175	G1279	G1423	U1671	C1804	C2023	C2023	C2477	C2475	
	G1176		G1424	C1674	U1805	C2024	C2024	C2478	C2476	
	A1177	U1292	C1293		C1816	C2025	C2025	C2479		
	C1178	C1293	C1428		G1817	C2026	C2026	C2480		
	C1179	G1299	G1429		G1824	C2027	C2027	C2481		
	C1185	U1300	U1431		A1825	C2028	C2028	C2482		
	G1186	A1301				C2029	C2029	C2483		
						C2030	C2030	C2484		
						C2031	C2031	C2485		
						C2032	C2032	C2486		
						C2033	C2033	C2487		
						C2034	C2034	C2488		
						C2035	C2035	C2489		
						C2036	C2036	C2490		
						C2037	C2037	C2491		
						C2038	C2038	C2492		
						C2039	C2039	C2493		
						C2040	C2040	C2494		
						C2041	C2041	C2495		
						C2042	C2042	C2496		
						C2043	C2043	C2497		
						C2044	C2044	C2498		
						C2045	C2045	C2499		
						C2046	C2046	C2500		
						C2047	C2047	C2501		
						C2048	C2048	C2502		
						C2049	C2049	C2503		
						C2050	C2050	C2504		
						C2051	C2051	C2505		
						C2052	C2052	C2506		
						C2053	C2053	C2507		
						C2054	C2054	C2508		
						C2055	C2055	C2509		
						C2056	C2056	C2510		
						C2057	C2057	C2511		
						C2058	C2058	C2512		
						C2059	C2059	C2513		
						C2060	C2060	C2514		
						C2061	C2061	C2515		
						C2062	C2062	C2516		
						C2063	C2063	C2517		
						C2064	C2064	C2518		
						C2065	C2065	C2519		
						C2066	C2066	C2520		
						C2067	C2067	C2521		
						C2068	C2068	C2522		
						C2069	C2069	C2523		
						C2070	C2070	C2524		
						C2071	C2071	C2525		
						C2072	C2072	C2526		
						C2073	C2073	C2527		
						C2074	C2074	C2528		
						C2075	C2075	C2529		
						C2076	C2076	C2530		
						C2077	C2077	C2531		
						C2078	C2078	C2532		
						C2079	C2079	C2533		
						C2080	C2080	C2534		
						C2081	C2081	C2535		
						C2082	C2082	C2536		
						C2083	C2083	C2537		
						C2084	C2084	C2538		
						C2085	C2085	C2539		
						C2086	C2086	C2540		
						C2087	C2087	C2541		
						C2088	C2088	C2542		
						C2089	C2089	C2543		
						C2090	C2090	C2544		
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						C2093	C2093	C2547		
						C2094	C2094	C2548		
						C2095	C2095	C2549		
						C2096	C2096	C2550		
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						C2099	C2099	C2553		
						C2100	C2100	C2554		
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						C2104	C2104	C2558		
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						C2110	C2110	C2564		
						C2111	C2111	C2565		
						C2112	C2112	C2566		
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						C2114	C2114	C2568		
						C2115	C2115	C2569		
						C2116	C2116	C2570		
						C2117	C2117	C2571		
						C2118	C2118	C2572		
						C2119	C2119	C2573		
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						C2122	C2122	C2576		
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						C2132	C2132	C2586		
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						C2143	C2143	C2597		
						C2144	C2144	C2598		
						C2145	C2145	C2599		
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						C2148	C2148	C2602		



• Molecule 1: 23S Ribosomal RNA







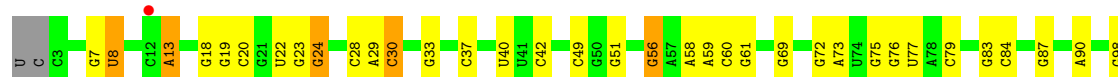
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 81% 16%



• Molecule 2: 5S Ribosomal RNA

Chain 2B: 65% 29%



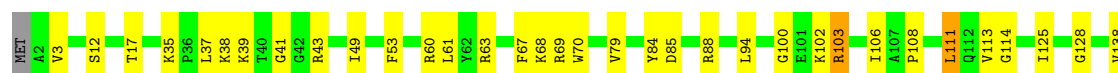
• Molecule 3: 50S ribosomal protein L2

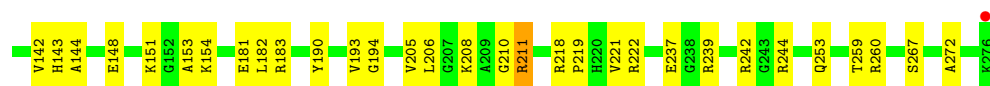
Chain 1D: 71% 26%



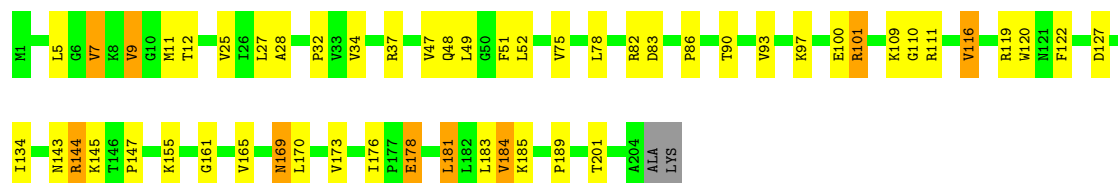
• Molecule 3: 50S ribosomal protein L2

Chain 2D: 76% 22%

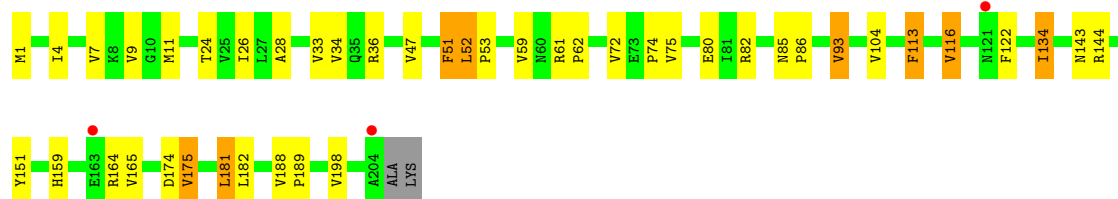
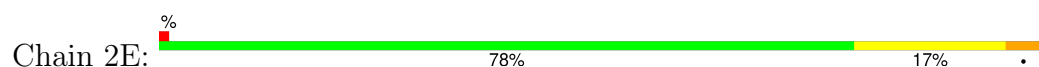




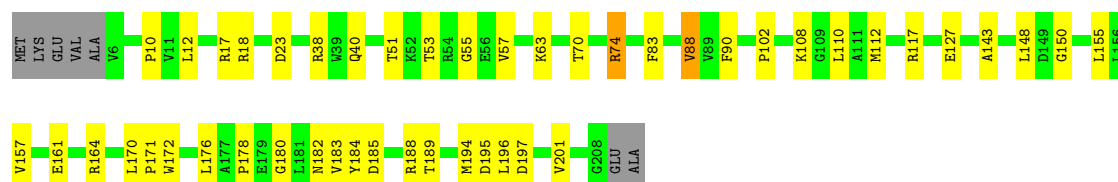
• Molecule 4: 50S ribosomal protein L3



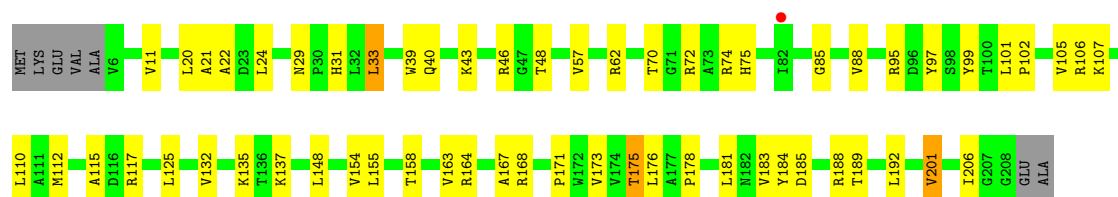
• Molecule 4: 50S ribosomal protein L3



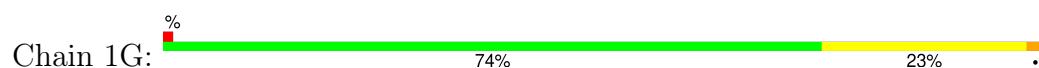
• Molecule 5: 50S ribosomal protein L4



• Molecule 5: 50S ribosomal protein L4

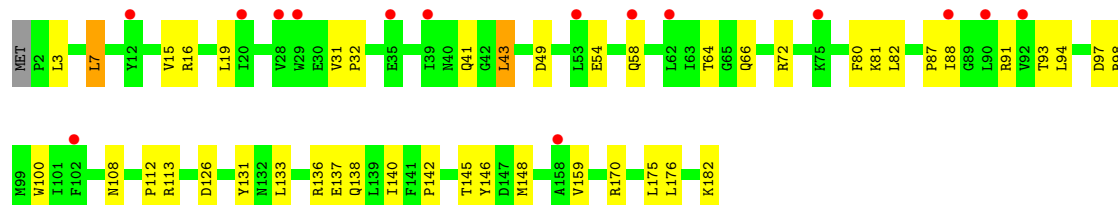
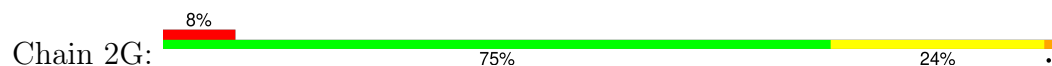


• Molecule 6: 50S ribosomal protein L5

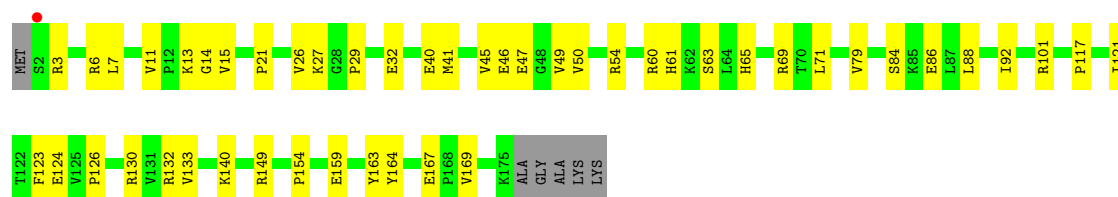




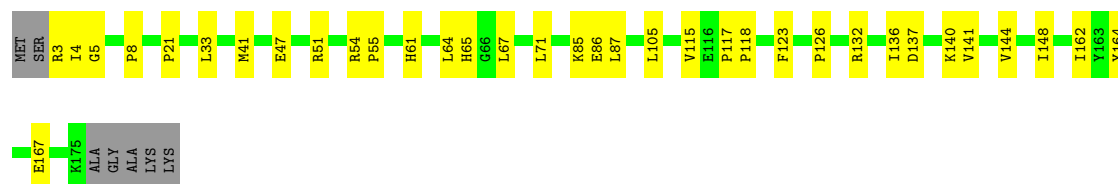
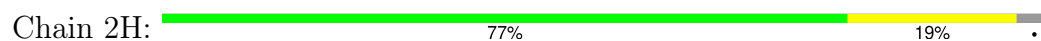
- Molecule 6: 50S ribosomal protein L5



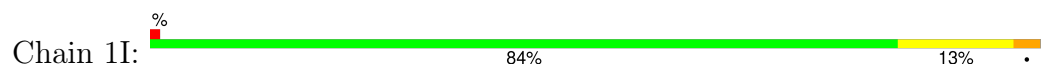
- Molecule 7: 50S ribosomal protein L6



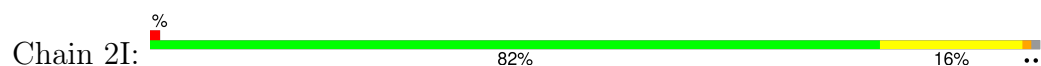
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9

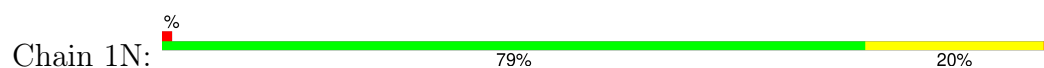


- Molecule 8: 50S ribosomal protein L9

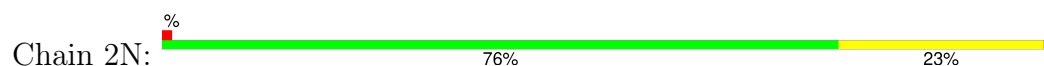




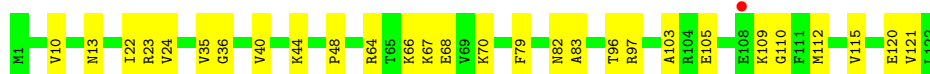
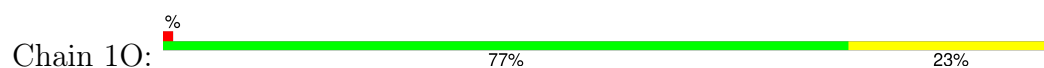
- Molecule 9: 50S ribosomal protein L13



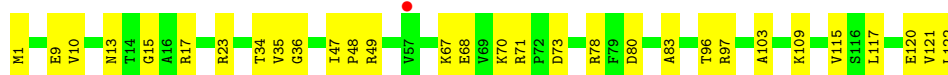
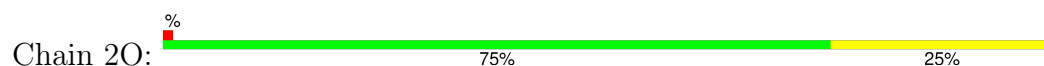
- Molecule 9: 50S ribosomal protein L13



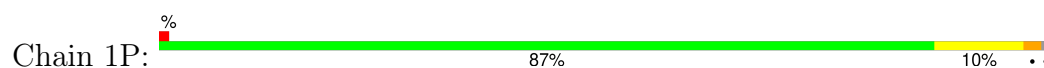
- Molecule 10: 50S ribosomal protein L14



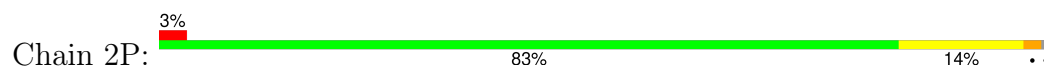
- Molecule 10: 50S ribosomal protein L14



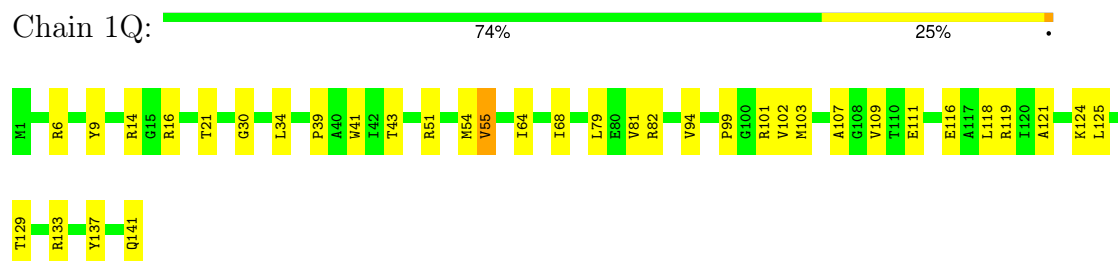
- Molecule 11: 50S ribosomal protein L15



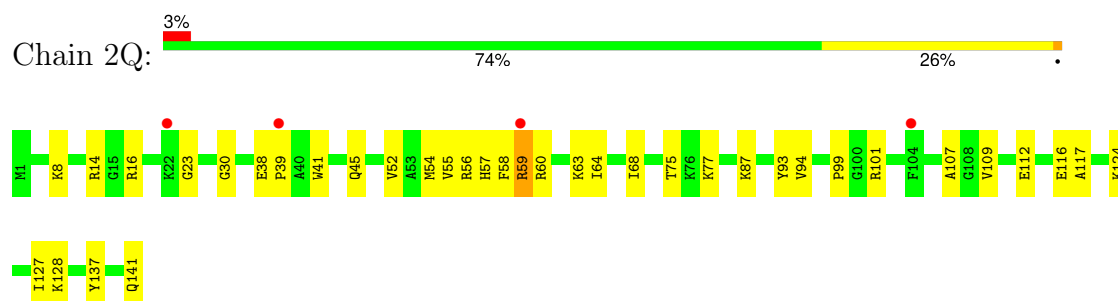
- Molecule 11: 50S ribosomal protein L15



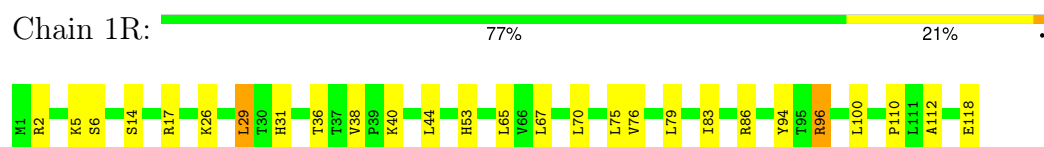
- Molecule 12: 50S ribosomal protein L16



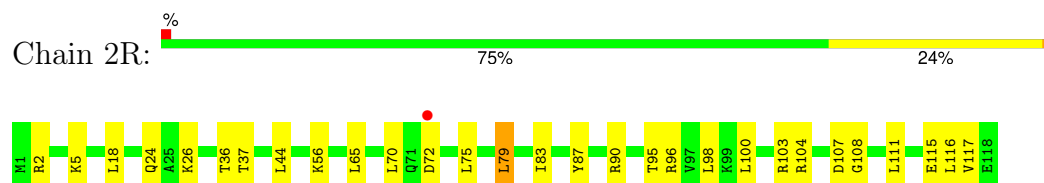
- Molecule 12: 50S ribosomal protein L16



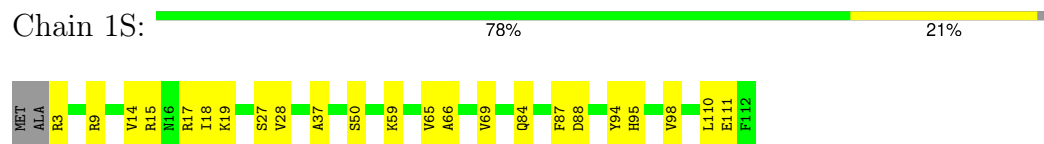
- Molecule 13: 50S ribosomal protein L17



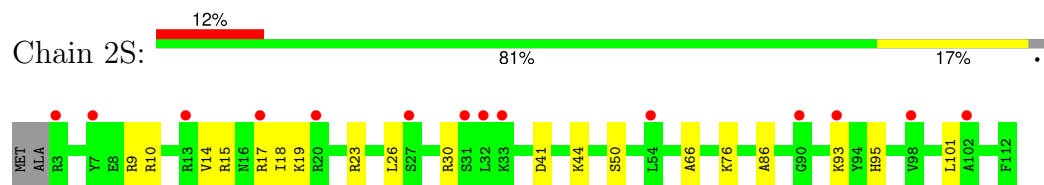
- Molecule 13: 50S ribosomal protein L17



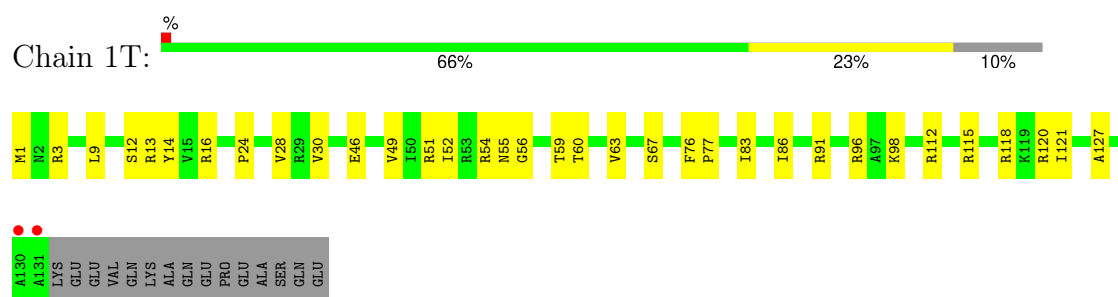
- Molecule 14: 50S ribosomal protein L18



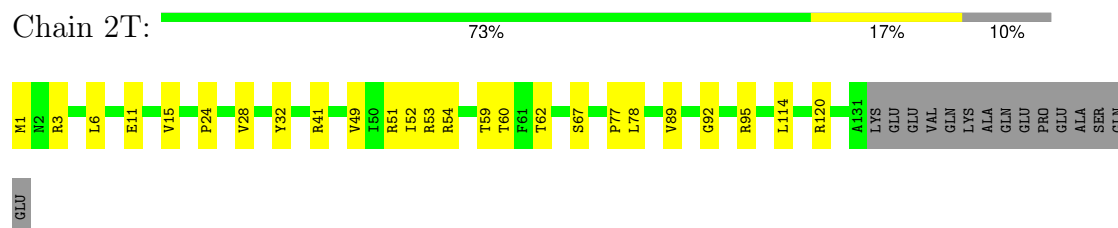
- Molecule 14: 50S ribosomal protein L18



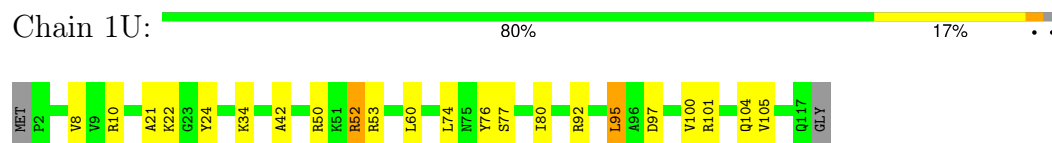
- Molecule 15: 50S ribosomal protein L19



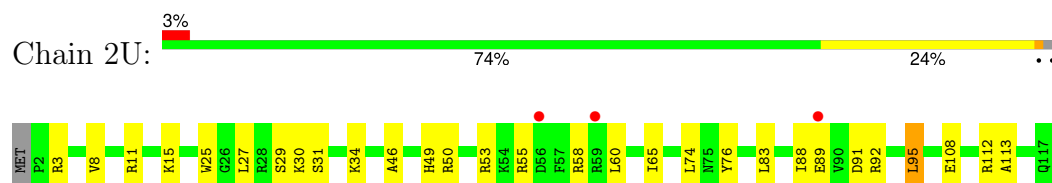
- Molecule 15: 50S ribosomal protein L19



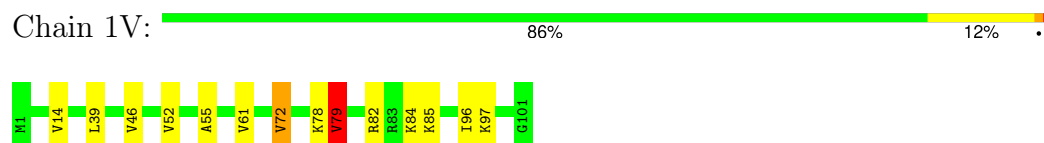
- Molecule 16: 50S ribosomal protein L20



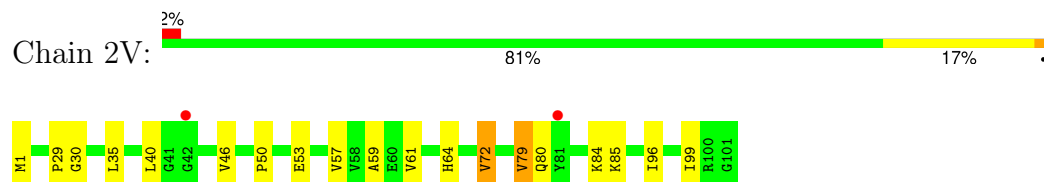
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21

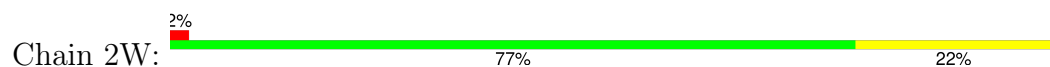


- Molecule 18: 50S ribosomal protein L22

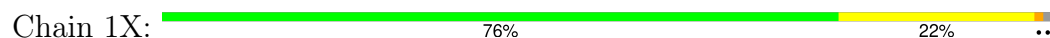




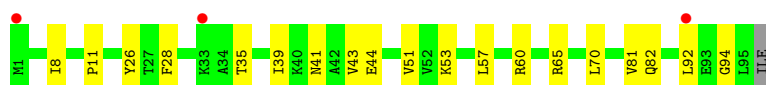
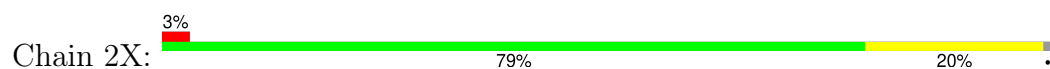
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



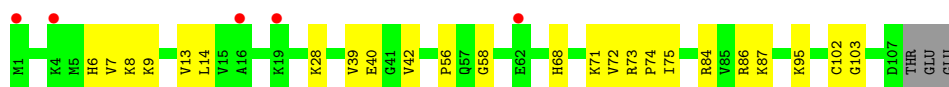
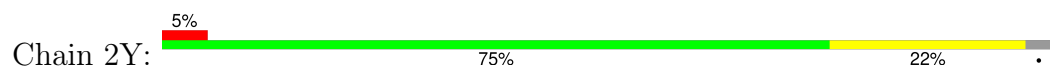
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



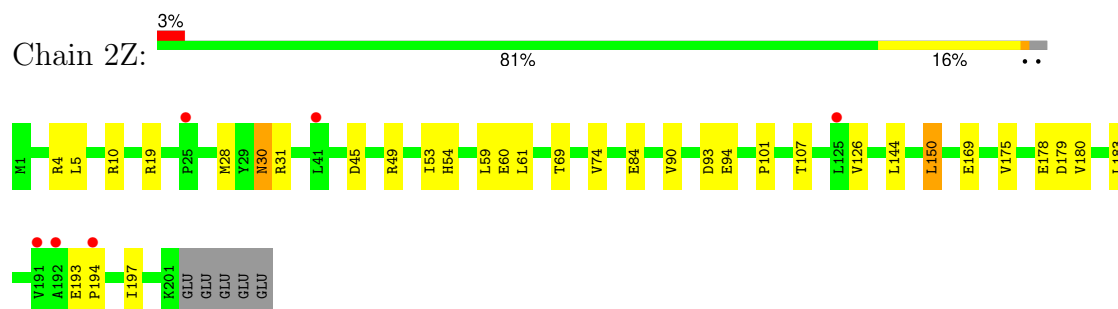
- Molecule 20: 50S ribosomal protein L24



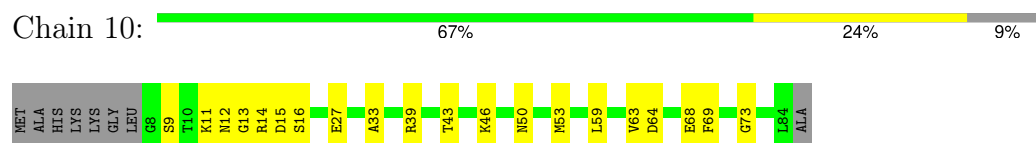
- Molecule 21: 50S ribosomal protein L25



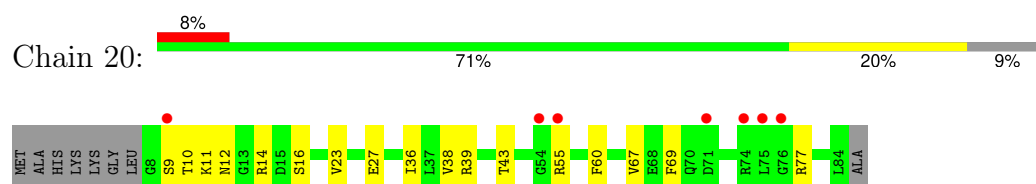
- Molecule 21: 50S ribosomal protein L25



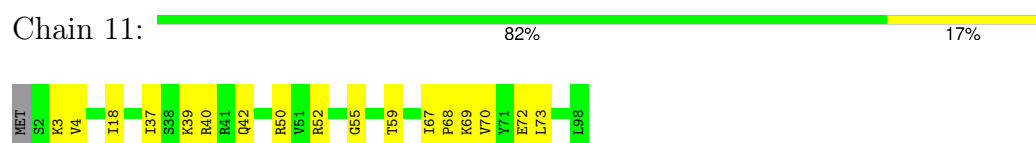
- Molecule 22: 50S ribosomal protein L27



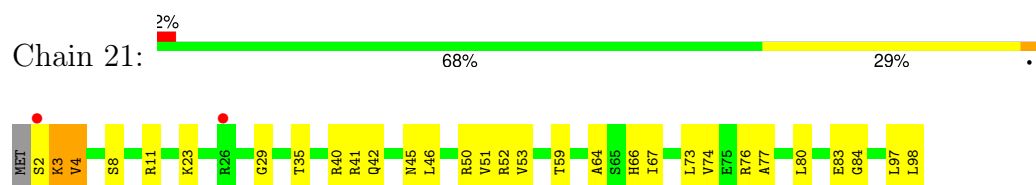
- Molecule 22: 50S ribosomal protein L27



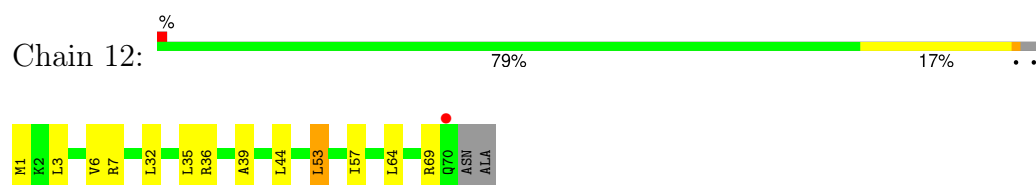
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28

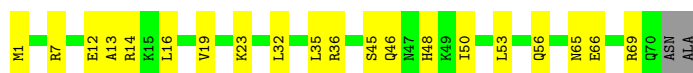


- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29

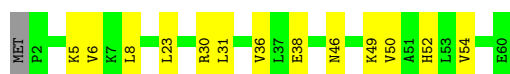
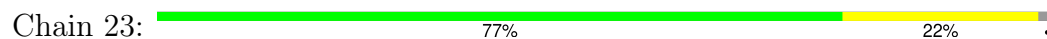




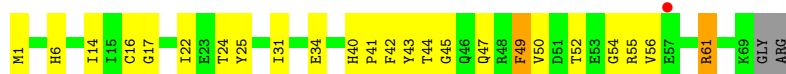
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



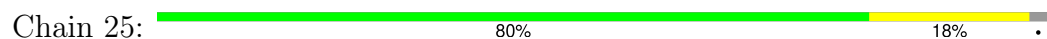
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

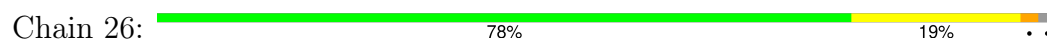


- Molecule 28: 50S ribosomal protein L33

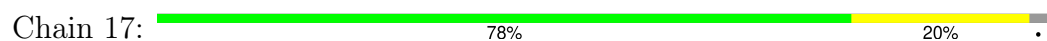




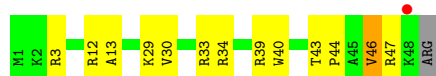
- Molecule 28: 50S ribosomal protein L33



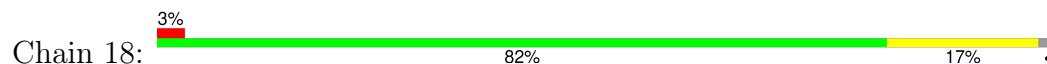
- Molecule 29: 50S ribosomal protein L34



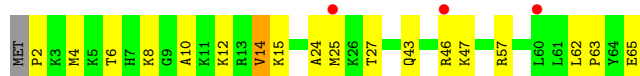
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



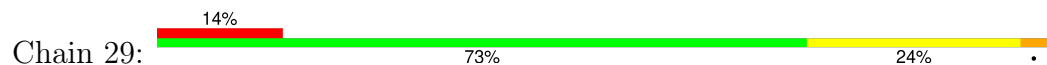
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

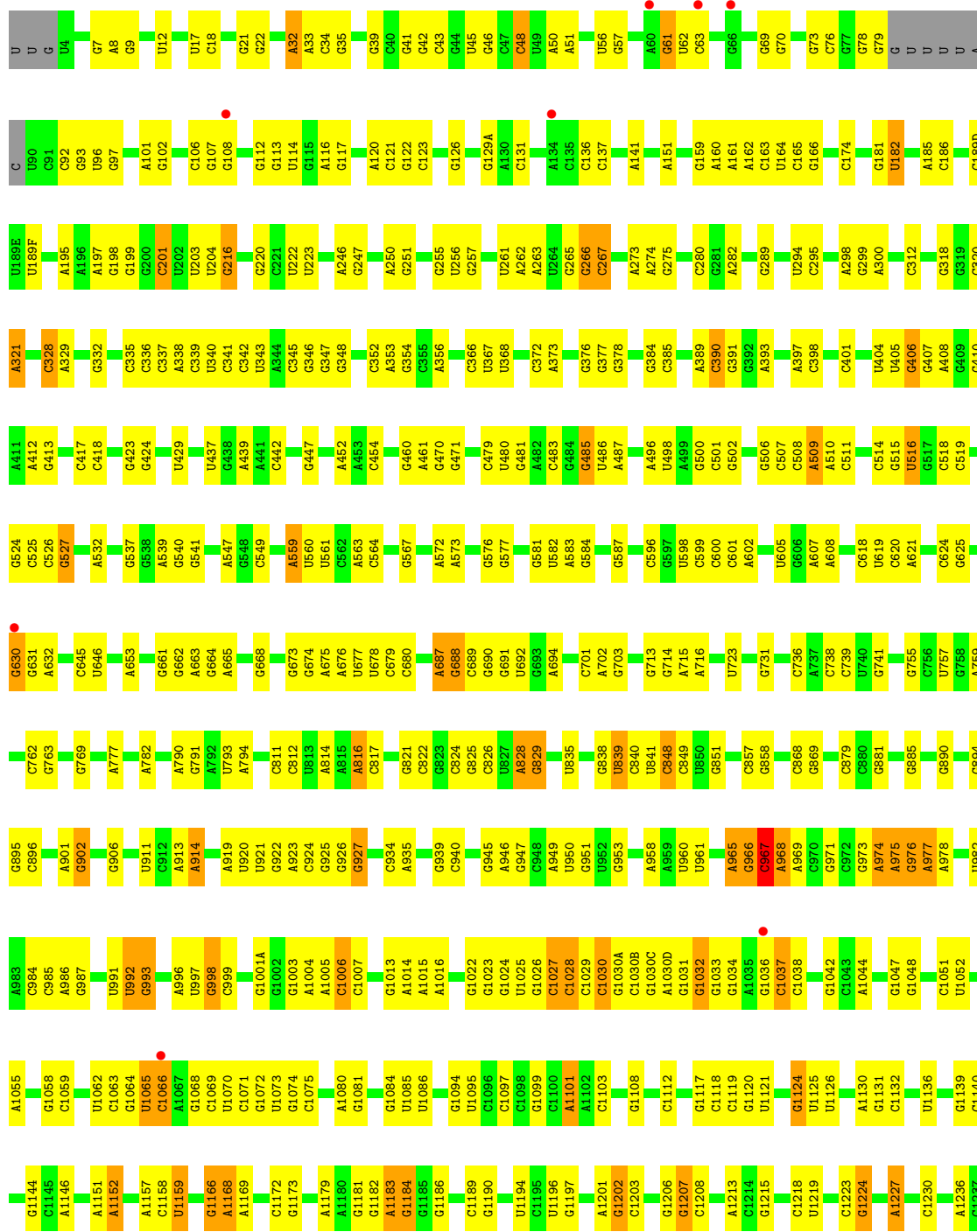


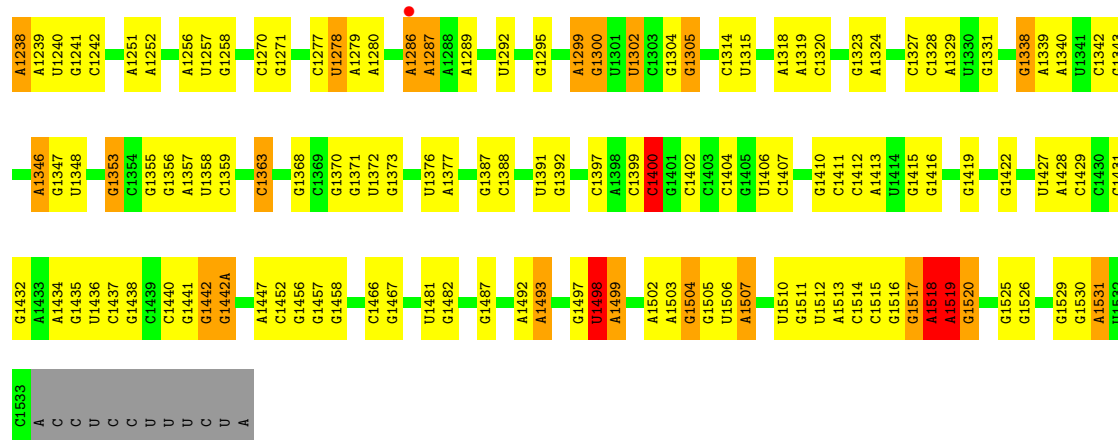
- Molecule 31: 50S ribosomal protein L36



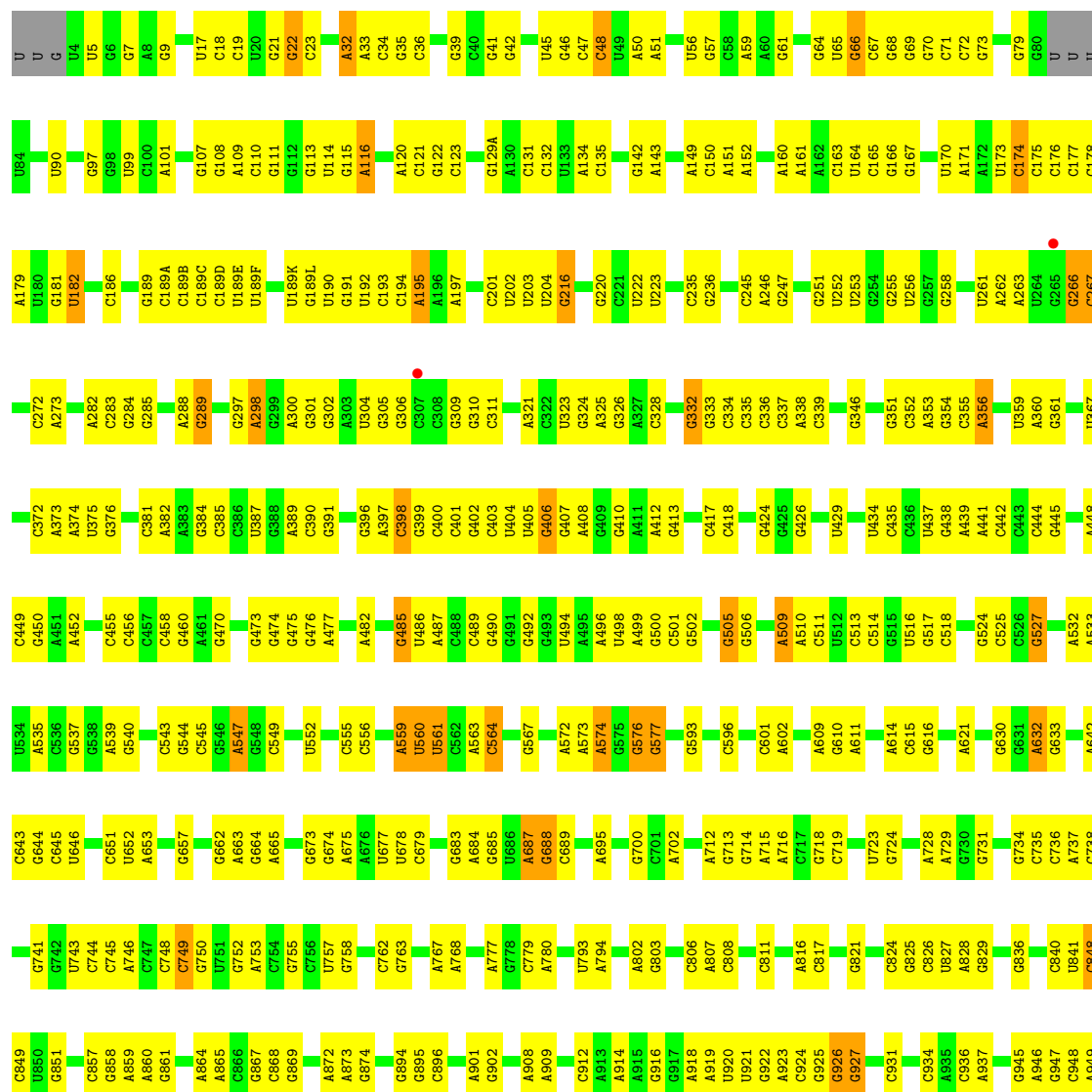


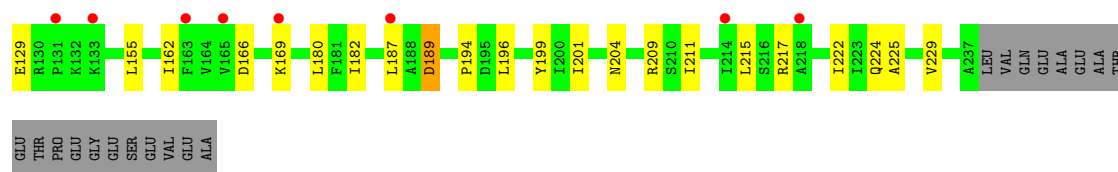
• Molecule 32: 16S Ribosomal RNA



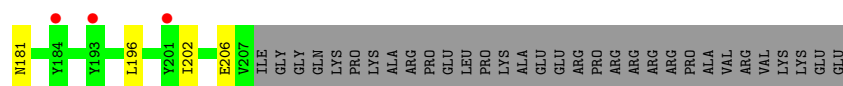


• Molecule 32: 16S Ribosomal RNA

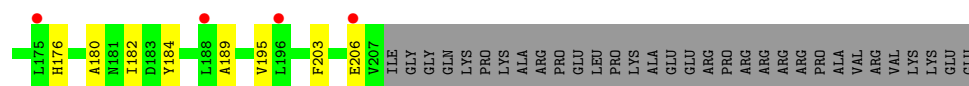




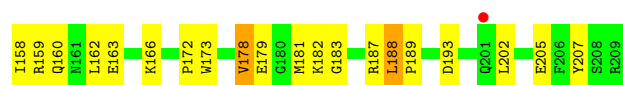
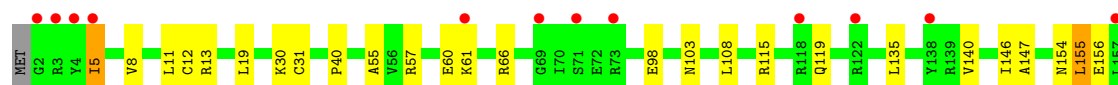
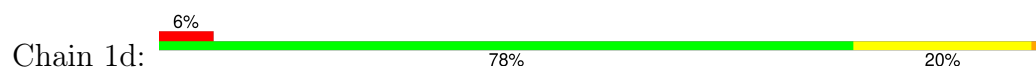
- Molecule 34: 30S ribosomal protein S3



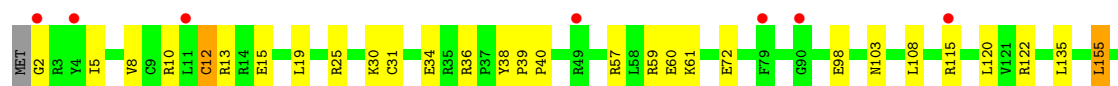
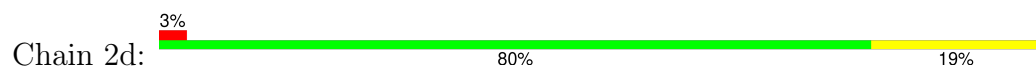
- Molecule 34: 30S ribosomal protein S3



- Molecule 35: 30S ribosomal protein S4

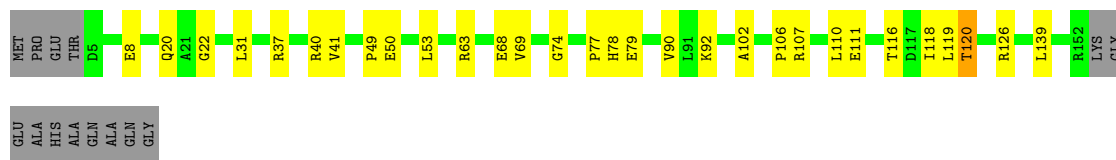


- Molecule 35: 30S ribosomal protein S4



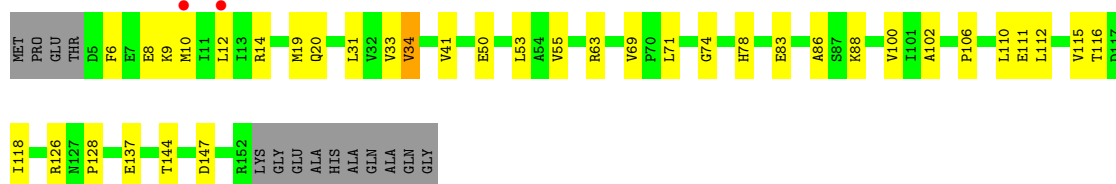
- Molecule 36: 30S ribosomal protein S5

Chain 1e:  73% 18% 9%



- Molecule 36: 30S ribosomal protein S5

Chain 2e:  69% 22% 9%



- Molecule 37: 30S ribosomal protein S6

Chain 1f:  78% 21%



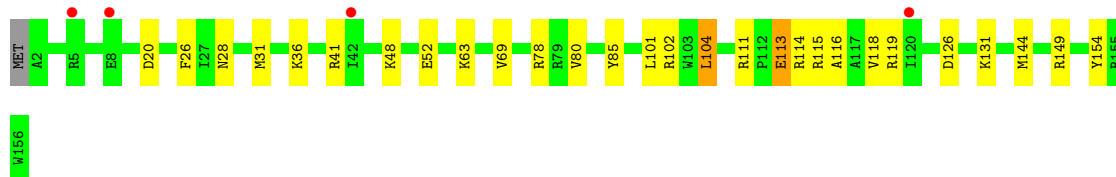
- Molecule 37: 30S ribosomal protein S6

Chain 2f:  73% 25%



- Molecule 38: 30S ribosomal protein S7

Chain 1g:  3% 81% 17%



- Molecule 38: 30S ribosomal protein S7

Chain 2g:  3% 81% 17%



W156

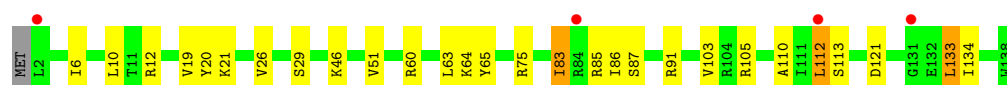
- Molecule 39: 30S ribosomal protein S8

Chain 1h:  73% 25% ..

L133
W138

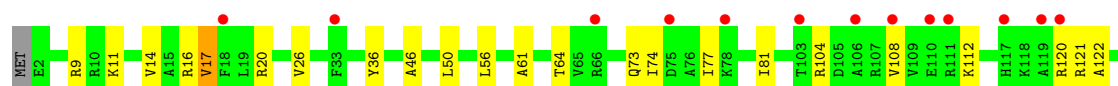
- Molecule 39: 30S ribosomal protein S8

Chain 2h:  3% 79% 18% ..



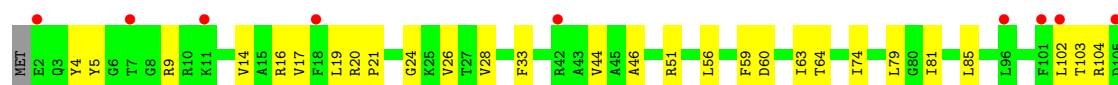
- Molecule 40: 30S ribosomal protein S9

Chain 1i:  12% 80% 18% ..

Y125
S126
K127
R128

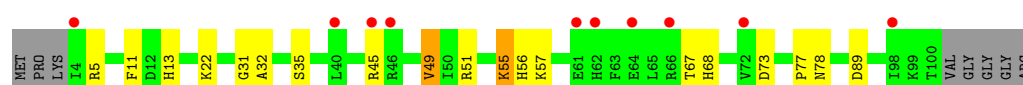
- Molecule 40: 30S ribosomal protein S9

Chain 2i:  21% 74% 24% .

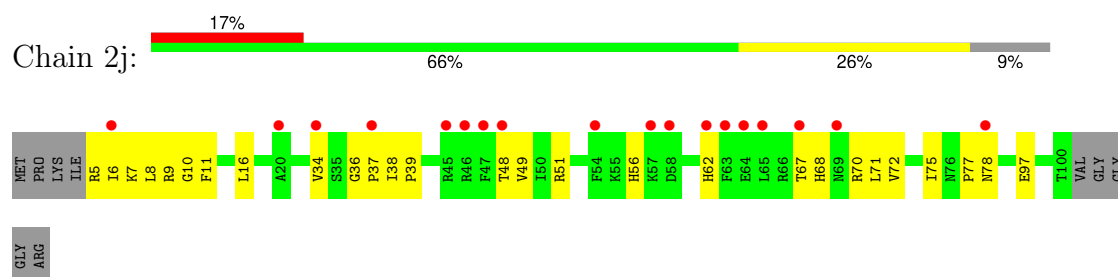
A106
R107
V108
E109
E110
R111
K112
K113
Y114
G115
K116
H117
K118
A119
R120
R121
A122
P123
Q124
Y125
S126
K127
ARG

- Molecule 41: 30S ribosomal protein S10

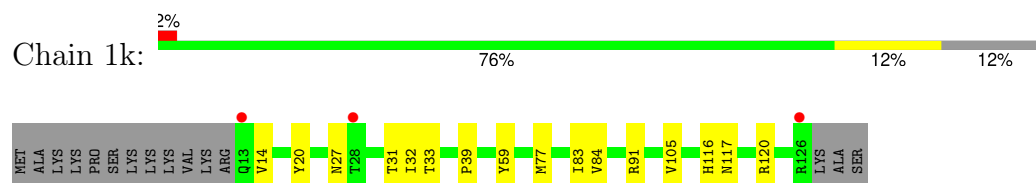
Chain 1j:  10% 74% 16% 8%



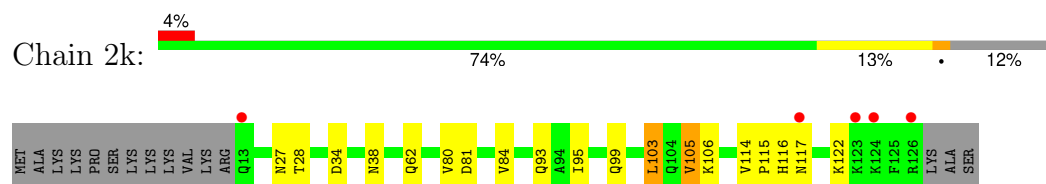
- Molecule 41: 30S ribosomal protein S10



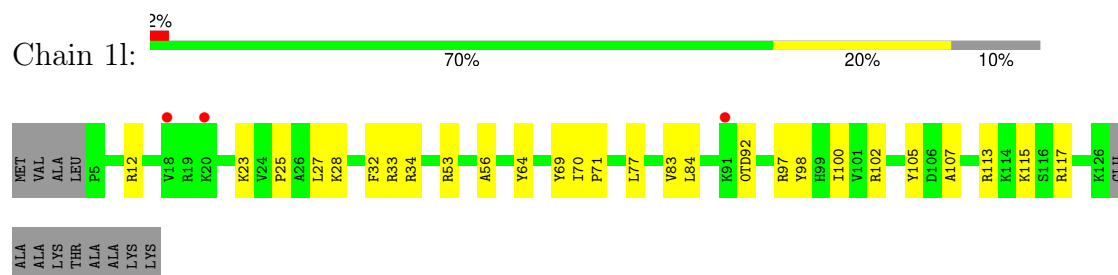
- Molecule 42: 30S ribosomal protein S11



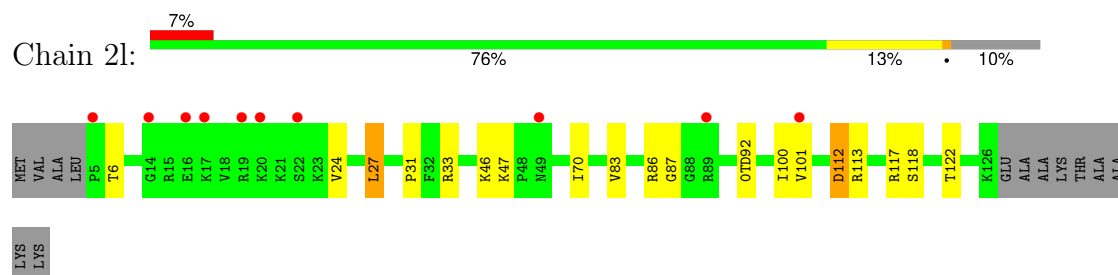
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12

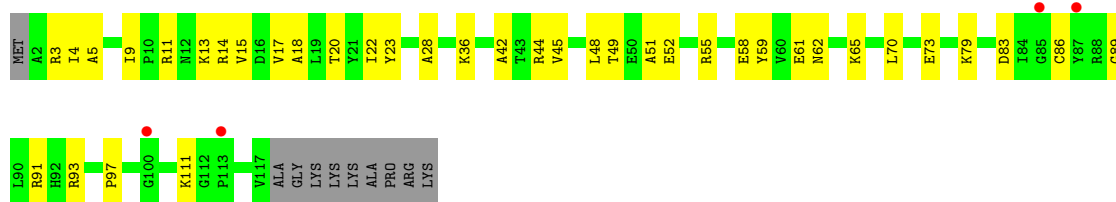


- Molecule 43: 30S ribosomal protein S12

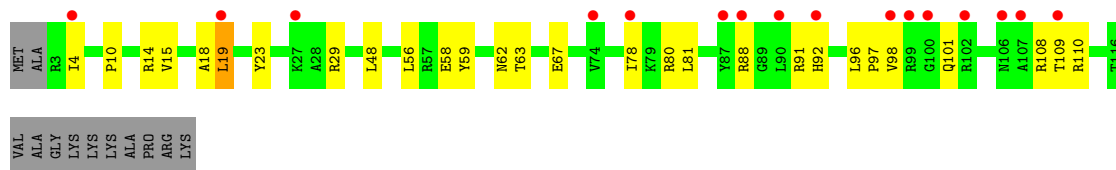


- Molecule 44: 30S ribosomal protein S13

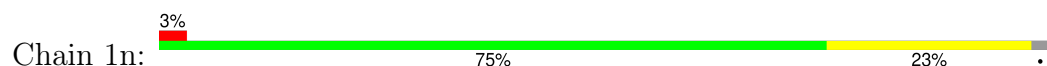




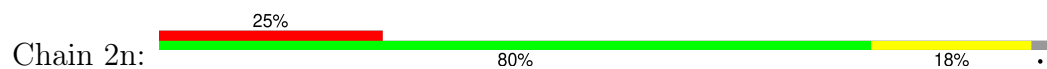
- Molecule 44: 30S ribosomal protein S13



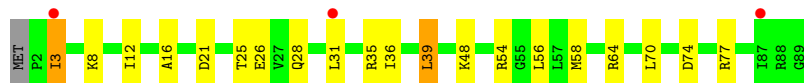
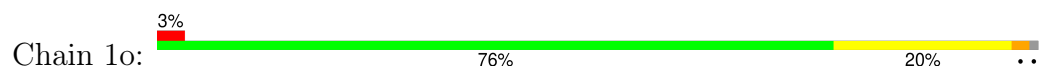
- Molecule 45: 30S ribosomal protein S14 type Z



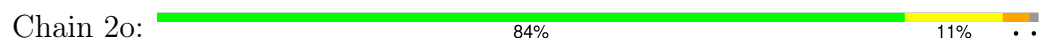
- Molecule 45: 30S ribosomal protein S14 type Z



- 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 S18



- Molecule 48: 30S ribosomal protein S18



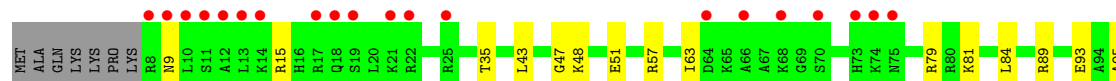
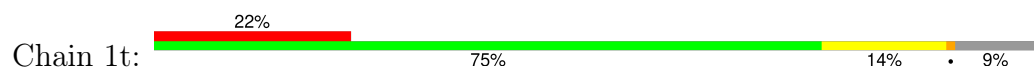
- Molecule 49: 30S ribosomal protein S19



- Molecule 49: 30S ribosomal protein S19

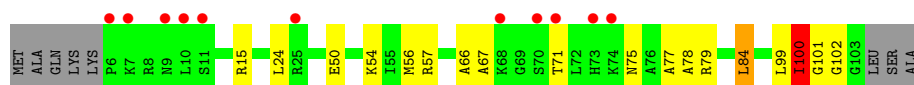
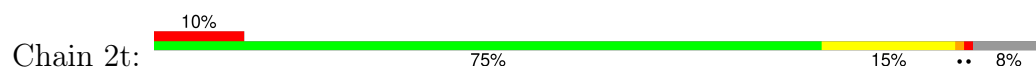


- Molecule 50: 30S ribosomal protein S20

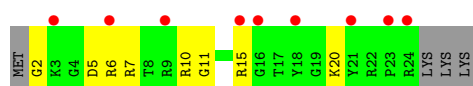




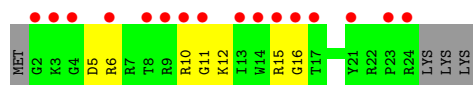
- Molecule 50: 30S ribosomal protein S20



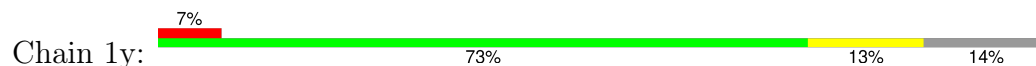
- Molecule 51: 30S ribosomal protein Thx



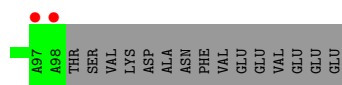
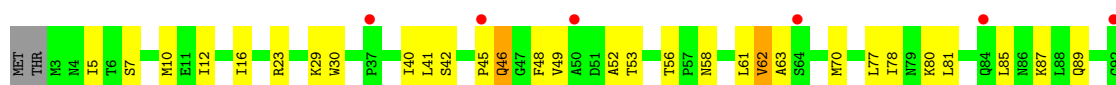
- Molecule 51: 30S ribosomal protein Thx



- Molecule 52: Ribosome-associated inhibitor A



- Molecule 52: 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	210.81Å 450.83Å 621.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 3.25 49.93 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.93-3.25) 99.9 (49.93-3.25)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.25Å)	Xtriage
Refinement program	PHENIX dev_2747	Depositor
R, R_{free}	0.226 , 0.270 0.225 , 0.268	Depositor DCC
R_{free} test set	46130 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	290709	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: MG, 2MG, OMG, 0TD, OMC, G7M, MPD, M2G, 5MC, 4OC, MA6, 2MA, ZN, SF4, 5MU, UR3, OMU, 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	0.17	0/68792	0.31	2/107386 (0.0%)
1	2A	0.14	0/68686	0.28	0/107216
2	1B	0.15	0/2837	0.29	0/4426
2	2B	0.13	0/2837	0.28	0/4426
3	1D	0.18	0/2181	0.40	0/2940
3	2D	0.16	0/2186	0.37	0/2944
4	1E	0.18	0/1592	0.38	0/2149
4	2E	0.15	0/1592	0.36	0/2149
5	1F	0.17	0/1621	0.36	0/2196
5	2F	0.14	0/1617	0.36	0/2191
6	1G	0.15	0/1452	0.39	1/1962 (0.1%)
6	2G	0.12	0/1450	0.31	0/1958
7	1H	0.16	0/1356	0.33	0/1834
7	2H	0.12	0/1350	0.30	0/1826
8	1I	0.14	0/1110	0.33	0/1513
8	2I	0.12	0/1092	0.28	0/1491
9	1N	0.17	0/1148	0.35	0/1547
9	2N	0.13	0/1144	0.31	0/1543
10	1O	0.17	0/942	0.35	0/1268
10	2O	0.14	0/942	0.34	0/1268
11	1P	0.18	0/1152	0.39	0/1533
11	2P	0.15	0/1152	0.37	0/1533
12	1Q	0.17	0/1142	0.37	0/1525
12	2Q	0.14	0/1142	0.32	0/1525
13	1R	0.19	0/982	0.42	0/1312
13	2R	0.15	0/982	0.35	0/1312
14	1S	0.17	0/887	0.39	0/1180
14	2S	0.13	0/880	0.33	0/1172
15	1T	0.17	0/1105	0.39	0/1476
15	2T	0.15	0/1097	0.35	0/1467
16	1U	0.20	0/977	0.39	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.14	0/977	0.32	0/1301
17	1V	0.18	0/786	0.37	0/1053
17	2V	0.13	0/782	0.32	0/1049
18	1W	0.19	0/897	0.38	0/1205
18	2W	0.14	0/897	0.34	0/1205
19	1X	0.17	0/764	0.38	0/1025
19	2X	0.13	0/764	0.33	0/1025
20	1Y	0.16	0/823	0.38	0/1099
20	2Y	0.13	0/823	0.32	0/1100
21	1Z	0.15	0/1620	0.35	0/2200
21	2Z	0.13	0/1590	0.31	0/2162
22	10	0.17	0/614	0.40	0/818
22	20	0.14	0/614	0.35	0/818
23	11	0.18	0/763	0.35	0/1016
23	21	0.15	0/768	0.31	0/1021
24	12	0.17	0/590	0.36	0/781
24	22	0.14	0/594	0.29	0/785
25	13	0.17	0/474	0.37	0/635
25	23	0.12	0/469	0.30	0/630
26	14	0.15	0/559	0.50	0/754
26	24	0.18	0/549	0.48	0/741
27	15	0.18	0/474	0.39	0/640
27	25	0.15	0/470	0.32	0/636
28	16	0.17	0/460	0.39	0/613
28	26	0.15	0/456	0.35	0/608
29	17	0.20	0/426	0.41	0/561
29	27	0.16	0/426	0.38	0/561
30	18	0.18	0/525	0.34	0/691
30	28	0.15	0/525	0.34	0/691
31	19	0.19	0/310	0.41	0/407
31	29	0.14	0/310	0.32	0/407
32	1a	0.14	0/35799	0.29	0/55871
32	2a	0.14	1/35894 (0.0%)	0.31	0/56019
33	1b	0.13	0/1876	0.34	0/2533
33	2b	0.14	0/1860	0.35	0/2518
34	1c	0.12	0/1582	0.30	0/2137
34	2c	0.12	0/1566	0.30	0/2119
35	1d	0.14	0/1695	0.34	0/2274
35	2d	0.14	0/1698	0.33	0/2277
36	1e	0.14	0/1149	0.35	0/1548
36	2e	0.13	0/1149	0.34	0/1548
37	1f	0.13	0/827	0.29	0/1120
37	2f	0.12	0/829	0.29	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.12	0/1254	0.30	0/1683
38	2g	0.12	0/1248	0.30	0/1676
39	1h	0.14	0/1118	0.33	0/1506
39	2h	0.12	0/1108	0.31	0/1494
40	1i	0.13	0/1005	0.33	0/1350
40	2i	0.13	0/985	0.33	0/1328
41	1j	0.13	0/732	0.32	0/993
41	2j	0.13	0/723	0.33	0/984
42	1k	0.14	0/849	0.31	0/1150
42	2k	0.13	0/848	0.34	0/1149
43	1l	0.14	0/937	0.33	0/1260
43	2l	0.14	0/937	0.37	0/1260
44	1m	0.13	0/924	0.36	0/1242
44	2m	0.13	0/905	0.32	0/1217
45	1n	0.13	0/501	0.34	0/664
45	2n	0.12	0/501	0.33	0/664
46	1o	0.13	0/739	0.32	0/985
46	2o	0.12	0/739	0.31	0/985
47	1p	0.13	0/697	0.35	0/939
47	2p	0.13	0/693	0.34	0/935
48	1r	0.14	0/560	0.35	0/746
48	2r	0.12	0/560	0.29	0/746
49	1s	0.11	0/663	0.31	0/895
49	2s	0.11	0/660	0.29	0/893
50	1t	0.14	0/733	0.36	0/968
50	2t	0.14	0/735	0.33	0/975
51	1u	0.13	0/203	0.35	0/266
51	2u	0.14	0/203	0.38	0/266
52	1y	0.12	0/776	0.29	0/1048
52	2y	0.11	0/761	0.28	0/1030
All	All	0.15	1/307745 (0.0%)	0.31	3/460191 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	527	G7M	O3'-P	5.13	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2552	OMU	O3'-P-O5'	9.99	122.97	104.00
6	1G	96	ARG	CB-CA-C	-5.77	109.94	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2552	OMU	P-O3'-C3'	-5.25	113.41	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61654	0	31088	554	0
1	2A	61564	0	31051	641	0
2	1B	2536	0	1284	14	0
2	2B	2536	0	1284	32	0
3	1D	2131	0	2207	56	0
3	2D	2136	0	2218	45	0
4	1E	1559	0	1618	30	0
4	2E	1559	0	1618	29	0
5	1F	1586	0	1631	30	0
5	2F	1582	0	1626	35	0
6	1G	1427	0	1447	28	0
6	2G	1425	0	1443	25	0
7	1H	1330	0	1407	27	0
7	2H	1324	0	1402	19	0
8	1I	1095	0	1129	14	0
8	2I	1077	0	1096	12	0
9	1N	1121	0	1195	17	0
9	2N	1117	0	1184	16	0
10	1O	932	0	994	21	0
10	2O	932	0	994	20	0
11	1P	1135	0	1212	13	0
11	2P	1135	0	1212	20	0
12	1Q	1121	0	1179	24	0
12	2Q	1121	0	1179	31	0
13	1R	968	0	1033	15	0
13	2R	968	0	1033	19	0
14	1S	877	0	938	16	0
14	2S	870	0	923	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	1T	1091	0	1156	23	0
15	2T	1083	0	1141	14	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	22	0
17	1V	775	0	840	8	0
17	2V	771	0	830	12	0
18	1W	886	0	940	20	0
18	2W	886	0	939	18	0
19	1X	750	0	814	15	0
19	2X	750	0	814	11	0
20	1Y	810	0	893	16	0
20	2Y	810	0	888	18	0
21	1Z	1587	0	1598	26	0
21	2Z	1557	0	1564	24	0
22	10	606	0	622	10	0
22	20	606	0	622	11	0
23	11	756	0	823	9	0
23	21	761	0	837	23	0
24	12	588	0	643	8	0
24	22	592	0	654	12	0
25	13	469	0	518	13	0
25	23	464	0	514	7	0
26	14	546	0	523	14	0
26	24	536	0	518	19	0
27	15	460	0	480	10	0
27	25	456	0	469	8	0
28	16	453	0	473	10	0
28	26	449	0	469	6	0
29	17	418	0	467	6	0
29	27	418	0	467	10	0
30	18	517	0	582	9	0
30	28	517	0	582	15	0
31	19	307	0	335	7	0
31	29	307	0	336	8	0
32	1a	32249	0	16293	389	0
32	2a	32334	0	16338	502	0
33	1b	1842	0	1862	39	0
33	2b	1825	0	1828	29	0
34	1c	1558	0	1557	19	0
34	2c	1542	0	1517	21	0
35	1d	1665	0	1691	29	0
35	2d	1668	0	1707	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	1e	1133	0	1191	20	0
36	2e	1133	0	1191	23	0
37	1f	814	0	808	14	0
37	2f	816	0	808	17	0
38	1g	1235	0	1249	17	0
38	2g	1229	0	1238	18	0
39	1h	1098	0	1143	24	0
39	2h	1088	0	1126	18	0
40	1i	987	0	996	19	0
40	2i	967	0	959	20	0
41	1j	719	0	672	13	0
41	2j	710	0	661	17	0
42	1k	834	0	838	9	0
42	2k	833	0	836	13	0
43	1l	932	0	981	17	0
43	2l	932	0	981	13	0
44	1m	914	0	954	22	0
44	2m	895	0	920	21	0
45	1n	492	0	529	11	0
45	2n	492	0	529	10	0
46	1o	728	0	760	13	0
46	2o	728	0	760	7	0
47	1p	681	0	697	16	0
47	2p	677	0	686	16	0
48	1r	555	0	618	7	0
48	2r	555	0	618	8	0
49	1s	648	0	658	12	0
49	2s	645	0	635	13	0
50	1t	731	0	807	11	0
50	2t	732	0	793	13	0
51	1u	199	0	208	6	0
51	2u	199	0	208	5	0
52	1y	764	0	785	8	0
52	2y	749	0	757	19	0
53	18	8	0	14	1	0
53	1A	8	0	14	0	0
53	1T	8	0	14	0	0
53	1a	8	0	14	1	0
53	2A	16	0	28	1	0
53	2B	8	0	14	2	0
54	10	6	0	0	0	0
54	11	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	13	2	0	0	0	0
54	15	3	0	0	0	0
54	16	1	0	0	0	0
54	17	3	0	0	0	0
54	19	2	0	0	0	0
54	1A	900	0	0	0	0
54	1B	29	0	0	0	0
54	1D	12	0	0	0	0
54	1E	5	0	0	0	0
54	1F	12	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	3	0	0	0	0
54	1O	1	0	0	0	0
54	1P	5	0	0	0	0
54	1Q	3	0	0	0	0
54	1R	7	0	0	0	0
54	1T	5	0	0	0	0
54	1U	3	0	0	0	0
54	1V	3	0	0	0	0
54	1W	4	0	0	0	0
54	1X	2	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	257	0	0	0	0
54	1b	1	0	0	0	0
54	1d	6	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
54	1h	1	0	0	0	0
54	1l	2	0	0	0	0
54	1n	2	0	0	0	0
54	1o	1	0	0	0	0
54	1t	2	0	0	0	0
54	1y	4	0	0	0	0
54	20	1	0	0	0	0
54	21	4	0	0	0	0
54	23	1	0	0	0	0
54	28	1	0	0	0	0
54	2A	641	0	0	0	0
54	2B	16	0	0	0	0
54	2D	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2E	2	0	0	0	0
54	2F	2	0	0	0	0
54	2G	3	0	0	0	0
54	2I	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	3	0	0	0	0
54	2T	5	0	0	0	0
54	2V	1	0	0	0	0
54	2W	2	0	0	0	0
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	164	0	0	0	0
54	2e	1	0	0	0	0
54	2f	1	0	0	0	0
54	2i	1	0	0	0	0
54	2j	1	0	0	0	0
54	2k	1	0	0	0	0
54	2l	2	0	0	0	0
54	2p	1	0	0	0	0
54	2t	1	0	0	0	0
55	1B	12	0	12	0	0
55	1F	12	0	12	1	0
56	14	1	0	0	0	0
56	15	1	0	0	0	0
56	16	1	0	0	0	0
56	19	1	0	0	0	0
56	1Y	1	0	0	0	0
56	1n	1	0	0	0	0
56	24	1	0	0	0	0
56	25	1	0	0	0	0
56	26	1	0	0	0	0
56	29	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2n	1	0	0	0	0
57	1d	8	0	0	0	0
57	2d	8	0	0	0	0
58	10	5	0	0	0	0
58	11	3	0	0	0	0
58	13	6	0	0	1	0
58	15	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	16	2	0	0	0	0
58	17	1	0	0	0	0
58	18	7	0	0	0	0
58	19	3	0	0	0	0
58	1A	1801	0	0	105	0
58	1B	56	0	0	3	0
58	1D	14	0	0	0	0
58	1E	17	0	0	0	0
58	1F	16	0	0	0	0
58	1G	5	0	0	0	0
58	1H	5	0	0	0	0
58	1N	7	0	0	0	0
58	1O	2	0	0	0	0
58	1P	17	0	0	0	0
58	1Q	5	0	0	0	0
58	1R	5	0	0	0	0
58	1T	8	0	0	0	0
58	1U	6	0	0	0	0
58	1V	5	0	0	0	0
58	1W	2	0	0	0	0
58	1X	6	0	0	0	0
58	1Y	1	0	0	0	0
58	1Z	1	0	0	0	0
58	1a	424	0	0	19	0
58	1c	1	0	0	0	0
58	1d	8	0	0	0	0
58	1e	4	0	0	0	0
58	1f	1	0	0	0	0
58	1h	1	0	0	0	0
58	1j	1	0	0	0	0
58	1l	3	0	0	0	0
58	1m	1	0	0	0	0
58	1o	3	0	0	0	0
58	1p	1	0	0	0	0
58	1t	2	0	0	0	0
58	1y	3	0	0	0	0
58	20	2	0	0	0	0
58	21	1	0	0	0	0
58	23	2	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	27	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	28	5	0	0	0	0
58	2A	1310	0	0	106	0
58	2B	32	0	0	3	0
58	2D	16	0	0	1	0
58	2E	10	0	0	0	0
58	2F	6	0	0	1	0
58	2G	1	0	0	0	0
58	2N	1	0	0	0	0
58	2O	3	0	0	0	0
58	2P	14	0	0	1	0
58	2Q	5	0	0	0	0
58	2R	1	0	0	0	0
58	2T	4	0	0	0	0
58	2V	2	0	0	0	0
58	2W	3	0	0	0	0
58	2X	4	0	0	1	0
58	2Y	1	0	0	0	0
58	2a	282	0	0	17	0
58	2e	1	0	0	0	0
58	2j	2	0	0	1	0
58	2l	1	0	0	0	0
58	2t	2	0	0	0	0
58	2y	3	0	0	0	0
All	All	290709	0	192529	3328	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 3328 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:2552:OMU:C4'	1:1A:2552:OMU:O4'	1.67	1.18
1:2A:2552:OMU:O4'	1:2A:2552:OMU:C4'	1.67	1.18
1:2A:2131:G:H5''	1:2A:2132:U:H5'	1.53	0.91
1:2A:1920:OMC:HM21	32:2a:1496:C:H4'	1.52	0.91
32:1a:1051:C:N3	32:1a:1207:2MG:N1	2.20	0.88

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24	55
4	2E	202/206 (98%)	187 (93%)	13 (6%)	2 (1%)	12	40
5	1F	201/210 (96%)	193 (96%)	8 (4%)	0	100	100
5	2F	201/210 (96%)	189 (94%)	12 (6%)	0	100	100
6	1G	179/182 (98%)	164 (92%)	13 (7%)	2 (1%)	11	38
6	2G	179/182 (98%)	162 (90%)	15 (8%)	2 (1%)	11	38
7	1H	172/180 (96%)	161 (94%)	7 (4%)	4 (2%)	5	24
7	2H	171/180 (95%)	156 (91%)	13 (8%)	2 (1%)	10	36
8	1I	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
8	2I	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	18	48
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
10	1O	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	48
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	18	48
13	1R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	6	28
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	115 (89%)	12 (9%)	2 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	40
17	2V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6	26
18	1W	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
18	2W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
19	1X	93/96 (97%)	87 (94%)	4 (4%)	2 (2%)	5	25
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	38
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	201/206 (98%)	191 (95%)	9 (4%)	1 (0%)	24	55
21	2Z	199/206 (97%)	187 (94%)	11 (6%)	1 (0%)	24	55
22	10	75/85 (88%)	71 (95%)	3 (4%)	1 (1%)	9	34
22	20	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	38
24	12	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	8
26	24	67/71 (94%)	52 (78%)	13 (19%)	2 (3%)	3	19
27	15	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
27	25	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	199 (87%)	22 (10%)	8 (4%)	3	17
33	2b	229/256 (90%)	203 (89%)	22 (10%)	4 (2%)	7	29
34	1c	204/239 (85%)	190 (93%)	13 (6%)	1 (0%)	24	55
34	2c	204/239 (85%)	192 (94%)	11 (5%)	1 (0%)	24	55
35	1d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	24	55
35	2d	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
36	1e	146/162 (90%)	137 (94%)	9 (6%)	0	100	100
36	2e	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
38	2g	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
40	1i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
40	2i	124/128 (97%)	111 (90%)	12 (10%)	1 (1%)	16	44
41	1j	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	3	18
41	2j	94/105 (90%)	85 (90%)	4 (4%)	5 (5%)	1	9
42	1k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	14	42
42	2k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	14	42
43	1l	119/135 (88%)	111 (93%)	8 (7%)	0	100	100
43	2l	119/135 (88%)	109 (92%)	10 (8%)	0	100	100
44	1m	114/126 (90%)	106 (93%)	7 (6%)	1 (1%)	14	42
44	2m	112/126 (89%)	106 (95%)	5 (4%)	1 (1%)	14	42
45	1n	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	36
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	34
48	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
48	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	1s	81/93 (87%)	74 (91%)	5 (6%)	2 (2%)	4	22
49	2s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
50	1t	94/106 (89%)	91 (97%)	2 (2%)	1 (1%)	11	38
50	2t	96/106 (91%)	90 (94%)	4 (4%)	2 (2%)	5	25
51	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
51	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	1y	95/113 (84%)	92 (97%)	3 (3%)	0	100	100
52	2y	94/113 (83%)	91 (97%)	2 (2%)	1 (1%)	11	38
All	All	11435/12150 (94%)	10717 (94%)	646 (6%)	72 (1%)	21	51

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	10	13	GLY
26	14	55	ARG
33	1b	125	PRO
41	1j	77	PRO
33	2b	17	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	197 (92%)	17 (8%)	11	35
3	2D	215/218 (99%)	204 (95%)	11 (5%)	21	49
4	1E	164/166 (99%)	149 (91%)	15 (9%)	9	30
4	2E	164/166 (99%)	152 (93%)	12 (7%)	13	38
5	1F	161/166 (97%)	152 (94%)	9 (6%)	19	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	160/166 (96%)	152 (95%)	8 (5%)	22	49
6	1G	144/156 (92%)	139 (96%)	5 (4%)	32	56
6	2G	142/156 (91%)	136 (96%)	6 (4%)	26	53
7	1H	144/148 (97%)	142 (99%)	2 (1%)	59	72
7	2H	143/148 (97%)	139 (97%)	4 (3%)	38	60
8	1I	111/124 (90%)	104 (94%)	7 (6%)	16	43
8	2I	108/124 (87%)	104 (96%)	4 (4%)	30	55
9	1N	119/119 (100%)	112 (94%)	7 (6%)	18	45
9	2N	118/119 (99%)	107 (91%)	11 (9%)	8	29
10	1O	100/100 (100%)	99 (99%)	1 (1%)	68	75
10	2O	100/100 (100%)	98 (98%)	2 (2%)	48	66
11	1P	115/116 (99%)	111 (96%)	4 (4%)	32	56
11	2P	115/116 (99%)	111 (96%)	4 (4%)	32	56
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	24	52
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	51	69
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	30
13	2R	101/101 (100%)	94 (93%)	7 (7%)	14	41
14	1S	87/88 (99%)	85 (98%)	2 (2%)	44	65
14	2S	85/88 (97%)	85 (100%)	0	100	100
15	1T	115/128 (90%)	114 (99%)	1 (1%)	70	76
15	2T	113/128 (88%)	109 (96%)	4 (4%)	32	56
16	1U	93/94 (99%)	86 (92%)	7 (8%)	12	37
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20	47
17	1V	81/82 (99%)	76 (94%)	5 (6%)	16	43
17	2V	80/82 (98%)	77 (96%)	3 (4%)	29	55
18	1W	90/92 (98%)	82 (91%)	8 (9%)	9	30
18	2W	90/92 (98%)	89 (99%)	1 (1%)	65	75
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	62
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	62
20	1Y	86/91 (94%)	83 (96%)	3 (4%)	32	56
20	2Y	86/91 (94%)	85 (99%)	1 (1%)	63	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	169/179 (94%)	164 (97%)	5 (3%)	36	59
21	2Z	165/179 (92%)	160 (97%)	5 (3%)	36	59
22	10	61/67 (91%)	59 (97%)	2 (3%)	33	57
22	20	61/67 (91%)	59 (97%)	2 (3%)	33	57
23	11	79/83 (95%)	79 (100%)	0	100	100
23	21	81/83 (98%)	80 (99%)	1 (1%)	63	74
24	12	65/67 (97%)	62 (95%)	3 (5%)	24	51
24	22	66/67 (98%)	63 (96%)	3 (4%)	24	52
25	13	51/52 (98%)	48 (94%)	3 (6%)	18	45
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	44
26	14	58/63 (92%)	53 (91%)	5 (9%)	10	32
26	24	54/63 (86%)	51 (94%)	3 (6%)	19	46
27	15	51/52 (98%)	47 (92%)	4 (8%)	11	36
27	25	50/52 (96%)	49 (98%)	1 (2%)	48	66
28	16	51/52 (98%)	49 (96%)	2 (4%)	28	54
28	26	50/52 (96%)	47 (94%)	3 (6%)	17	44
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	50
29	27	41/42 (98%)	39 (95%)	2 (5%)	22	50
30	18	54/55 (98%)	54 (100%)	0	100	100
30	28	54/55 (98%)	53 (98%)	1 (2%)	50	67
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	60
33	1b	191/220 (87%)	184 (96%)	7 (4%)	30	55
33	2b	187/220 (85%)	178 (95%)	9 (5%)	23	50
34	1c	144/188 (77%)	142 (99%)	2 (1%)	59	72
34	2c	140/188 (74%)	136 (97%)	4 (3%)	37	60
35	1d	171/181 (94%)	166 (97%)	5 (3%)	37	60
35	2d	172/181 (95%)	166 (96%)	6 (4%)	32	56
36	1e	114/123 (93%)	112 (98%)	2 (2%)	51	69
36	2e	114/123 (93%)	109 (96%)	5 (4%)	25	52
37	1f	85/90 (94%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	83 (98%)	2 (2%)	43	64
38	1g	120/127 (94%)	117 (98%)	3 (2%)	42	63
38	2g	119/127 (94%)	117 (98%)	2 (2%)	53	69
39	1h	116/119 (98%)	111 (96%)	5 (4%)	26	52
39	2h	114/119 (96%)	109 (96%)	5 (4%)	25	52
40	1i	91/99 (92%)	89 (98%)	2 (2%)	45	65
40	2i	88/99 (89%)	85 (97%)	3 (3%)	32	57
41	1j	68/92 (74%)	67 (98%)	1 (2%)	57	71
41	2j	68/92 (74%)	67 (98%)	1 (2%)	57	71
42	1k	83/99 (84%)	81 (98%)	2 (2%)	43	64
42	2k	83/99 (84%)	81 (98%)	2 (2%)	43	64
43	1l	96/110 (87%)	93 (97%)	3 (3%)	35	59
43	2l	96/110 (87%)	91 (95%)	5 (5%)	21	48
44	1m	90/101 (89%)	88 (98%)	2 (2%)	45	65
44	2m	87/101 (86%)	85 (98%)	2 (2%)	44	65
45	1n	49/50 (98%)	47 (96%)	2 (4%)	27	53
45	2n	49/50 (98%)	48 (98%)	1 (2%)	48	66
46	1o	78/80 (98%)	75 (96%)	3 (4%)	29	55
46	2o	78/80 (98%)	76 (97%)	2 (3%)	40	62
47	1p	69/74 (93%)	64 (93%)	5 (7%)	13	39
47	2p	68/74 (92%)	64 (94%)	4 (6%)	18	45
48	1r	59/77 (77%)	58 (98%)	1 (2%)	53	69
48	2r	59/77 (77%)	58 (98%)	1 (2%)	53	69
49	1s	68/80 (85%)	66 (97%)	2 (3%)	37	60
49	2s	67/80 (84%)	67 (100%)	0	100	100
50	1t	71/82 (87%)	69 (97%)	2 (3%)	38	60
50	2t	70/82 (85%)	67 (96%)	3 (4%)	26	52
51	1u	18/22 (82%)	18 (100%)	0	100	100
51	2u	18/22 (82%)	18 (100%)	0	100	100
52	1y	82/98 (84%)	81 (99%)	1 (1%)	63	74
52	2y	79/98 (81%)	74 (94%)	5 (6%)	16	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9338/10072 (93%)	8979 (96%)	359 (4%)	29 55

5 of 359 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	2N	28	THR
26	24	36	CYS
9	2N	73	THR
16	2U	8	VAL
33	2b	127	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
4	2E	180	ASN
15	2T	58	ASN
45	2n	52	GLN
4	2E	192	ASN
10	2O	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2857/2894 (98%)	391 (13%)	17 (0%)
1	2A	2850/2894 (98%)	429 (15%)	25 (0%)
2	1B	117/120 (97%)	8 (6%)	0
2	2B	117/120 (97%)	10 (8%)	0
32	1a	1497/1522 (98%)	215 (14%)	0
32	2a	1501/1522 (98%)	224 (14%)	0
All	All	8939/9072 (98%)	1277 (14%)	42 (0%)

5 of 1277 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	63	U
1	1A	71	A

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1067	A
1	2A	2126	A
1	2A	1073	A
1	2A	1491	G
1	2A	2172	U

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

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	967	32	19,22,23	2.20	6 (31%)	26,32,35	1.32	2 (7%)
1	PSU	2A	1911	1	18,21,22	2.04	7 (38%)	21,30,33	1.80	5 (23%)
1	OMG	1A	2251	1	23,26,27	1.60	4 (17%)	32,38,41	2.00	9 (28%)
32	G7M	1a	527	32,54	23,26,27	1.57	4 (17%)	34,39,42	1.50	6 (17%)
32	MA6	1a	1519	32	23,26,27	1.51	6 (26%)	33,38,41	2.19	10 (30%)
32	5MC	2a	967	32	19,22,23	2.19	6 (31%)	26,32,35	1.13	2 (7%)
32	M2G	2a	966	32,54	24,27,28	1.62	4 (16%)	33,40,43	1.82	8 (24%)
32	2MG	1a	1207	32,54	23,26,27	1.62	3 (13%)	33,38,41	2.09	7 (21%)
32	UR3	1a	1498	32	19,22,23	1.79	5 (26%)	26,32,35	1.25	2 (7%)
1	5MU	2A	1939	1,54	19,22,23	2.06	8 (42%)	27,32,35	2.26	6 (22%)
1	2MA	1A	2503	1,54	22,25,26	1.08	2 (9%)	32,37,40	2.23	7 (21%)
1	5MC	2A	1942	1	19,22,23	2.14	6 (31%)	26,32,35	1.14	1 (3%)
1	OMG	2A	2251	1,54	23,26,27	1.61	5 (21%)	32,38,41	1.88	6 (18%)
32	5MC	1a	1400	32	19,22,23	2.17	6 (31%)	26,32,35	1.10	2 (7%)
1	OMU	2A	2552	1,54	19,22,23	3.94	11 (57%)	25,31,34	1.92	6 (24%)
1	5MU	2A	1915	1	19,22,23	1.98	7 (36%)	27,32,35	2.31	8 (29%)
32	5MC	2a	1400	32	19,22,23	2.22	6 (31%)	26,32,35	1.07	1 (3%)
32	4OC	2a	1402	32	20,23,24	1.61	4 (20%)	25,32,35	0.93	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MA	2A	2503	1,54	22,25,26	1.09	2 (9%)	32,37,40	2.06	8 (25%)
1	5MC	1A	1962	1,54	19,22,23	2.18	6 (31%)	26,32,35	1.13	1 (3%)
32	MA6	1a	1518	32	23,26,27	1.52	7 (30%)	33,38,41	2.14	10 (30%)
32	4OC	1a	1402	32	20,23,24	1.62	4 (20%)	25,32,35	0.96	1 (4%)
1	PSU	1A	2605	1	18,21,22	2.04	8 (44%)	21,30,33	2.11	4 (19%)
1	5MC	1A	1942	1	19,22,23	2.18	6 (31%)	26,32,35	1.11	2 (7%)
1	OMU	1A	2552	1,54	19,22,23	3.98	11 (57%)	25,31,34	2.01	7 (28%)
32	5MC	2a	1404	32	19,22,23	2.16	6 (31%)	26,32,35	1.06	2 (7%)
1	PSU	2A	1917	1	18,21,22	2.02	8 (44%)	21,30,33	2.10	3 (14%)
1	5MU	1A	1915	1,54	19,22,23	2.00	7 (36%)	27,32,35	2.37	10 (37%)
1	5MC	2A	1962	1,54	19,22,23	2.16	6 (31%)	26,32,35	1.04	1 (3%)
43	0TD	1l	92	43	8,9,10	1.50	0	6,11,13	1.48	1 (16%)
32	5MC	2a	1407	32	19,22,23	2.24	5 (26%)	26,32,35	1.23	2 (7%)
32	5MC	1a	1404	32	19,22,23	2.16	6 (31%)	26,32,35	1.04	1 (3%)
32	UR3	2a	1498	32,54	19,22,23	1.75	5 (26%)	26,32,35	1.24	4 (15%)
32	M2G	1a	966	32	24,27,28	1.62	4 (16%)	33,40,43	1.79	8 (24%)
32	G7M	2a	527	32,54	23,26,27	1.58	5 (21%)	34,39,42	1.54	6 (17%)
32	5MC	1a	1407	32	19,22,23	2.13	6 (31%)	26,32,35	1.16	2 (7%)
32	PSU	1a	516	32	18,21,22	2.10	9 (50%)	21,30,33	2.12	4 (19%)
32	PSU	2a	516	32,54	18,21,22	2.02	9 (50%)	21,30,33	2.15	5 (23%)
1	OMC	2A	1920	1	19,22,23	1.75	5 (26%)	25,31,34	0.99	2 (8%)
1	PSU	1A	1917	1	18,21,22	2.11	8 (44%)	21,30,33	2.23	5 (23%)
1	PSU	1A	1911	1	18,21,22	1.93	6 (33%)	21,30,33	1.69	4 (19%)
32	MA6	2a	1518	32	23,26,27	1.59	8 (34%)	33,38,41	2.16	10 (30%)
32	MA6	2a	1519	32	23,26,27	1.53	7 (30%)	33,38,41	2.26	11 (33%)
32	2MG	2a	1207	32	23,26,27	1.65	5 (21%)	33,38,41	2.23	10 (30%)
1	PSU	2A	2605	1	18,21,22	1.99	8 (44%)	21,30,33	2.08	4 (19%)
1	OMC	1A	1920	1,54	19,22,23	1.75	4 (21%)	25,31,34	1.12	4 (16%)
43	0TD	2l	92	43	8,9,10	1.67	1 (12%)	6,11,13	2.30	2 (33%)
1	5MU	1A	1939	1,54	19,22,23	2.09	8 (42%)	27,32,35	2.53	7 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1	-	1/9/27/28	0/3/3/3
32	G7M	1a	527	32,54	-	3/7/25/26	0/3/3/3
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
32	M2G	2a	966	32,54	-	6/11/29/30	0/3/3/3
32	2MG	1a	1207	32,54	-	3/9/27/28	0/3/3/3
32	UR3	1a	1498	32	-	2/7/25/26	0/2/2/2
1	5MU	2A	1939	1,54	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,54	-	0/7/25/26	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	3/9/27/28	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	OMU	2A	2552	1,54	-	0/9/27/28	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
1	2MA	2A	2503	1,54	-	0/7/25/26	0/3/3/3
1	5MC	1A	1962	1,54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,54	-	0/9/27/28	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1,54	-	2/7/25/26	0/2/2/2
1	5MC	2A	1962	1,54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	5MC	2a	1407	32	-	2/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32,54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	G7M	2a	527	32,54	-	2/7/25/26	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/11/29/30	0/3/3/3
32	MA6	2a	1519	32	-	6/11/29/30	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1,54	-	1/9/27/28	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	5MU	1A	1939	1,54	-	2/7/25/26	0/2/2/2

The worst 5 of 280 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	O4'-C4'	10.19	1.67	1.45
1	2A	2552	OMU	O4'-C4'	10.14	1.67	1.45
1	1A	2552	OMU	C3'-C4'	-9.74	1.28	1.53
1	2A	2552	OMU	C3'-C4'	-9.61	1.28	1.53
32	2a	966	M2G	C2-N2	6.11	1.46	1.35

The worst 5 of 231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	2MA	C5-C4-N3	-7.74	119.03	127.18
32	2a	1207	2MG	C2-N3-C4	7.16	120.96	112.00
1	2A	2503	2MA	C5-C4-N3	-7.12	119.68	127.18
32	1a	1207	2MG	C2-N3-C4	6.84	120.56	112.00
1	1A	1917	PSU	N1-C2-N3	6.35	121.87	115.17

There are no chirality outliers.

5 of 56 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
1	1A	1939	5MU	C3'-C4'-C5'-O5'
1	1A	1939	5MU	O4'-C4'-C5'-O5'
1	1A	2251	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

29 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	967	5MC	2	0
1	2A	1911	PSU	2	0
32	1a	1519	MA6	1	0
32	2a	967	5MC	3	0
32	2a	966	M2G	1	0
32	1a	1207	2MG	3	0
32	1a	1498	UR3	3	0
1	2A	1939	5MU	1	0
1	1A	2503	2MA	3	0
1	2A	2251	OMG	1	0
32	1a	1400	5MC	1	0
1	2A	2552	OMU	3	0
1	2A	1915	5MU	1	0
32	2a	1400	5MC	2	0
1	2A	2503	2MA	1	0
32	1a	1518	MA6	2	0
1	1A	2552	OMU	2	0
32	2a	1404	5MC	3	0
1	2A	1917	PSU	1	0
1	2A	1962	5MC	1	0
32	1a	966	M2G	1	0
32	1a	516	PSU	1	0
1	2A	1920	OMC	3	0
1	1A	1911	PSU	3	0
32	2a	1518	MA6	1	0
32	2a	1519	MA6	1	0
32	2a	1207	2MG	2	0
1	1A	1920	OMC	1	0
1	1A	1939	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2199 ligands modelled in this entry, 2188 are monoatomic - leaving 11 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	ARG	1B	1001	-	10,11,11	0.74	1 (10%)	9,13,13	1.06	1 (11%)
53	MPD	2A	3002	-	7,7,7	0.31	0	9,10,10	0.17	0
53	MPD	1T	2001	-	7,7,7	0.31	0	9,10,10	0.29	0
55	ARG	1F	303	-	10,11,11	0.74	1 (10%)	9,13,13	1.03	1 (11%)
53	MPD	1a	1601	-	7,7,7	0.33	0	9,10,10	0.36	0
53	MPD	1A	3001	-	7,7,7	0.31	0	9,10,10	0.22	0
53	MPD	2A	3001	-	7,7,7	0.34	0	9,10,10	0.33	0
53	MPD	2B	201	-	7,7,7	0.29	0	9,10,10	0.15	0
57	SF4	2d	501	-	0,12,12	-	-	-	-	-
57	SF4	1d	501	-	0,12,12	-	-	-	-	-
53	MPD	18	101	-	7,7,7	0.31	0	9,10,10	0.35	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	ARG	1B	1001	-	-	1/11/11/11	-
53	MPD	2A	3002	-	-	4/5/5/5	-
53	MPD	1T	2001	-	-	0/5/5/5	-
55	ARG	1F	303	-	-	2/11/11/11	-
53	MPD	1a	1601	-	-	1/5/5/5	-
53	MPD	1A	3001	-	-	1/5/5/5	-
53	MPD	2A	3001	-	-	2/5/5/5	-
53	MPD	2B	201	-	-	5/5/5/5	-
57	SF4	2d	501	-	-	-	0/6/5/5
57	SF4	1d	501	-	-	-	0/6/5/5
53	MPD	18	101	-	-	3/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1F	303	ARG	OXT-C	-2.19	1.23	1.30
55	1B	1001	ARG	OXT-C	-2.13	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1B	1001	ARG	OXT-C-O	-3.12	117.00	124.08
55	1F	303	ARG	OXT-C-O	-2.98	117.31	124.08

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1B	1001	ARG	NE-CD-CG-CB
55	1F	303	ARG	O-C-CA-N
53	1a	1601	MPD	C2-C3-C4-O4
53	2B	201	MPD	C2-C3-C4-O4
53	18	101	MPD	C1-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1F	303	ARG	1	0
53	1a	1601	MPD	1	0
53	2A	3001	MPD	1	0
53	2B	201	MPD	2	0
53	18	101	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2851/2894 (98%)	-0.51	31 (1%) 78 60	26, 52, 150, 184	0
1	2A	2847/2894 (98%)	-0.25	41 (1%) 73 54	46, 77, 156, 186	0
2	1B	118/120 (98%)	-0.47	0 100 100	45, 72, 90, 110	0
2	2B	118/120 (98%)	0.34	1 (0%) 82 68	86, 116, 133, 144	0
3	1D	275/276 (99%)	-0.13	2 (0%) 84 70	29, 47, 64, 93	0
3	2D	275/276 (99%)	0.06	1 (0%) 88 78	43, 67, 83, 106	0
4	1E	204/206 (99%)	-0.07	0 100 100	29, 58, 79, 112	0
4	2E	204/206 (99%)	0.12	3 (1%) 72 53	45, 73, 98, 109	0
5	1F	203/210 (96%)	-0.15	0 100 100	27, 55, 90, 120	0
5	2F	203/210 (96%)	0.18	1 (0%) 87 76	44, 89, 109, 129	0
6	1G	181/182 (99%)	0.16	1 (0%) 85 73	67, 91, 111, 134	0
6	2G	181/182 (99%)	0.78	15 (8%) 17 13	106, 127, 139, 147	0
7	1H	174/180 (96%)	-0.10	1 (0%) 85 73	45, 71, 91, 101	0
7	2H	173/180 (96%)	0.37	0 100 100	81, 113, 130, 142	0
8	1I	147/148 (99%)	0.08	1 (0%) 84 70	61, 104, 121, 131	0
8	2I	146/148 (98%)	0.30	2 (1%) 73 54	70, 109, 126, 136	0
9	1N	140/140 (100%)	-0.04	1 (0%) 84 70	39, 52, 75, 100	0
9	2N	140/140 (100%)	0.45	1 (0%) 84 70	58, 90, 111, 122	0
10	1O	122/122 (100%)	-0.14	1 (0%) 82 68	36, 57, 77, 86	0
10	2O	122/122 (100%)	0.08	1 (0%) 82 68	50, 68, 83, 92	0
11	1P	149/150 (99%)	0.07	1 (0%) 84 70	25, 63, 91, 116	0
11	2P	149/150 (99%)	0.42	4 (2%) 56 38	53, 91, 116, 128	0
12	1Q	141/141 (100%)	0.07	0 100 100	39, 56, 70, 99	0
12	2Q	141/141 (100%)	0.59	4 (2%) 55 36	68, 87, 104, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.02	0 100 100	34, 50, 67, 83	0
13	2R	118/118 (100%)	0.25	1 (0%) 82 68	54, 68, 89, 99	0
14	1S	110/112 (98%)	0.06	0 100 100	52, 69, 84, 95	0
14	2S	110/112 (98%)	0.91	14 (12%) 8 6	95, 108, 118, 125	0
15	1T	131/146 (89%)	0.17	2 (1%) 72 53	49, 63, 109, 117	0
15	2T	131/146 (89%)	0.04	0 100 100	53, 74, 104, 123	0
16	1U	116/118 (98%)	-0.09	0 100 100	31, 45, 68, 83	0
16	2U	116/118 (98%)	0.33	3 (2%) 57 38	59, 85, 101, 117	0
17	1V	101/101 (100%)	-0.16	0 100 100	31, 58, 77, 87	0
17	2V	101/101 (100%)	0.26	2 (1%) 65 46	60, 100, 115, 129	0
18	1W	112/113 (99%)	-0.22	0 100 100	35, 48, 71, 91	0
18	2W	112/113 (99%)	0.08	2 (1%) 67 48	48, 66, 96, 140	0
19	1X	95/96 (98%)	-0.08	0 100 100	39, 53, 74, 97	0
19	2X	95/96 (98%)	0.49	3 (3%) 50 34	58, 79, 106, 116	0
20	1Y	107/110 (97%)	0.08	0 100 100	44, 66, 88, 103	0
20	2Y	107/110 (97%)	0.69	5 (4%) 36 24	75, 94, 111, 121	0
21	1Z	203/206 (98%)	0.05	0 100 100	57, 81, 105, 117	0
21	2Z	201/206 (97%)	0.58	6 (2%) 52 35	89, 111, 124, 141	0
22	10	77/85 (90%)	-0.06	0 100 100	40, 52, 66, 79	0
22	20	77/85 (90%)	0.77	7 (9%) 15 11	67, 86, 98, 117	0
23	11	97/98 (98%)	0.04	0 100 100	36, 55, 88, 114	0
23	21	97/98 (98%)	0.36	2 (2%) 63 44	49, 75, 100, 112	0
24	12	70/72 (97%)	0.15	1 (1%) 73 54	47, 66, 80, 108	0
24	22	70/72 (97%)	0.26	0 100 100	80, 93, 103, 105	0
25	13	59/60 (98%)	-0.06	0 100 100	38, 53, 87, 91	0
25	23	59/60 (98%)	0.58	0 100 100	75, 90, 116, 126	0
26	14	69/71 (97%)	0.31	1 (1%) 73 54	83, 113, 141, 146	0
26	24	69/71 (97%)	0.63	1 (1%) 73 54	125, 144, 158, 160	0
27	15	59/60 (98%)	-0.22	0 100 100	34, 44, 79, 89	0
27	25	59/60 (98%)	-0.02	0 100 100	49, 74, 88, 100	0
28	16	53/54 (98%)	-0.16	0 100 100	45, 55, 71, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.10	0 100 100	71, 81, 93, 103	0
29	17	48/49 (97%)	0.06	0 100 100	37, 46, 77, 81	0
29	27	48/49 (97%)	0.25	1 (2%) 63 44	53, 62, 83, 86	0
30	18	64/65 (98%)	0.14	2 (3%) 51 34	39, 49, 61, 83	0
30	28	64/65 (98%)	0.84	3 (4%) 36 24	59, 73, 85, 90	0
31	19	37/37 (100%)	0.11	1 (2%) 56 38	40, 54, 64, 72	0
31	29	37/37 (100%)	1.15	5 (13%) 7 6	80, 89, 100, 105	0
32	1a	1488/1522 (97%)	-0.03	9 (0%) 85 73	50, 99, 152, 187	0
32	2a	1492/1522 (98%)	0.11	22 (1%) 72 53	63, 108, 154, 188	0
33	1b	231/256 (90%)	0.46	6 (2%) 57 38	100, 119, 139, 151	0
33	2b	231/256 (90%)	0.64	15 (6%) 25 17	111, 134, 146, 154	0
34	1c	206/239 (86%)	0.29	8 (3%) 43 29	86, 108, 129, 139	0
34	2c	206/239 (86%)	0.73	15 (7%) 21 15	104, 131, 139, 145	0
35	1d	208/209 (99%)	0.77	13 (6%) 26 18	84, 107, 124, 131	0
35	2d	208/209 (99%)	0.52	7 (3%) 48 32	76, 95, 107, 114	0
36	1e	148/162 (91%)	0.20	0 100 100	71, 91, 106, 126	0
36	2e	148/162 (91%)	0.40	2 (1%) 73 54	87, 104, 117, 144	0
37	1f	100/101 (99%)	0.09	0 100 100	65, 88, 107, 116	0
37	2f	100/101 (99%)	0.24	0 100 100	79, 99, 110, 114	0
38	1g	155/156 (99%)	0.37	4 (2%) 57 38	89, 106, 117, 133	0
38	2g	155/156 (99%)	0.62	5 (3%) 50 34	112, 122, 133, 150	0
39	1h	137/138 (99%)	0.48	2 (1%) 72 53	76, 94, 104, 107	0
39	2h	137/138 (99%)	0.55	4 (2%) 53 36	96, 109, 120, 128	0
40	1i	127/128 (99%)	0.84	16 (12%) 8 7	91, 117, 133, 142	0
40	2i	126/128 (98%)	1.42	27 (21%) 2 2	116, 137, 147, 153	0
41	1j	97/105 (92%)	0.98	10 (10%) 12 10	87, 121, 140, 149	0
41	2j	96/105 (91%)	1.32	18 (18%) 3 3	113, 137, 147, 164	0
42	1k	114/129 (88%)	0.09	3 (2%) 57 38	60, 83, 101, 108	0
42	2k	114/129 (88%)	0.31	5 (4%) 39 25	84, 106, 122, 131	0
43	1l	121/135 (89%)	0.39	3 (2%) 58 39	64, 80, 96, 114	0
43	2l	121/135 (89%)	0.52	10 (8%) 17 13	70, 87, 105, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.56	4 (3%) 48 32	90, 109, 119, 125	0
44	2m	114/126 (90%)	1.04	16 (14%) 6 5	111, 134, 141, 146	0
45	1n	60/61 (98%)	0.87	2 (3%) 49 33	95, 105, 115, 120	0
45	2n	60/61 (98%)	1.47	15 (25%) 2 1	116, 130, 138, 140	0
46	1o	88/89 (98%)	0.46	3 (3%) 48 32	67, 87, 107, 114	0
46	2o	88/89 (98%)	0.44	0 100 100	78, 101, 120, 127	0
47	1p	82/88 (93%)	1.06	9 (10%) 10 9	83, 111, 127, 138	0
47	2p	82/88 (93%)	0.75	5 (6%) 27 19	77, 92, 110, 120	0
48	1r	68/88 (77%)	0.12	0 100 100	69, 86, 111, 119	0
48	2r	68/88 (77%)	0.31	0 100 100	90, 106, 120, 129	0
49	1s	83/93 (89%)	0.79	8 (9%) 13 11	89, 116, 132, 142	0
49	2s	83/93 (89%)	1.16	12 (14%) 6 5	116, 138, 146, 152	0
50	1t	96/106 (90%)	1.31	23 (23%) 2 2	95, 109, 124, 134	0
50	2t	98/106 (92%)	0.93	11 (11%) 10 9	78, 100, 117, 122	0
51	1u	23/27 (85%)	2.01	9 (39%) 1 1	101, 107, 112, 117	0
51	2u	23/27 (85%)	2.57	16 (69%) 0 0	120, 125, 130, 130	0
52	1y	97/113 (85%)	0.55	8 (8%) 17 14	64, 85, 106, 116	0
52	2y	96/113 (84%)	0.99	8 (8%) 17 13	99, 115, 130, 140	0
All	All	20545/21222 (96%)	0.11	528 (2%) 57 38	25, 86, 140, 188	0

The worst 5 of 528 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1091	G	8.3
40	2i	109	VAL	7.2
1	1A	1087	G	6.1
35	2d	4	TYR	5.9
1	1A	1076	C	5.9

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
32	5MC	2a	967	21/22	0.72	0.20	112,121,129,135	0
1	PSU	1A	1911	20/21	0.81	0.11	94,100,105,113	0
1	5MU	2A	1915	21/22	0.82	0.08	114,125,132,139	0
32	2MG	2a	1207	24/25	0.82	0.11	138,142,147,153	0
1	PSU	1A	1917	20/21	0.83	0.09	91,102,109,109	0
1	OMC	2A	1920	21/22	0.83	0.13	91,103,111,113	0
32	2MG	1a	1207	24/25	0.86	0.11	109,112,119,126	0
1	PSU	2A	1911	20/21	0.86	0.08	97,107,115,117	0
1	PSU	2A	1917	20/21	0.87	0.07	106,117,121,124	0
32	PSU	2a	516	20/21	0.88	0.08	97,104,116,117	0
1	5MU	1A	1915	21/22	0.89	0.08	100,108,116,117	0
32	M2G	2a	966	25/26	0.89	0.17	111,117,124,126	0
1	5MC	2A	1942	21/22	0.90	0.09	69,75,78,79	0
32	5MC	1a	967	21/22	0.90	0.11	88,92,101,102	0
32	PSU	1a	516	20/21	0.90	0.08	80,90,97,98	0
32	5MC	1a	1407	21/22	0.90	0.13	71,77,85,86	0
43	0TD	1l	92	10/11	0.90	0.13	85,89,94,102	0
43	0TD	2l	92	10/11	0.90	0.16	80,82,89,105	0
32	5MC	2a	1407	21/22	0.91	0.12	88,96,104,106	0
32	G7M	2a	527	24/25	0.92	0.11	84,91,98,100	0
32	5MC	2a	1400	21/22	0.92	0.12	97,105,110,111	0
32	M2G	1a	966	25/26	0.93	0.11	83,88,97,99	0
32	4OC	2a	1402	22/23	0.93	0.11	81,94,100,103	0
32	5MC	2a	1404	21/22	0.94	0.10	88,94,102,105	0
32	G7M	1a	527	24/25	0.94	0.11	64,79,84,88	0
32	5MC	1a	1404	21/22	0.94	0.10	60,65,71,72	0
32	MA6	1a	1518	24/25	0.95	0.10	61,66,70,74	0
1	PSU	2A	2605	20/21	0.95	0.10	53,63,70,75	0
1	OMC	1A	1920	21/22	0.95	0.09	74,83,97,101	0
32	MA6	2a	1518	24/25	0.95	0.12	78,87,92,95	0
32	UR3	1a	1498	21/22	0.95	0.09	60,68,72,84	0
1	OMU	1A	2552	21/22	0.96	0.08	43,48,52,59	0
32	MA6	1a	1519	24/25	0.96	0.11	57,67,73,75	0
1	PSU	1A	2605	20/21	0.96	0.08	37,41,47,48	0
32	5MC	1a	1400	21/22	0.96	0.09	64,71,76,84	0
32	4OC	1a	1402	22/23	0.96	0.09	61,68,71,73	0
1	5MU	1A	1939	21/22	0.96	0.11	34,46,54,57	0
1	5MC	1A	1942	21/22	0.96	0.07	46,55,61,63	0
1	5MU	2A	1939	21/22	0.96	0.09	53,57,61,62	0
1	OMG	1A	2251	24/25	0.96	0.08	31,36,42,46	0
1	5MC	2A	1962	21/22	0.96	0.07	54,59,69,74	0
32	UR3	2a	1498	21/22	0.96	0.08	83,86,91,94	0
1	OMG	2A	2251	24/25	0.96	0.08	52,60,65,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MA6	2a	1519	24/25	0.96	0.12	78,89,96,98	0
1	2MA	2A	2503	23/24	0.96	0.10	44,50,59,61	0
1	5MC	1A	1962	21/22	0.97	0.07	50,56,61,63	0
1	OMU	2A	2552	21/22	0.97	0.07	49,54,59,62	0
1	2MA	1A	2503	23/24	0.98	0.07	21,35,41,44	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	1a	1761	1/1	0.02	0.29	114,114,114,114	0
54	MG	2a	1645	1/1	0.13	0.14	120,120,120,120	0
54	MG	2a	1655	1/1	0.13	0.36	114,114,114,114	0
54	MG	2A	3301	1/1	0.24	0.13	103,103,103,103	0
54	MG	2a	1663	1/1	0.24	0.15	110,110,110,110	0
54	MG	2A	3087	1/1	0.30	0.32	99,99,99,99	0
54	MG	1A	3260	1/1	0.33	0.15	141,141,141,141	0
54	MG	2A	3565	1/1	0.34	0.14	155,155,155,155	0
54	MG	1a	1743	1/1	0.36	0.18	103,103,103,103	0
54	MG	1t	201	1/1	0.40	0.18	110,110,110,110	0
54	MG	2i	201	1/1	0.42	0.62	103,103,103,103	0
54	MG	1a	1831	1/1	0.44	0.11	96,96,96,96	0
54	MG	2a	1701	1/1	0.45	0.32	101,101,101,101	0
54	MG	2a	1636	1/1	0.46	0.16	99,99,99,99	0
54	MG	2A	3392	1/1	0.46	0.15	81,81,81,81	0
54	MG	1a	1774	1/1	0.47	0.19	103,103,103,103	0
54	MG	1a	1779	1/1	0.47	0.20	81,81,81,81	0
54	MG	2a	1658	1/1	0.48	0.26	102,102,102,102	0
54	MG	2a	1659	1/1	0.48	0.26	87,87,87,87	0
54	MG	1A	3591	1/1	0.48	0.15	87,87,87,87	0
54	MG	2A	3541	1/1	0.48	0.17	85,85,85,85	0
54	MG	1a	1681	1/1	0.48	0.14	113,113,113,113	0
54	MG	1y	204	1/1	0.50	0.17	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3114	1/1	0.52	0.34	68,68,68,68	0
54	MG	2a	1690	1/1	0.52	0.17	94,94,94,94	0
54	MG	1a	1639	1/1	0.53	0.20	97,97,97,97	0
54	MG	1P	205	1/1	0.53	0.10	117,117,117,117	0
54	MG	1a	1820	1/1	0.54	0.17	124,124,124,124	0
54	MG	2a	1664	1/1	0.54	0.32	94,94,94,94	0
54	MG	1A	3600	1/1	0.54	0.39	74,74,74,74	0
54	MG	2B	207	1/1	0.54	0.30	99,99,99,99	0
54	MG	1b	301	1/1	0.54	0.14	116,116,116,116	0
54	MG	2A	3110	1/1	0.55	0.12	107,107,107,107	0
54	MG	2a	1693	1/1	0.55	0.18	84,84,84,84	0
54	MG	1A	3730	1/1	0.55	0.16	75,75,75,75	0
54	MG	2A	3118	1/1	0.55	0.33	81,81,81,81	0
54	MG	2A	3083	1/1	0.56	0.15	87,87,87,87	0
54	MG	2B	204	1/1	0.56	0.14	110,110,110,110	0
54	MG	2a	1709	1/1	0.58	0.16	83,83,83,83	0
54	MG	1A	3818	1/1	0.59	0.17	59,59,59,59	0
54	MG	2A	3209	1/1	0.59	0.21	59,59,59,59	0
54	MG	2A	3257	1/1	0.59	0.22	89,89,89,89	0
54	MG	2a	1635	1/1	0.59	0.24	78,78,78,78	0
53	MPD	2B	201	8/8	0.60	0.45	101,115,117,121	0
54	MG	1a	1828	1/1	0.60	0.15	116,116,116,116	0
54	MG	1a	1784	1/1	0.60	0.36	82,82,82,82	0
54	MG	1a	1819	1/1	0.60	0.13	97,97,97,97	0
54	MG	2A	3244	1/1	0.60	0.17	72,72,72,72	0
54	MG	2A	3461	1/1	0.61	0.17	87,87,87,87	0
54	MG	1a	1839	1/1	0.61	0.22	95,95,95,95	0
54	MG	1a	1760	1/1	0.61	0.10	128,128,128,128	0
54	MG	1A	3834	1/1	0.62	0.16	90,90,90,90	0
54	MG	2A	3005	1/1	0.62	0.19	68,68,68,68	0
54	MG	2A	3105	1/1	0.63	0.42	95,95,95,95	0
54	MG	2A	3149	1/1	0.63	0.17	78,78,78,78	0
54	MG	2O	202	1/1	0.63	0.13	94,94,94,94	0
54	MG	2A	3322	1/1	0.63	0.11	90,90,90,90	0
54	MG	2A	3193	1/1	0.63	0.14	104,104,104,104	0
54	MG	1n	103	1/1	0.63	0.28	100,100,100,100	0
54	MG	2A	3228	1/1	0.63	0.17	99,99,99,99	0
54	MG	1A	3165	1/1	0.63	0.27	78,78,78,78	0
54	MG	2a	1698	1/1	0.64	0.17	95,95,95,95	0
54	MG	1a	1747	1/1	0.64	0.20	109,109,109,109	0
54	MG	1B	1018	1/1	0.64	0.15	84,84,84,84	0
54	MG	1a	1822	1/1	0.64	0.12	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3194	1/1	0.65	0.15	60,60,60,60	0
54	MG	1A	3283	1/1	0.65	0.22	64,64,64,64	0
54	MG	1a	1762	1/1	0.65	0.14	108,108,108,108	0
54	MG	1a	1763	1/1	0.65	0.10	96,96,96,96	0
54	MG	1a	1765	1/1	0.65	0.12	103,103,103,103	0
54	MG	1a	1646	1/1	0.65	0.18	102,102,102,102	0
54	MG	2A	3102	1/1	0.65	0.12	95,95,95,95	0
54	MG	1a	1614	1/1	0.66	0.22	94,94,94,94	0
54	MG	2A	3373	1/1	0.66	0.17	87,87,87,87	0
54	MG	1A	3850	1/1	0.66	0.22	54,54,54,54	0
54	MG	2B	206	1/1	0.66	0.19	61,61,61,61	0
54	MG	1a	1696	1/1	0.66	0.18	80,80,80,80	0
54	MG	1a	1735	1/1	0.67	0.15	83,83,83,83	0
54	MG	1A	3173	1/1	0.67	0.28	80,80,80,80	0
54	MG	1a	1796	1/1	0.67	0.18	81,81,81,81	0
54	MG	1a	1806	1/1	0.67	0.28	85,85,85,85	0
54	MG	1a	1832	1/1	0.67	0.20	90,90,90,90	0
54	MG	2I	201	1/1	0.67	0.11	87,87,87,87	0
54	MG	2a	1739	1/1	0.67	0.10	98,98,98,98	0
54	MG	1G	202	1/1	0.67	0.11	79,79,79,79	0
54	MG	2a	1681	1/1	0.68	0.18	94,94,94,94	0
54	MG	2A	3051	1/1	0.68	0.16	78,78,78,78	0
54	MG	1A	3555	1/1	0.68	0.20	79,79,79,79	0
54	MG	2A	3522	1/1	0.68	0.16	96,96,96,96	0
54	MG	2A	3086	1/1	0.68	0.15	94,94,94,94	0
54	MG	1A	3423	1/1	0.68	0.25	81,81,81,81	0
54	MG	2A	3094	1/1	0.68	0.24	74,74,74,74	0
54	MG	2a	1668	1/1	0.68	0.18	90,90,90,90	0
54	MG	2a	1625	1/1	0.69	0.19	94,94,94,94	0
54	MG	2B	203	1/1	0.69	0.12	74,74,74,74	0
54	MG	2A	3225	1/1	0.69	0.38	80,80,80,80	0
54	MG	2a	1657	1/1	0.70	0.27	89,89,89,89	0
54	MG	1a	1625	1/1	0.70	0.33	54,54,54,54	0
54	MG	1V	203	1/1	0.70	0.15	86,86,86,86	0
54	MG	1a	1709	1/1	0.70	0.19	99,99,99,99	0
54	MG	1A	3030	1/1	0.70	0.34	69,69,69,69	0
54	MG	1f	201	1/1	0.70	0.11	68,68,68,68	0
54	MG	2A	3076	1/1	0.70	0.22	76,76,76,76	0
54	MG	2k	201	1/1	0.70	0.13	83,83,83,83	0
54	MG	2A	3463	1/1	0.71	0.11	90,90,90,90	0
54	MG	2a	1667	1/1	0.71	0.30	79,79,79,79	0
54	MG	1a	1811	1/1	0.71	0.19	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3241	1/1	0.71	0.13	93,93,93,93	0
54	MG	1A	3317	1/1	0.71	0.22	76,76,76,76	0
54	MG	1a	1856	1/1	0.71	0.15	83,83,83,83	0
54	MG	1A	3384	1/1	0.71	0.13	74,74,74,74	0
54	MG	2a	1656	1/1	0.71	0.20	106,106,106,106	0
54	MG	2B	205	1/1	0.71	0.28	70,70,70,70	0
54	MG	10	106	1/1	0.71	0.18	81,81,81,81	0
54	MG	2A	3219	1/1	0.71	0.13	70,70,70,70	0
54	MG	2A	3080	1/1	0.71	0.14	130,130,130,130	0
54	MG	1A	3562	1/1	0.72	0.15	81,81,81,81	0
54	MG	1a	1634	1/1	0.72	0.16	62,62,62,62	0
54	MG	2A	3333	1/1	0.72	0.20	57,57,57,57	0
54	MG	1A	3703	1/1	0.72	0.13	41,41,41,41	0
54	MG	2A	3377	1/1	0.72	0.25	57,57,57,57	0
54	MG	2B	211	1/1	0.72	0.24	89,89,89,89	0
54	MG	2B	213	1/1	0.72	0.09	97,97,97,97	0
54	MG	1a	1807	1/1	0.72	0.14	87,87,87,87	0
54	MG	2A	3447	1/1	0.72	0.10	69,69,69,69	0
54	MG	2a	1615	1/1	0.72	0.09	77,77,77,77	0
54	MG	2A	3454	1/1	0.72	0.31	66,66,66,66	0
54	MG	1a	1602	1/1	0.72	0.13	63,63,63,63	0
54	MG	1A	3052	1/1	0.72	0.16	85,85,85,85	0
54	MG	1a	1686	1/1	0.72	0.24	88,88,88,88	0
54	MG	2A	3077	1/1	0.72	0.33	67,67,67,67	0
54	MG	1e	203	1/1	0.72	0.14	89,89,89,89	0
54	MG	2A	3410	1/1	0.73	0.11	75,75,75,75	0
54	MG	1a	1667	1/1	0.73	0.15	85,85,85,85	0
54	MG	2A	3236	1/1	0.73	0.16	70,70,70,70	0
54	MG	1a	1672	1/1	0.73	0.15	85,85,85,85	0
54	MG	2A	3150	1/1	0.73	0.12	135,135,135,135	0
54	MG	2R	202	1/1	0.73	0.28	70,70,70,70	0
54	MG	2A	3508	1/1	0.73	0.16	64,64,64,64	0
54	MG	1A	3426	1/1	0.73	0.13	47,47,47,47	0
54	MG	1A	3518	1/1	0.73	0.16	56,56,56,56	0
54	MG	2A	3206	1/1	0.73	0.19	67,67,67,67	0
54	MG	1a	1687	1/1	0.73	0.26	72,72,72,72	0
54	MG	2a	1654	1/1	0.73	0.19	100,100,100,100	0
53	MPD	1a	1601	8/8	0.73	0.21	97,116,129,130	0
54	MG	2e	201	1/1	0.73	0.19	85,85,85,85	0
54	MG	1A	3672	1/1	0.73	0.22	78,78,78,78	0
54	MG	2j	201	1/1	0.73	0.10	112,112,112,112	0
54	MG	2A	3397	1/1	0.73	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	1680	1/1	0.74	0.24	121,121,121,121	0
54	MG	2B	210	1/1	0.74	0.18	84,84,84,84	0
54	MG	1a	1794	1/1	0.74	0.19	78,78,78,78	0
54	MG	1a	1745	1/1	0.74	0.13	78,78,78,78	0
54	MG	2F	301	1/1	0.74	0.09	54,54,54,54	0
54	MG	1a	1680	1/1	0.74	0.18	105,105,105,105	0
54	MG	1a	1628	1/1	0.74	0.25	67,67,67,67	0
54	MG	1A	3432	1/1	0.74	0.11	53,53,53,53	0
54	MG	1A	3828	1/1	0.74	0.15	64,64,64,64	0
54	MG	1t	202	1/1	0.74	0.49	92,92,92,92	0
54	MG	2A	3115	1/1	0.74	0.15	73,73,73,73	0
54	MG	2A	3359	1/1	0.74	0.16	73,73,73,73	0
54	MG	2A	3169	1/1	0.75	0.15	80,80,80,80	0
54	MG	2G	202	1/1	0.75	0.13	108,108,108,108	0
54	MG	1a	1793	1/1	0.75	0.11	89,89,89,89	0
54	MG	2A	3050	1/1	0.75	0.33	70,70,70,70	0
54	MG	2Q	201	1/1	0.75	0.27	83,83,83,83	0
54	MG	2A	3356	1/1	0.75	0.13	91,91,91,91	0
54	MG	2a	1612	1/1	0.75	0.16	96,96,96,96	0
54	MG	2A	3199	1/1	0.75	0.12	64,64,64,64	0
54	MG	2A	3637	1/1	0.75	0.15	64,64,64,64	0
54	MG	1a	1741	1/1	0.75	0.25	89,89,89,89	0
54	MG	1A	3324	1/1	0.75	0.13	57,57,57,57	0
54	MG	15	104	1/1	0.75	0.09	72,72,72,72	0
54	MG	1a	1780	1/1	0.75	0.17	83,83,83,83	0
54	MG	1A	3872	1/1	0.75	0.20	77,77,77,77	0
54	MG	1y	202	1/1	0.75	0.10	98,98,98,98	0
54	MG	1a	1789	1/1	0.75	0.17	107,107,107,107	0
54	MG	2A	3152	1/1	0.75	0.19	71,71,71,71	0
54	MG	2A	3022	1/1	0.76	0.18	80,80,80,80	0
54	MG	2A	3165	1/1	0.76	0.11	72,72,72,72	0
54	MG	2a	1720	1/1	0.76	0.11	117,117,117,117	0
54	MG	1A	3402	1/1	0.76	0.11	58,58,58,58	0
54	MG	1A	3250	1/1	0.76	0.13	61,61,61,61	0
54	MG	2a	1609	1/1	0.76	0.16	62,62,62,62	0
54	MG	2a	1652	1/1	0.76	0.20	88,88,88,88	0
54	MG	2A	3210	1/1	0.76	0.13	61,61,61,61	0
54	MG	1A	3783	1/1	0.77	0.17	51,51,51,51	0
54	MG	1A	3481	1/1	0.77	0.16	74,74,74,74	0
54	MG	2A	3309	1/1	0.77	0.12	94,94,94,94	0
54	MG	2A	3120	1/1	0.77	0.24	82,82,82,82	0
54	MG	1a	1821	1/1	0.77	0.21	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MPD	1T	2001	8/8	0.77	0.28	77,82,86,94	0
54	MG	1A	3548	1/1	0.77	0.17	63,63,63,63	0
54	MG	2a	1660	1/1	0.77	0.20	79,79,79,79	0
54	MG	1A	3319	1/1	0.77	0.25	72,72,72,72	0
54	MG	1a	1713	1/1	0.77	0.12	92,92,92,92	0
54	MG	2A	3385	1/1	0.77	0.10	73,73,73,73	0
54	MG	1A	3709	1/1	0.77	0.12	58,58,58,58	0
54	MG	1a	1849	1/1	0.77	0.14	62,62,62,62	0
54	MG	1a	1739	1/1	0.77	0.34	81,81,81,81	0
54	MG	1B	1004	1/1	0.77	0.17	60,60,60,60	0
54	MG	2a	1692	1/1	0.77	0.21	75,75,75,75	0
54	MG	1d	502	1/1	0.77	0.25	101,101,101,101	0
54	MG	2A	3090	1/1	0.77	0.30	81,81,81,81	0
54	MG	1B	1009	1/1	0.77	0.11	77,77,77,77	0
54	MG	2A	3481	1/1	0.77	0.14	92,92,92,92	0
54	MG	1A	3714	1/1	0.77	0.14	44,44,44,44	0
54	MG	2a	1634	1/1	0.77	0.20	101,101,101,101	0
54	MG	1A	3479	1/1	0.77	0.09	70,70,70,70	0
54	MG	1A	3748	1/1	0.77	0.09	92,92,92,92	0
54	MG	2a	1639	1/1	0.77	0.13	124,124,124,124	0
54	MG	1A	3749	1/1	0.77	0.13	74,74,74,74	0
54	MG	1A	3418	1/1	0.78	0.14	39,39,39,39	0
54	MG	1a	1754	1/1	0.78	0.14	78,78,78,78	0
54	MG	2A	3261	1/1	0.78	0.14	74,74,74,74	0
54	MG	2A	3451	1/1	0.78	0.14	63,63,63,63	0
54	MG	2A	3272	1/1	0.78	0.14	64,64,64,64	0
54	MG	1a	1670	1/1	0.78	0.50	91,91,91,91	0
54	MG	2A	3060	1/1	0.78	0.13	66,66,66,66	0
54	MG	1A	3137	1/1	0.78	0.19	74,74,74,74	0
54	MG	1A	3143	1/1	0.78	0.17	70,70,70,70	0
54	MG	1B	1006	1/1	0.78	0.10	69,69,69,69	0
54	MG	1A	3530	1/1	0.78	0.09	103,103,103,103	0
54	MG	1A	3191	1/1	0.78	0.15	64,64,64,64	0
54	MG	2a	1741	1/1	0.78	0.17	97,97,97,97	0
54	MG	2a	1757	1/1	0.78	0.17	92,92,92,92	0
54	MG	2T	201	1/1	0.78	0.13	61,61,61,61	0
54	MG	1a	1809	1/1	0.78	0.14	87,87,87,87	0
54	MG	2A	3151	1/1	0.78	0.12	72,72,72,72	0
54	MG	1a	1695	1/1	0.78	0.12	94,94,94,94	0
54	MG	2A	3133	1/1	0.79	0.22	66,66,66,66	0
54	MG	2A	3313	1/1	0.79	0.08	90,90,90,90	0
54	MG	1B	1011	1/1	0.79	0.13	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	3045	1/1	0.79	0.15	74,74,74,74	0
54	MG	1A	3478	1/1	0.79	0.18	50,50,50,50	0
54	MG	2A	3464	1/1	0.79	0.16	69,69,69,69	0
54	MG	2A	3472	1/1	0.79	0.14	69,69,69,69	0
54	MG	1B	1029	1/1	0.79	0.09	80,80,80,80	0
54	MG	2a	1653	1/1	0.79	0.15	86,86,86,86	0
54	MG	1a	1661	1/1	0.79	0.27	86,86,86,86	0
54	MG	1A	3735	1/1	0.79	0.14	58,58,58,58	0
54	MG	2A	3384	1/1	0.79	0.15	76,76,76,76	0
54	MG	1a	1616	1/1	0.79	0.20	106,106,106,106	0
54	MG	2a	1745	1/1	0.79	0.14	85,85,85,85	0
54	MG	2a	1750	1/1	0.79	0.23	79,79,79,79	0
54	MG	1A	3837	1/1	0.79	0.13	56,56,56,56	0
54	MG	2V	201	1/1	0.79	0.11	101,101,101,101	0
54	MG	2a	1605	1/1	0.79	0.14	91,91,91,91	0
54	MG	1a	1788	1/1	0.79	0.17	106,106,106,106	0
54	MG	1A	3570	1/1	0.79	0.14	81,81,81,81	0
54	MG	1A	3557	1/1	0.80	0.45	41,41,41,41	0
54	MG	1a	1664	1/1	0.80	0.25	80,80,80,80	0
54	MG	1A	3169	1/1	0.80	0.13	56,56,56,56	0
54	MG	2A	3543	1/1	0.80	0.14	89,89,89,89	0
54	MG	2A	3007	1/1	0.80	0.17	63,63,63,63	0
54	MG	1T	2002	1/1	0.80	0.13	54,54,54,54	0
54	MG	2A	3642	1/1	0.80	0.25	87,87,87,87	0
54	MG	2B	202	1/1	0.80	0.14	99,99,99,99	0
54	MG	1A	3244	1/1	0.80	0.16	87,87,87,87	0
54	MG	1A	3724	1/1	0.80	0.20	91,91,91,91	0
54	MG	2A	3332	1/1	0.80	0.16	82,82,82,82	0
54	MG	1A	3727	1/1	0.80	0.46	58,58,58,58	0
54	MG	2A	3346	1/1	0.80	0.08	89,89,89,89	0
54	MG	2A	3052	1/1	0.80	0.21	75,75,75,75	0
54	MG	2A	3161	1/1	0.80	0.20	59,59,59,59	0
54	MG	1A	3439	1/1	0.80	0.15	114,114,114,114	0
54	MG	2a	1671	1/1	0.80	0.27	79,79,79,79	0
54	MG	1A	3732	1/1	0.80	0.35	60,60,60,60	0
54	MG	2G	201	1/1	0.80	0.14	114,114,114,114	0
54	MG	2A	3172	1/1	0.80	0.27	80,80,80,80	0
54	MG	1A	3152	1/1	0.80	0.08	52,52,52,52	0
54	MG	1a	1617	1/1	0.80	0.12	79,79,79,79	0
54	MG	2A	3196	1/1	0.80	0.22	58,58,58,58	0
54	MG	1A	3604	1/1	0.80	0.33	55,55,55,55	0
54	MG	2a	1706	1/1	0.80	0.17	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3445	1/1	0.80	0.16	68,68,68,68	0
54	MG	1A	3629	1/1	0.80	0.21	73,73,73,73	0
54	MG	1a	1714	1/1	0.80	0.21	83,83,83,83	0
54	MG	1a	1725	1/1	0.80	0.07	104,104,104,104	0
54	MG	2a	1610	1/1	0.80	0.13	106,106,106,106	0
54	MG	2A	3093	1/1	0.80	0.15	81,81,81,81	0
53	MPD	2A	3001	8/8	0.80	0.34	54,73,76,82	0
54	MG	2a	1759	1/1	0.80	0.18	80,80,80,80	0
54	MG	2a	1762	1/1	0.80	0.12	105,105,105,105	0
54	MG	2a	1618	1/1	0.80	0.14	97,97,97,97	0
54	MG	1a	1636	1/1	0.80	0.15	77,77,77,77	0
54	MG	1A	3796	1/1	0.80	0.13	66,66,66,66	0
54	MG	1B	1030	1/1	0.80	0.11	78,78,78,78	0
54	MG	1a	1675	1/1	0.81	0.10	68,68,68,68	0
54	MG	1A	3253	1/1	0.81	0.08	61,61,61,61	0
54	MG	2A	3297	1/1	0.81	0.13	66,66,66,66	0
54	MG	2A	3135	1/1	0.81	0.12	69,69,69,69	0
54	MG	2A	3139	1/1	0.81	0.25	74,74,74,74	0
54	MG	1A	3445	1/1	0.81	0.17	43,43,43,43	0
54	MG	2A	3317	1/1	0.81	0.21	103,103,103,103	0
54	MG	1A	3641	1/1	0.81	0.14	33,33,33,33	0
54	MG	1a	1858	1/1	0.81	0.20	90,90,90,90	0
54	MG	2A	3074	1/1	0.81	0.13	80,80,80,80	0
54	MG	2A	3334	1/1	0.81	0.14	49,49,49,49	0
54	MG	2A	3342	1/1	0.81	0.17	69,69,69,69	0
54	MG	2A	3154	1/1	0.81	0.28	66,66,66,66	0
54	MG	1a	1641	1/1	0.81	0.14	60,60,60,60	0
54	MG	1a	1802	1/1	0.81	0.08	142,142,142,142	0
54	MG	1d	507	1/1	0.81	0.08	116,116,116,116	0
54	MG	1a	1645	1/1	0.81	0.26	73,73,73,73	0
54	MG	2A	3180	1/1	0.81	0.17	61,61,61,61	0
54	MG	1A	3502	1/1	0.81	0.10	91,91,91,91	0
54	MG	1a	1705	1/1	0.81	0.13	93,93,93,93	0
54	MG	1D	312	1/1	0.81	0.15	62,62,62,62	0
54	MG	2a	1694	1/1	0.81	0.23	95,95,95,95	0
54	MG	2A	3091	1/1	0.81	0.13	67,67,67,67	0
54	MG	1a	1711	1/1	0.81	0.14	82,82,82,82	0
54	MG	23	101	1/1	0.81	0.23	81,81,81,81	0
54	MG	2a	1603	1/1	0.81	0.14	58,58,58,58	0
54	MG	2a	1604	1/1	0.81	0.28	91,91,91,91	0
54	MG	1F	312	1/1	0.81	0.26	52,52,52,52	0
54	MG	2A	3097	1/1	0.81	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	3728	1/1	0.81	0.17	60,60,60,60	0
54	MG	1A	3690	1/1	0.81	0.33	51,51,51,51	0
54	MG	1a	1734	1/1	0.81	0.08	130,130,130,130	0
54	MG	2a	1617	1/1	0.81	0.19	73,73,73,73	0
54	MG	2a	1761	1/1	0.81	0.17	90,90,90,90	0
54	MG	2A	3230	1/1	0.81	0.18	58,58,58,58	0
54	MG	2A	3235	1/1	0.81	0.13	84,84,84,84	0
54	MG	2A	3010	1/1	0.81	0.18	62,62,62,62	0
54	MG	1A	3122	1/1	0.81	0.16	59,59,59,59	0
54	MG	2A	3023	1/1	0.81	0.26	50,50,50,50	0
54	MG	1B	1026	1/1	0.82	0.15	94,94,94,94	0
54	MG	1A	3618	1/1	0.82	0.18	68,68,68,68	0
54	MG	2A	3141	1/1	0.82	0.30	78,78,78,78	0
54	MG	1A	3220	1/1	0.82	0.20	54,54,54,54	0
54	MG	1A	3544	1/1	0.82	0.12	69,69,69,69	0
54	MG	1A	3577	1/1	0.82	0.13	72,72,72,72	0
54	MG	1A	3855	1/1	0.82	0.13	54,54,54,54	0
54	MG	2A	3071	1/1	0.82	0.28	51,51,51,51	0
54	MG	1A	3856	1/1	0.82	0.17	53,53,53,53	0
54	MG	1R	203	1/1	0.82	0.11	52,52,52,52	0
54	MG	1A	3858	1/1	0.82	0.18	77,77,77,77	0
54	MG	1a	1652	1/1	0.82	0.21	74,74,74,74	0
54	MG	1a	1654	1/1	0.82	0.14	80,80,80,80	0
54	MG	2A	3187	1/1	0.82	0.23	70,70,70,70	0
54	MG	1d	503	1/1	0.82	0.26	85,85,85,85	0
54	MG	1a	1716	1/1	0.82	0.12	77,77,77,77	0
54	MG	1a	1656	1/1	0.82	0.18	73,73,73,73	0
54	MG	2a	1675	1/1	0.82	0.18	87,87,87,87	0
54	MG	1A	3588	1/1	0.82	0.12	82,82,82,82	0
54	MG	2A	3386	1/1	0.82	0.20	86,86,86,86	0
54	MG	1g	203	1/1	0.82	0.05	62,62,62,62	0
54	MG	2A	3395	1/1	0.82	0.12	97,97,97,97	0
54	MG	1A	3163	1/1	0.82	0.08	50,50,50,50	0
54	MG	1a	1800	1/1	0.82	0.13	100,100,100,100	0
54	MG	2A	3435	1/1	0.82	0.17	81,81,81,81	0
54	MG	2Y	201	1/1	0.82	0.12	66,66,66,66	0
54	MG	2A	3211	1/1	0.82	0.20	69,69,69,69	0
54	MG	1a	1737	1/1	0.82	0.22	94,94,94,94	0
54	MG	1a	1666	1/1	0.82	0.16	78,78,78,78	0
54	MG	1A	3704	1/1	0.82	0.23	61,61,61,61	0
54	MG	2a	1608	1/1	0.82	0.37	68,68,68,68	0
54	MG	2A	3113	1/1	0.82	0.20	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3592	1/1	0.82	0.15	68,68,68,68	0
54	MG	2a	1751	1/1	0.82	0.13	60,60,60,60	0
54	MG	1A	3449	1/1	0.82	0.15	72,72,72,72	0
54	MG	2A	3466	1/1	0.82	0.09	70,70,70,70	0
54	MG	1A	3356	1/1	0.82	0.10	88,88,88,88	0
54	MG	2A	3017	1/1	0.82	0.24	76,76,76,76	0
54	MG	2A	3491	1/1	0.82	0.13	52,52,52,52	0
54	MG	2a	1629	1/1	0.82	0.15	110,110,110,110	0
54	MG	2A	3493	1/1	0.82	0.14	65,65,65,65	0
54	MG	1a	1750	1/1	0.82	0.10	89,89,89,89	0
54	MG	1A	3243	1/1	0.83	0.15	45,45,45,45	0
54	MG	1A	3386	1/1	0.83	0.10	67,67,67,67	0
54	MG	1a	1764	1/1	0.83	0.14	92,92,92,92	0
54	MG	2a	1638	1/1	0.83	0.24	77,77,77,77	0
54	MG	2A	3542	1/1	0.83	0.11	90,90,90,90	0
54	MG	2a	1640	1/1	0.83	0.16	100,100,100,100	0
54	MG	2a	1642	1/1	0.83	0.13	61,61,61,61	0
54	MG	1A	3619	1/1	0.83	0.15	55,55,55,55	0
54	MG	2A	3075	1/1	0.83	0.29	70,70,70,70	0
54	MG	2A	3615	1/1	0.83	0.14	75,75,75,75	0
54	MG	2A	3163	1/1	0.83	0.18	67,67,67,67	0
54	MG	1a	1770	1/1	0.83	0.09	99,99,99,99	0
54	MG	1a	1700	1/1	0.83	0.13	77,77,77,77	0
54	MG	1A	3621	1/1	0.83	0.11	67,67,67,67	0
54	MG	1A	3392	1/1	0.83	0.09	80,80,80,80	0
54	MG	2A	3186	1/1	0.83	0.10	65,65,65,65	0
54	MG	2A	3372	1/1	0.83	0.10	63,63,63,63	0
54	MG	1d	505	1/1	0.83	0.08	56,56,56,56	0
54	MG	1A	3879	1/1	0.83	0.20	100,100,100,100	0
54	MG	1a	1650	1/1	0.83	0.24	74,74,74,74	0
54	MG	1T	2006	1/1	0.83	0.08	83,83,83,83	0
54	MG	1U	202	1/1	0.83	0.16	37,37,37,37	0
54	MG	1A	3880	1/1	0.83	0.14	50,50,50,50	0
54	MG	2a	1676	1/1	0.83	0.20	93,93,93,93	0
54	MG	2A	3096	1/1	0.83	0.13	57,57,57,57	0
54	MG	1A	3309	1/1	0.83	0.18	59,59,59,59	0
54	MG	2A	3403	1/1	0.83	0.13	74,74,74,74	0
54	MG	1a	1662	1/1	0.83	0.16	69,69,69,69	0
54	MG	2A	3414	1/1	0.83	0.21	74,74,74,74	0
54	MG	2A	3418	1/1	0.83	0.11	71,71,71,71	0
54	MG	2A	3431	1/1	0.83	0.11	46,46,46,46	0
54	MG	1A	3170	1/1	0.83	0.19	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2I	104	1/1	0.83	0.09	95,95,95,95	0
54	MG	2A	3444	1/1	0.83	0.09	68,68,68,68	0
54	MG	1A	3227	1/1	0.83	0.14	88,88,88,88	0
54	MG	2a	1737	1/1	0.83	0.15	131,131,131,131	0
54	MG	1a	1605	1/1	0.83	0.31	96,96,96,96	0
54	MG	1a	1669	1/1	0.83	0.15	110,110,110,110	0
54	MG	1A	3322	1/1	0.83	0.15	58,58,58,58	0
54	MG	1A	3589	1/1	0.83	0.15	43,43,43,43	0
54	MG	1A	3528	1/1	0.83	0.16	66,66,66,66	0
54	MG	2a	1754	1/1	0.83	0.11	121,121,121,121	0
54	MG	1a	1751	1/1	0.83	0.26	80,80,80,80	0
54	MG	2A	3041	1/1	0.83	0.20	81,81,81,81	0
54	MG	2A	3263	1/1	0.83	0.10	85,85,85,85	0
54	MG	1a	1622	1/1	0.83	0.09	106,106,106,106	0
54	MG	2a	1620	1/1	0.83	0.17	60,60,60,60	0
54	MG	2a	1621	1/1	0.83	0.23	52,52,52,52	0
54	MG	1A	3211	1/1	0.83	0.17	50,50,50,50	0
54	MG	1A	3242	1/1	0.83	0.12	90,90,90,90	0
54	MG	1a	1748	1/1	0.84	0.12	86,86,86,86	0
54	MG	1A	3687	1/1	0.84	0.14	66,66,66,66	0
54	MG	2A	3214	1/1	0.84	0.12	48,48,48,48	0
54	MG	1a	1850	1/1	0.84	0.11	129,129,129,129	0
54	MG	2A	3456	1/1	0.84	0.11	71,71,71,71	0
54	MG	1A	3047	1/1	0.84	0.18	73,73,73,73	0
54	MG	1A	3851	1/1	0.84	0.19	75,75,75,75	0
54	MG	1A	3089	1/1	0.84	0.21	45,45,45,45	0
54	MG	2a	1637	1/1	0.84	0.20	65,65,65,65	0
54	MG	1A	3347	1/1	0.84	0.11	82,82,82,82	0
54	MG	1A	3707	1/1	0.84	0.22	91,91,91,91	0
54	MG	2A	3242	1/1	0.84	0.10	77,77,77,77	0
54	MG	1a	1676	1/1	0.84	0.28	85,85,85,85	0
54	MG	2A	3248	1/1	0.84	0.19	48,48,48,48	0
54	MG	2a	1646	1/1	0.84	0.08	69,69,69,69	0
54	MG	1A	3179	1/1	0.84	0.16	49,49,49,49	0
54	MG	1A	3472	1/1	0.84	0.14	43,43,43,43	0
54	MG	1A	3578	1/1	0.84	0.12	62,62,62,62	0
54	MG	1B	1002	1/1	0.84	0.12	57,57,57,57	0
54	MG	2A	3279	1/1	0.84	0.09	74,74,74,74	0
54	MG	1n	101	1/1	0.84	0.26	85,85,85,85	0
54	MG	2A	3597	1/1	0.84	0.10	101,101,101,101	0
54	MG	1a	1778	1/1	0.84	0.10	72,72,72,72	0
54	MG	1A	3474	1/1	0.84	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3359	1/1	0.84	0.14	38,38,38,38	0
54	MG	1B	1008	1/1	0.84	0.21	64,64,64,64	0
54	MG	1a	1785	1/1	0.84	0.15	84,84,84,84	0
54	MG	2A	3328	1/1	0.84	0.11	78,78,78,78	0
54	MG	1A	3150	1/1	0.84	0.10	41,41,41,41	0
54	MG	1A	3199	1/1	0.84	0.25	58,58,58,58	0
54	MG	1a	1635	1/1	0.84	0.09	80,80,80,80	0
54	MG	2A	3336	1/1	0.84	0.11	92,92,92,92	0
54	MG	2A	3338	1/1	0.84	0.18	64,64,64,64	0
54	MG	2a	1685	1/1	0.84	0.34	71,71,71,71	0
54	MG	1B	1017	1/1	0.84	0.19	65,65,65,65	0
54	MG	2B	215	1/1	0.84	0.09	112,112,112,112	0
54	MG	2A	3021	1/1	0.84	0.12	59,59,59,59	0
54	MG	1A	3101	1/1	0.84	0.24	46,46,46,46	0
54	MG	2a	1695	1/1	0.84	0.08	95,95,95,95	0
54	MG	1A	3510	1/1	0.84	0.12	57,57,57,57	0
54	MG	2A	3157	1/1	0.84	0.14	56,56,56,56	0
54	MG	1B	1028	1/1	0.84	0.07	75,75,75,75	0
54	MG	1a	1729	1/1	0.84	0.20	92,92,92,92	0
54	MG	1A	3395	1/1	0.84	0.21	57,57,57,57	0
54	MG	1A	3524	1/1	0.84	0.12	59,59,59,59	0
54	MG	1D	301	1/1	0.84	0.19	22,22,22,22	0
54	MG	2A	3174	1/1	0.84	0.12	72,72,72,72	0
54	MG	2A	3058	1/1	0.84	0.14	70,70,70,70	0
54	MG	1a	1738	1/1	0.84	0.17	78,78,78,78	0
54	MG	2A	3067	1/1	0.84	0.34	46,46,46,46	0
54	MG	1A	3217	1/1	0.84	0.15	48,48,48,48	0
54	MG	1a	1740	1/1	0.84	0.12	77,77,77,77	0
54	MG	2a	1606	1/1	0.84	0.22	57,57,57,57	0
54	MG	1A	3815	1/1	0.84	0.10	61,61,61,61	0
54	MG	1A	3109	1/1	0.84	0.19	46,46,46,46	0
54	MG	1A	3049	1/1	0.84	0.18	69,69,69,69	0
54	MG	2A	3439	1/1	0.84	0.08	65,65,65,65	0
54	MG	2A	3443	1/1	0.84	0.07	111,111,111,111	0
54	MG	1A	3124	1/1	0.84	0.09	67,67,67,67	0
54	MG	2t	201	1/1	0.84	0.26	71,71,71,71	0
54	MG	2A	3117	1/1	0.85	0.14	45,45,45,45	0
53	MPD	2A	3002	8/8	0.85	0.28	89,92,94,95	0
54	MG	2A	3046	1/1	0.85	0.13	69,69,69,69	0
54	MG	2A	3047	1/1	0.85	0.17	61,61,61,61	0
54	MG	1a	1722	1/1	0.85	0.11	85,85,85,85	0
54	MG	1A	3666	1/1	0.85	0.12	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	3424	1/1	0.85	0.08	88,88,88,88	0
54	MG	1G	203	1/1	0.85	0.18	91,91,91,91	0
54	MG	1a	1626	1/1	0.85	0.24	70,70,70,70	0
54	MG	1A	3372	1/1	0.85	0.13	59,59,59,59	0
54	MG	2A	3441	1/1	0.85	0.15	88,88,88,88	0
54	MG	2A	3442	1/1	0.85	0.13	74,74,74,74	0
54	MG	1a	1633	1/1	0.85	0.09	85,85,85,85	0
54	MG	1A	3224	1/1	0.85	0.10	45,45,45,45	0
54	MG	1A	3051	1/1	0.85	0.14	77,77,77,77	0
54	MG	1A	3017	1/1	0.85	0.24	57,57,57,57	0
54	MG	1a	1679	1/1	0.85	0.16	57,57,57,57	0
54	MG	2A	3307	1/1	0.85	0.10	75,75,75,75	0
54	MG	2a	1683	1/1	0.85	0.21	83,83,83,83	0
54	MG	1A	3484	1/1	0.85	0.10	64,64,64,64	0
54	MG	2a	1687	1/1	0.85	0.10	70,70,70,70	0
54	MG	2A	3078	1/1	0.85	0.18	58,58,58,58	0
54	MG	1A	3117	1/1	0.85	0.20	26,26,26,26	0
54	MG	1a	1683	1/1	0.85	0.12	73,73,73,73	0
54	MG	1a	1643	1/1	0.85	0.14	87,87,87,87	0
54	MG	2A	3176	1/1	0.85	0.21	54,54,54,54	0
54	MG	2a	1697	1/1	0.85	0.08	75,75,75,75	0
54	MG	1A	3861	1/1	0.85	0.10	133,133,133,133	0
54	MG	1a	1693	1/1	0.85	0.24	68,68,68,68	0
54	MG	1A	3054	1/1	0.85	0.13	57,57,57,57	0
54	MG	2a	1708	1/1	0.85	0.18	72,72,72,72	0
54	MG	2A	3501	1/1	0.85	0.12	60,60,60,60	0
54	MG	2a	1718	1/1	0.85	0.09	95,95,95,95	0
54	MG	2A	3337	1/1	0.85	0.12	69,69,69,69	0
54	MG	2a	1731	1/1	0.85	0.12	86,86,86,86	0
54	MG	1a	1649	1/1	0.85	0.17	95,95,95,95	0
54	MG	2a	1738	1/1	0.85	0.12	93,93,93,93	0
54	MG	1A	3808	1/1	0.85	0.10	63,63,63,63	0
54	MG	1a	1603	1/1	0.85	0.18	118,118,118,118	0
54	MG	1a	1827	1/1	0.85	0.16	95,95,95,95	0
54	MG	2a	1627	1/1	0.85	0.18	69,69,69,69	0
54	MG	2A	3203	1/1	0.85	0.20	66,66,66,66	0
54	MG	2A	3566	1/1	0.85	0.12	81,81,81,81	0
54	MG	2A	3101	1/1	0.85	0.15	56,56,56,56	0
54	MG	1A	3452	1/1	0.85	0.08	52,52,52,52	0
54	MG	2A	3620	1/1	0.85	0.14	101,101,101,101	0
54	MG	2A	3628	1/1	0.85	0.14	60,60,60,60	0
54	MG	1A	3461	1/1	0.85	0.16	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1659	1/1	0.85	0.24	70,70,70,70	0
54	MG	2A	3034	1/1	0.85	0.19	62,62,62,62	0
54	MG	2A	3038	1/1	0.85	0.16	71,71,71,71	0
54	MG	1F	311	1/1	0.85	0.15	90,90,90,90	0
55	ARG	1F	303	12/12	0.85	0.22	56,82,107,107	0
54	MG	2a	1643	1/1	0.86	0.11	51,51,51,51	0
54	MG	2A	3598	1/1	0.86	0.12	64,64,64,64	0
54	MG	1a	1708	1/1	0.86	0.17	64,64,64,64	0
54	MG	2a	1650	1/1	0.86	0.18	59,59,59,59	0
54	MG	1A	3895	1/1	0.86	0.16	56,56,56,56	0
54	MG	2A	3622	1/1	0.86	0.09	97,97,97,97	0
54	MG	1A	3382	1/1	0.86	0.12	63,63,63,63	0
54	MG	1A	3307	1/1	0.86	0.10	41,41,41,41	0
54	MG	2A	3189	1/1	0.86	0.21	83,83,83,83	0
54	MG	1W	204	1/1	0.86	0.17	52,52,52,52	0
54	MG	2A	3088	1/1	0.86	0.18	52,52,52,52	0
54	MG	1A	3757	1/1	0.86	0.12	44,44,44,44	0
54	MG	2A	3197	1/1	0.86	0.20	78,78,78,78	0
54	MG	1a	1719	1/1	0.86	0.17	102,102,102,102	0
54	MG	1a	1657	1/1	0.86	0.12	95,95,95,95	0
54	MG	2B	208	1/1	0.86	0.27	79,79,79,79	0
54	MG	1a	1790	1/1	0.86	0.13	95,95,95,95	0
54	MG	1A	3013	1/1	0.86	0.18	36,36,36,36	0
54	MG	1A	3665	1/1	0.86	0.12	59,59,59,59	0
54	MG	2A	3004	1/1	0.86	0.16	65,65,65,65	0
54	MG	2A	3413	1/1	0.86	0.09	77,77,77,77	0
54	MG	2F	302	1/1	0.86	0.14	69,69,69,69	0
54	MG	1a	1795	1/1	0.86	0.12	81,81,81,81	0
54	MG	2A	3415	1/1	0.86	0.11	59,59,59,59	0
54	MG	2A	3103	1/1	0.86	0.10	82,82,82,82	0
54	MG	2A	3220	1/1	0.86	0.17	70,70,70,70	0
54	MG	1a	1733	1/1	0.86	0.15	76,76,76,76	0
54	MG	2A	3008	1/1	0.86	0.14	61,61,61,61	0
54	MG	1A	3125	1/1	0.86	0.18	37,37,37,37	0
54	MG	1a	1604	1/1	0.86	0.25	65,65,65,65	0
54	MG	1A	3476	1/1	0.86	0.24	65,65,65,65	0
54	MG	1A	3057	1/1	0.86	0.14	56,56,56,56	0
54	MG	1A	3115	1/1	0.86	0.16	42,42,42,42	0
54	MG	2A	3119	1/1	0.86	0.21	76,76,76,76	0
54	MG	1A	3172	1/1	0.86	0.13	71,71,71,71	0
54	MG	2A	3132	1/1	0.86	0.18	54,54,54,54	0
54	MG	1a	1620	1/1	0.86	0.11	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3585	1/1	0.86	0.08	62,62,62,62	0
54	MG	2a	1725	1/1	0.86	0.09	73,73,73,73	0
54	MG	1A	3077	1/1	0.86	0.10	64,64,64,64	0
54	MG	2A	3285	1/1	0.86	0.15	68,68,68,68	0
54	MG	1A	3493	1/1	0.86	0.19	68,68,68,68	0
54	MG	1A	3258	1/1	0.86	0.11	81,81,81,81	0
54	MG	2A	3304	1/1	0.86	0.11	65,65,65,65	0
54	MG	1A	3037	1/1	0.86	0.14	56,56,56,56	0
54	MG	1A	3599	1/1	0.86	0.10	49,49,49,49	0
54	MG	1A	3435	1/1	0.86	0.16	51,51,51,51	0
54	MG	1A	3366	1/1	0.86	0.10	45,45,45,45	0
54	MG	1N	202	1/1	0.86	0.16	66,66,66,66	0
54	MG	1a	1694	1/1	0.86	0.14	73,73,73,73	0
54	MG	1A	3369	1/1	0.86	0.15	37,37,37,37	0
54	MG	1Q	201	1/1	0.86	0.14	51,51,51,51	0
54	MG	1A	3230	1/1	0.86	0.16	49,49,49,49	0
54	MG	2A	3171	1/1	0.86	0.18	84,84,84,84	0
54	MG	1A	3890	1/1	0.86	0.60	45,45,45,45	0
54	MG	2A	3586	1/1	0.86	0.11	104,104,104,104	0
54	MG	2p	101	1/1	0.86	0.17	55,55,55,55	0
54	MG	2A	3593	1/1	0.86	0.09	99,99,99,99	0
54	MG	1a	1772	1/1	0.86	0.12	83,83,83,83	0
54	MG	1a	1629	1/1	0.87	0.22	68,68,68,68	0
54	MG	1A	3701	1/1	0.87	0.14	47,47,47,47	0
54	MG	1A	3605	1/1	0.87	0.12	71,71,71,71	0
54	MG	1a	1797	1/1	0.87	0.18	68,68,68,68	0
54	MG	2a	1672	1/1	0.87	0.38	55,55,55,55	0
54	MG	1A	3351	1/1	0.87	0.10	66,66,66,66	0
54	MG	2A	3482	1/1	0.87	0.10	106,106,106,106	0
54	MG	2A	3124	1/1	0.87	0.12	93,93,93,93	0
54	MG	2A	3345	1/1	0.87	0.16	70,70,70,70	0
54	MG	1a	1756	1/1	0.87	0.10	78,78,78,78	0
54	MG	2A	3213	1/1	0.87	0.11	73,73,73,73	0
54	MG	1a	1759	1/1	0.87	0.15	101,101,101,101	0
54	MG	2A	3538	1/1	0.87	0.14	42,42,42,42	0
54	MG	1A	3527	1/1	0.87	0.11	56,56,56,56	0
54	MG	1A	3799	1/1	0.87	0.18	53,53,53,53	0
54	MG	1a	1673	1/1	0.87	0.16	59,59,59,59	0
54	MG	2A	3380	1/1	0.87	0.12	48,48,48,48	0
54	MG	1a	1640	1/1	0.87	0.19	75,75,75,75	0
54	MG	1A	3807	1/1	0.87	0.13	64,64,64,64	0
54	MG	2a	1699	1/1	0.87	0.09	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3383	1/1	0.87	0.07	80,80,80,80	0
54	MG	2A	3391	1/1	0.87	0.14	65,65,65,65	0
54	MG	1A	3234	1/1	0.87	0.14	59,59,59,59	0
54	MG	2A	3153	1/1	0.87	0.17	78,78,78,78	0
54	MG	1a	1608	1/1	0.87	0.16	78,78,78,78	0
54	MG	2A	3246	1/1	0.87	0.18	88,88,88,88	0
54	MG	1a	1613	1/1	0.87	0.12	69,69,69,69	0
54	MG	2A	3412	1/1	0.87	0.11	70,70,70,70	0
54	MG	2A	3638	1/1	0.87	0.12	55,55,55,55	0
54	MG	2A	3256	1/1	0.87	0.12	54,54,54,54	0
54	MG	1a	1830	1/1	0.87	0.07	62,62,62,62	0
54	MG	1A	3265	1/1	0.87	0.13	86,86,86,86	0
54	MG	1A	3185	1/1	0.87	0.16	61,61,61,61	0
54	MG	2A	3264	1/1	0.87	0.13	98,98,98,98	0
54	MG	1A	3506	1/1	0.87	0.09	65,65,65,65	0
54	MG	1a	1843	1/1	0.87	0.14	81,81,81,81	0
54	MG	1A	3729	1/1	0.87	0.10	46,46,46,46	0
54	MG	2A	3100	1/1	0.87	0.14	69,69,69,69	0
54	MG	1A	3507	1/1	0.87	0.14	50,50,50,50	0
54	MG	1a	1851	1/1	0.87	0.09	76,76,76,76	0
54	MG	2A	3184	1/1	0.87	0.10	56,56,56,56	0
54	MG	1A	3684	1/1	0.87	0.21	74,74,74,74	0
54	MG	1A	3106	1/1	0.87	0.10	48,48,48,48	0
54	MG	2A	3107	1/1	0.87	0.26	85,85,85,85	0
54	MG	1a	1746	1/1	0.87	0.18	91,91,91,91	0
54	MG	2A	3049	1/1	0.87	0.17	65,65,65,65	0
55	ARG	1B	1001	12/12	0.87	0.14	49,55,69,72	0
54	MG	1A	3006	1/1	0.87	0.08	49,49,49,49	0
54	MG	2A	3073	1/1	0.88	0.15	60,60,60,60	0
54	MG	2A	3394	1/1	0.88	0.24	48,48,48,48	0
54	MG	1A	3136	1/1	0.88	0.16	43,43,43,43	0
54	MG	1A	3098	1/1	0.88	0.16	44,44,44,44	0
54	MG	1a	1847	1/1	0.88	0.08	62,62,62,62	0
54	MG	2A	3404	1/1	0.88	0.20	81,81,81,81	0
54	MG	1A	3363	1/1	0.88	0.14	52,52,52,52	0
54	MG	1A	3470	1/1	0.88	0.12	45,45,45,45	0
54	MG	1A	3864	1/1	0.88	0.20	50,50,50,50	0
54	MG	1a	1852	1/1	0.88	0.10	106,106,106,106	0
54	MG	1A	3558	1/1	0.88	0.30	81,81,81,81	0
54	MG	1A	3702	1/1	0.88	0.14	71,71,71,71	0
54	MG	2A	3419	1/1	0.88	0.14	55,55,55,55	0
54	MG	1A	3023	1/1	0.88	0.19	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	3430	1/1	0.88	0.09	64,64,64,64	0
54	MG	2A	3089	1/1	0.88	0.21	61,61,61,61	0
54	MG	2A	3432	1/1	0.88	0.10	66,66,66,66	0
54	MG	1A	3881	1/1	0.88	0.12	38,38,38,38	0
54	MG	2A	3436	1/1	0.88	0.13	73,73,73,73	0
54	MG	1A	3887	1/1	0.88	0.11	40,40,40,40	0
54	MG	1A	3144	1/1	0.88	0.11	56,56,56,56	0
54	MG	1A	3572	1/1	0.88	0.09	61,61,61,61	0
54	MG	1e	202	1/1	0.88	0.14	78,78,78,78	0
54	MG	2A	3221	1/1	0.88	0.17	65,65,65,65	0
54	MG	1A	3899	1/1	0.88	0.14	54,54,54,54	0
54	MG	2A	3098	1/1	0.88	0.14	58,58,58,58	0
54	MG	1a	1691	1/1	0.88	0.09	68,68,68,68	0
54	MG	2A	3452	1/1	0.88	0.12	70,70,70,70	0
54	MG	1g	202	1/1	0.88	0.18	85,85,85,85	0
54	MG	1A	3028	1/1	0.88	0.17	47,47,47,47	0
54	MG	1A	3206	1/1	0.88	0.32	40,40,40,40	0
54	MG	1A	3720	1/1	0.88	0.25	64,64,64,64	0
54	MG	1A	3584	1/1	0.88	0.10	70,70,70,70	0
54	MG	1A	3207	1/1	0.88	0.17	37,37,37,37	0
54	MG	1a	1701	1/1	0.88	0.18	93,93,93,93	0
54	MG	1A	3267	1/1	0.88	0.10	58,58,58,58	0
54	MG	2A	3003	1/1	0.88	0.22	49,49,49,49	0
54	MG	2A	3486	1/1	0.88	0.12	96,96,96,96	0
54	MG	1A	3270	1/1	0.88	0.25	59,59,59,59	0
53	MPD	1A	3001	8/8	0.88	0.23	58,65,67,67	0
54	MG	1A	3301	1/1	0.88	0.09	51,51,51,51	0
54	MG	2a	1662	1/1	0.88	0.16	64,64,64,64	0
54	MG	2A	3506	1/1	0.88	0.12	64,64,64,64	0
54	MG	2A	3275	1/1	0.88	0.18	75,75,75,75	0
54	MG	1A	3162	1/1	0.88	0.09	43,43,43,43	0
54	MG	2A	3527	1/1	0.88	0.13	55,55,55,55	0
54	MG	2a	1669	1/1	0.88	0.14	61,61,61,61	0
54	MG	2A	3531	1/1	0.88	0.17	74,74,74,74	0
54	MG	2A	3533	1/1	0.88	0.14	61,61,61,61	0
54	MG	2a	1673	1/1	0.88	0.21	69,69,69,69	0
54	MG	1A	3035	1/1	0.88	0.24	57,57,57,57	0
54	MG	2A	3539	1/1	0.88	0.13	74,74,74,74	0
54	MG	2A	3292	1/1	0.88	0.14	74,74,74,74	0
54	MG	2A	3125	1/1	0.88	0.10	73,73,73,73	0
54	MG	2A	3299	1/1	0.88	0.08	53,53,53,53	0
54	MG	2A	3546	1/1	0.88	0.13	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3300	1/1	0.88	0.09	51,51,51,51	0
54	MG	2A	3131	1/1	0.88	0.17	64,64,64,64	0
54	MG	2A	3302	1/1	0.88	0.14	59,59,59,59	0
54	MG	1A	3602	1/1	0.88	0.23	54,54,54,54	0
54	MG	1A	3164	1/1	0.88	0.12	49,49,49,49	0
54	MG	1A	3516	1/1	0.88	0.20	73,73,73,73	0
54	MG	2A	3605	1/1	0.88	0.14	65,65,65,65	0
54	MG	1A	3612	1/1	0.88	0.13	45,45,45,45	0
54	MG	2A	3031	1/1	0.88	0.20	75,75,75,75	0
54	MG	1a	1648	1/1	0.88	0.24	56,56,56,56	0
54	MG	2A	3036	1/1	0.88	0.19	64,64,64,64	0
54	MG	2A	3330	1/1	0.88	0.11	82,82,82,82	0
54	MG	1A	3613	1/1	0.88	0.10	32,32,32,32	0
54	MG	2a	1710	1/1	0.88	0.08	98,98,98,98	0
54	MG	1A	3806	1/1	0.88	0.17	85,85,85,85	0
54	MG	2A	3643	1/1	0.88	0.11	62,62,62,62	0
54	MG	1A	3614	1/1	0.88	0.12	57,57,57,57	0
54	MG	1A	3011	1/1	0.88	0.13	55,55,55,55	0
54	MG	2a	1732	1/1	0.88	0.12	91,91,91,91	0
54	MG	2a	1736	1/1	0.88	0.12	100,100,100,100	0
54	MG	2A	3156	1/1	0.88	0.10	57,57,57,57	0
54	MG	1A	3167	1/1	0.88	0.23	42,42,42,42	0
54	MG	1A	3038	1/1	0.88	0.12	53,53,53,53	0
54	MG	1A	3083	1/1	0.88	0.16	51,51,51,51	0
54	MG	2A	3164	1/1	0.88	0.21	62,62,62,62	0
54	MG	2a	1747	1/1	0.88	0.11	129,129,129,129	0
54	MG	1a	1823	1/1	0.88	0.10	99,99,99,99	0
54	MG	1a	1660	1/1	0.88	0.17	85,85,85,85	0
54	MG	2A	3055	1/1	0.88	0.25	66,66,66,66	0
54	MG	2B	214	1/1	0.88	0.08	101,101,101,101	0
54	MG	1A	3638	1/1	0.88	0.09	68,68,68,68	0
54	MG	2D	306	1/1	0.88	0.12	52,52,52,52	0
54	MG	2A	3374	1/1	0.88	0.10	60,60,60,60	0
54	MG	2a	1764	1/1	0.88	0.15	61,61,61,61	0
54	MG	1A	3018	1/1	0.88	0.20	40,40,40,40	0
54	MG	2f	201	1/1	0.88	0.10	79,79,79,79	0
54	MG	2A	3378	1/1	0.88	0.16	54,54,54,54	0
54	MG	2A	3061	1/1	0.88	0.13	61,61,61,61	0
54	MG	2A	3178	1/1	0.88	0.12	44,44,44,44	0
54	MG	1A	3532	1/1	0.88	0.15	46,46,46,46	0
54	MG	2A	3181	1/1	0.88	0.16	57,57,57,57	0
54	MG	2A	3388	1/1	0.88	0.24	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3543	1/1	0.88	0.16	42,42,42,42	0
54	MG	2A	3179	1/1	0.89	0.43	70,70,70,70	0
54	MG	1A	3142	1/1	0.89	0.15	36,36,36,36	0
54	MG	1a	1684	1/1	0.89	0.21	56,56,56,56	0
54	MG	1A	3777	1/1	0.89	0.16	35,35,35,35	0
54	MG	2A	3340	1/1	0.89	0.12	57,57,57,57	0
54	MG	1A	3581	1/1	0.89	0.11	66,66,66,66	0
54	MG	2a	1644	1/1	0.89	0.20	92,92,92,92	0
54	MG	1a	1813	1/1	0.89	0.14	76,76,76,76	0
54	MG	2A	3188	1/1	0.89	0.17	67,67,67,67	0
54	MG	2a	1649	1/1	0.89	0.11	40,40,40,40	0
54	MG	1A	3489	1/1	0.89	0.09	64,64,64,64	0
54	MG	1A	3537	1/1	0.89	0.15	39,39,39,39	0
54	MG	1a	1752	1/1	0.89	0.23	61,61,61,61	0
54	MG	1A	3249	1/1	0.89	0.14	45,45,45,45	0
54	MG	1A	3058	1/1	0.89	0.08	51,51,51,51	0
54	MG	2A	3580	1/1	0.89	0.19	97,97,97,97	0
54	MG	1A	3130	1/1	0.89	0.19	39,39,39,39	0
54	MG	13	101	1/1	0.89	0.18	76,76,76,76	0
54	MG	1A	3809	1/1	0.89	0.09	57,57,57,57	0
54	MG	2A	3207	1/1	0.89	0.16	61,61,61,61	0
54	MG	2A	3601	1/1	0.89	0.11	75,75,75,75	0
54	MG	2A	3032	1/1	0.89	0.25	61,61,61,61	0
54	MG	2A	3609	1/1	0.89	0.18	80,80,80,80	0
54	MG	1A	3471	1/1	0.89	0.12	62,62,62,62	0
54	MG	1A	3659	1/1	0.89	0.23	62,62,62,62	0
54	MG	2A	3212	1/1	0.89	0.14	58,58,58,58	0
54	MG	1a	1833	1/1	0.89	0.10	122,122,122,122	0
54	MG	2A	3393	1/1	0.89	0.11	77,77,77,77	0
54	MG	2A	3040	1/1	0.89	0.09	65,65,65,65	0
54	MG	2A	3641	1/1	0.89	0.11	88,88,88,88	0
54	MG	1A	3821	1/1	0.89	0.14	51,51,51,51	0
54	MG	2A	3044	1/1	0.89	0.06	71,71,71,71	0
54	MG	1A	3331	1/1	0.89	0.11	40,40,40,40	0
54	MG	2A	3122	1/1	0.89	0.17	74,74,74,74	0
54	MG	2A	3407	1/1	0.89	0.09	66,66,66,66	0
54	MG	1a	1845	1/1	0.89	0.09	63,63,63,63	0
54	MG	1a	1768	1/1	0.89	0.10	81,81,81,81	0
54	MG	2A	3127	1/1	0.89	0.15	49,49,49,49	0
54	MG	1a	1607	1/1	0.89	0.14	108,108,108,108	0
54	MG	1A	3373	1/1	0.89	0.09	67,67,67,67	0
54	MG	1A	3836	1/1	0.89	0.09	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	2A	3245	1/1	0.89	0.29	71,71,71,71	0
54	MG	2A	3134	1/1	0.89	0.11	71,71,71,71	0
54	MG	1a	1718	1/1	0.89	0.14	86,86,86,86	0
54	MG	2B	217	1/1	0.89	0.09	81,81,81,81	0
54	MG	2a	1705	1/1	0.89	0.13	93,93,93,93	0
54	MG	2A	3250	1/1	0.89	0.12	60,60,60,60	0
54	MG	2A	3136	1/1	0.89	0.15	62,62,62,62	0
54	MG	2A	3137	1/1	0.89	0.16	67,67,67,67	0
54	MG	2A	3138	1/1	0.89	0.31	49,49,49,49	0
54	MG	2A	3438	1/1	0.89	0.09	80,80,80,80	0
54	MG	2A	3053	1/1	0.89	0.23	56,56,56,56	0
54	MG	2A	3440	1/1	0.89	0.21	76,76,76,76	0
54	MG	2A	3140	1/1	0.89	0.10	61,61,61,61	0
54	MG	1A	3254	1/1	0.89	0.19	62,62,62,62	0
54	MG	1A	3847	1/1	0.89	0.09	38,38,38,38	0
54	MG	1A	3848	1/1	0.89	0.13	55,55,55,55	0
54	MG	2A	3280	1/1	0.89	0.10	53,53,53,53	0
54	MG	1a	1618	1/1	0.89	0.12	81,81,81,81	0
54	MG	2A	3450	1/1	0.89	0.15	49,49,49,49	0
54	MG	1a	1732	1/1	0.89	0.15	70,70,70,70	0
54	MG	2a	1746	1/1	0.89	0.09	119,119,119,119	0
54	MG	1A	3677	1/1	0.89	0.17	71,71,71,71	0
54	MG	2a	1748	1/1	0.89	0.11	100,100,100,100	0
54	MG	1A	3010	1/1	0.89	0.13	46,46,46,46	0
54	MG	2A	3455	1/1	0.89	0.14	68,68,68,68	0
54	MG	1A	3354	1/1	0.89	0.14	38,38,38,38	0
54	MG	2A	3457	1/1	0.89	0.16	79,79,79,79	0
54	MG	1A	3743	1/1	0.89	0.11	47,47,47,47	0
54	MG	1A	3744	1/1	0.89	0.11	55,55,55,55	0
54	MG	1g	201	1/1	0.89	0.14	87,87,87,87	0
54	MG	1A	3747	1/1	0.89	0.08	54,54,54,54	0
54	MG	1A	3042	1/1	0.89	0.12	63,63,63,63	0
54	MG	2A	3082	1/1	0.89	0.08	76,76,76,76	0
54	MG	1l	202	1/1	0.89	0.06	51,51,51,51	0
54	MG	1a	1799	1/1	0.89	0.09	96,96,96,96	0
54	MG	2A	3173	1/1	0.89	0.24	63,63,63,63	0
54	MG	1A	3869	1/1	0.89	0.21	58,58,58,58	0
54	MG	2A	3496	1/1	0.89	0.14	69,69,69,69	0
54	MG	1A	3697	1/1	0.89	0.11	72,72,72,72	0
54	MG	1a	1803	1/1	0.89	0.09	93,93,93,93	0
54	MG	2A	3298	1/1	0.90	0.08	82,82,82,82	0
54	MG	1a	1815	1/1	0.90	0.09	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3694	1/1	0.90	0.09	61,61,61,61	0
54	MG	1A	3105	1/1	0.90	0.18	52,52,52,52	0
54	MG	1A	3700	1/1	0.90	0.20	58,58,58,58	0
54	MG	1A	3810	1/1	0.90	0.07	59,59,59,59	0
54	MG	2A	3305	1/1	0.90	0.14	58,58,58,58	0
54	MG	1A	3374	1/1	0.90	0.08	73,73,73,73	0
54	MG	2A	3483	1/1	0.90	0.10	53,53,53,53	0
54	MG	1A	3321	1/1	0.90	0.14	61,61,61,61	0
54	MG	2A	3057	1/1	0.90	0.08	55,55,55,55	0
54	MG	1A	3025	1/1	0.90	0.19	38,38,38,38	0
54	MG	1F	304	1/1	0.90	0.18	43,43,43,43	0
54	MG	1F	305	1/1	0.90	0.24	50,50,50,50	0
54	MG	1A	3824	1/1	0.90	0.12	63,63,63,63	0
54	MG	1A	3825	1/1	0.90	0.19	72,72,72,72	0
54	MG	1G	201	1/1	0.90	0.07	92,92,92,92	0
54	MG	1A	3259	1/1	0.90	0.21	79,79,79,79	0
54	MG	1A	3706	1/1	0.90	0.09	50,50,50,50	0
54	MG	2A	3532	1/1	0.90	0.07	89,89,89,89	0
54	MG	1G	204	1/1	0.90	0.12	73,73,73,73	0
54	MG	1H	202	1/1	0.90	0.11	64,64,64,64	0
54	MG	1A	3835	1/1	0.90	0.15	50,50,50,50	0
54	MG	1A	3329	1/1	0.90	0.07	57,57,57,57	0
54	MG	2A	3343	1/1	0.90	0.11	47,47,47,47	0
54	MG	1A	3389	1/1	0.90	0.14	56,56,56,56	0
54	MG	2A	3544	1/1	0.90	0.07	86,86,86,86	0
54	MG	2A	3183	1/1	0.90	0.29	84,84,84,84	0
54	MG	2A	3553	1/1	0.90	0.09	100,100,100,100	0
54	MG	1a	1854	1/1	0.90	0.12	57,57,57,57	0
54	MG	1A	3839	1/1	0.90	0.11	61,61,61,61	0
54	MG	2A	3575	1/1	0.90	0.10	52,52,52,52	0
54	MG	2A	3363	1/1	0.90	0.24	76,76,76,76	0
54	MG	1a	1665	1/1	0.90	0.12	86,86,86,86	0
54	MG	2A	3589	1/1	0.90	0.10	67,67,67,67	0
54	MG	1A	3027	1/1	0.90	0.14	49,49,49,49	0
54	MG	1A	3715	1/1	0.90	0.10	71,71,71,71	0
54	MG	2A	3375	1/1	0.90	0.11	50,50,50,50	0
54	MG	1a	1668	1/1	0.90	0.23	69,69,69,69	0
54	MG	2a	1674	1/1	0.90	0.22	66,66,66,66	0
54	MG	1A	3341	1/1	0.90	0.14	30,30,30,30	0
54	MG	1A	3086	1/1	0.90	0.10	68,68,68,68	0
54	MG	2A	3381	1/1	0.90	0.12	99,99,99,99	0
54	MG	1A	3033	1/1	0.90	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	10	101	1/1	0.90	0.16	82,82,82,82	0
54	MG	2A	3202	1/1	0.90	0.25	73,73,73,73	0
54	MG	2A	3630	1/1	0.90	0.13	58,58,58,58	0
54	MG	10	105	1/1	0.90	0.08	57,57,57,57	0
54	MG	2A	3204	1/1	0.90	0.10	51,51,51,51	0
54	MG	1a	1769	1/1	0.90	0.11	90,90,90,90	0
54	MG	1A	3039	1/1	0.90	0.18	38,38,38,38	0
54	MG	1a	1771	1/1	0.90	0.20	89,89,89,89	0
54	MG	1A	3277	1/1	0.90	0.13	89,89,89,89	0
54	MG	2A	3396	1/1	0.90	0.08	82,82,82,82	0
54	MG	1A	3633	1/1	0.90	0.19	60,60,60,60	0
54	MG	17	103	1/1	0.90	0.10	62,62,62,62	0
54	MG	1A	3495	1/1	0.90	0.12	65,65,65,65	0
54	MG	2A	3405	1/1	0.90	0.12	81,81,81,81	0
54	MG	2a	1707	1/1	0.90	0.11	84,84,84,84	0
54	MG	2A	3108	1/1	0.90	0.09	50,50,50,50	0
54	MG	1A	3639	1/1	0.90	0.07	58,58,58,58	0
54	MG	1a	1782	1/1	0.90	0.10	86,86,86,86	0
54	MG	2a	1715	1/1	0.90	0.10	88,88,88,88	0
54	MG	1A	3497	1/1	0.90	0.11	44,44,44,44	0
54	MG	1A	3874	1/1	0.90	0.11	65,65,65,65	0
54	MG	1A	3500	1/1	0.90	0.20	73,73,73,73	0
54	MG	2a	1730	1/1	0.90	0.12	97,97,97,97	0
54	MG	1A	3662	1/1	0.90	0.13	43,43,43,43	0
54	MG	1a	1609	1/1	0.90	0.05	120,120,120,120	0
54	MG	2a	1733	1/1	0.90	0.10	86,86,86,86	0
54	MG	2A	3420	1/1	0.90	0.12	51,51,51,51	0
54	MG	1A	3221	1/1	0.90	0.04	100,100,100,100	0
54	MG	1A	3505	1/1	0.90	0.10	49,49,49,49	0
54	MG	1A	3888	1/1	0.90	0.31	80,80,80,80	0
54	MG	2G	203	1/1	0.90	0.12	104,104,104,104	0
54	MG	1A	3433	1/1	0.90	0.09	66,66,66,66	0
54	MG	1A	3759	1/1	0.90	0.12	51,51,51,51	0
54	MG	2A	3130	1/1	0.90	0.11	62,62,62,62	0
54	MG	1A	3763	1/1	0.90	0.15	46,46,46,46	0
54	MG	2A	3028	1/1	0.90	0.17	44,44,44,44	0
54	MG	2T	202	1/1	0.90	0.15	65,65,65,65	0
54	MG	1A	3768	1/1	0.90	0.07	51,51,51,51	0
54	MG	1A	3222	1/1	0.90	0.10	52,52,52,52	0
54	MG	20	101	1/1	0.90	0.18	80,80,80,80	0
54	MG	1A	3682	1/1	0.90	0.10	79,79,79,79	0
54	MG	1a	1804	1/1	0.90	0.27	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	1601	1/1	0.90	0.12	74,74,74,74	0
54	MG	2A	3269	1/1	0.90	0.10	88,88,88,88	0
54	MG	2A	3271	1/1	0.90	0.09	67,67,67,67	0
54	MG	1A	3071	1/1	0.90	0.17	54,54,54,54	0
54	MG	1A	3798	1/1	0.90	0.24	71,71,71,71	0
54	MG	1a	1631	1/1	0.90	0.13	68,68,68,68	0
54	MG	1a	1810	1/1	0.90	0.07	82,82,82,82	0
54	MG	1A	3251	1/1	0.90	0.08	41,41,41,41	0
54	MG	2A	3148	1/1	0.90	0.11	42,42,42,42	0
54	MG	1A	3225	1/1	0.90	0.17	54,54,54,54	0
54	MG	1a	1632	1/1	0.91	0.11	59,59,59,59	0
54	MG	1A	3274	1/1	0.91	0.13	22,22,22,22	0
54	MG	2X	101	1/1	0.91	0.09	84,84,84,84	0
54	MG	1A	3118	1/1	0.91	0.20	59,59,59,59	0
54	MG	2A	3217	1/1	0.91	0.35	60,60,60,60	0
54	MG	2I	103	1/1	0.91	0.08	60,60,60,60	0
54	MG	2A	3218	1/1	0.91	0.10	73,73,73,73	0
54	MG	1A	3430	1/1	0.91	0.07	82,82,82,82	0
54	MG	28	101	1/1	0.91	0.19	70,70,70,70	0
54	MG	1A	3210	1/1	0.91	0.13	37,37,37,37	0
54	MG	1a	1638	1/1	0.91	0.19	42,42,42,42	0
54	MG	2A	3095	1/1	0.91	0.24	58,58,58,58	0
54	MG	1D	303	1/1	0.91	0.12	47,47,47,47	0
54	MG	1D	307	1/1	0.91	0.17	36,36,36,36	0
54	MG	2A	3234	1/1	0.91	0.19	65,65,65,65	0
54	MG	1D	308	1/1	0.91	0.20	55,55,55,55	0
54	MG	1A	3299	1/1	0.91	0.17	58,58,58,58	0
54	MG	1A	3138	1/1	0.91	0.16	41,41,41,41	0
54	MG	2a	1614	1/1	0.91	0.10	82,82,82,82	0
54	MG	1A	3593	1/1	0.91	0.06	84,84,84,84	0
54	MG	2a	1616	1/1	0.91	0.08	80,80,80,80	0
54	MG	1A	3705	1/1	0.91	0.09	46,46,46,46	0
54	MG	1a	1749	1/1	0.91	0.17	100,100,100,100	0
54	MG	1A	3831	1/1	0.91	0.16	92,92,92,92	0
54	MG	2A	3449	1/1	0.91	0.13	65,65,65,65	0
54	MG	2a	1622	1/1	0.91	0.07	38,38,38,38	0
54	MG	1e	201	1/1	0.91	0.12	66,66,66,66	0
54	MG	1A	3216	1/1	0.91	0.16	66,66,66,66	0
54	MG	1A	3056	1/1	0.91	0.12	42,42,42,42	0
54	MG	2a	1632	1/1	0.91	0.19	63,63,63,63	0
54	MG	2a	1633	1/1	0.91	0.14	92,92,92,92	0
54	MG	1a	1653	1/1	0.91	0.07	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	1f	202	1/1	0.91	0.24	93,93,93,93	0
54	MG	1A	3447	1/1	0.91	0.26	70,70,70,70	0
54	MG	2A	3265	1/1	0.91	0.13	61,61,61,61	0
54	MG	2A	3266	1/1	0.91	0.10	59,59,59,59	0
54	MG	1A	3123	1/1	0.91	0.15	49,49,49,49	0
54	MG	1A	3252	1/1	0.91	0.17	45,45,45,45	0
54	MG	2a	1641	1/1	0.91	0.12	71,71,71,71	0
54	MG	2A	3465	1/1	0.91	0.11	69,69,69,69	0
54	MG	1A	3845	1/1	0.91	0.15	50,50,50,50	0
54	MG	1P	201	1/1	0.91	0.11	83,83,83,83	0
54	MG	2A	3477	1/1	0.91	0.13	83,83,83,83	0
54	MG	2A	3478	1/1	0.91	0.07	85,85,85,85	0
54	MG	2a	1647	1/1	0.91	0.20	67,67,67,67	0
54	MG	2a	1648	1/1	0.91	0.36	64,64,64,64	0
54	MG	1A	3718	1/1	0.91	0.09	69,69,69,69	0
54	MG	1A	3608	1/1	0.91	0.19	56,56,56,56	0
54	MG	2A	3281	1/1	0.91	0.10	65,65,65,65	0
54	MG	1R	202	1/1	0.91	0.23	41,41,41,41	0
54	MG	2A	3287	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3112	1/1	0.91	0.08	53,53,53,53	0
54	MG	1R	205	1/1	0.91	0.13	49,49,49,49	0
54	MG	1A	3465	1/1	0.91	0.18	46,46,46,46	0
54	MG	1A	3468	1/1	0.91	0.10	62,62,62,62	0
54	MG	1A	3615	1/1	0.91	0.10	57,57,57,57	0
54	MG	1V	201	1/1	0.91	0.21	56,56,56,56	0
54	MG	1a	1671	1/1	0.91	0.30	71,71,71,71	0
54	MG	2A	3529	1/1	0.91	0.09	73,73,73,73	0
54	MG	2A	3009	1/1	0.91	0.10	63,63,63,63	0
54	MG	2a	1666	1/1	0.91	0.15	79,79,79,79	0
54	MG	1A	3535	1/1	0.91	0.11	53,53,53,53	0
54	MG	2A	3014	1/1	0.91	0.17	66,66,66,66	0
54	MG	2A	3537	1/1	0.91	0.06	97,97,97,97	0
54	MG	1W	202	1/1	0.91	0.23	59,59,59,59	0
54	MG	2A	3310	1/1	0.91	0.26	55,55,55,55	0
54	MG	1A	3148	1/1	0.91	0.09	54,54,54,54	0
54	MG	2A	3143	1/1	0.91	0.12	61,61,61,61	0
54	MG	2A	3145	1/1	0.91	0.12	62,62,62,62	0
54	MG	2A	3326	1/1	0.91	0.08	75,75,75,75	0
54	MG	1A	3540	1/1	0.91	0.10	36,36,36,36	0
54	MG	2A	3329	1/1	0.91	0.09	93,93,93,93	0
54	MG	1A	3624	1/1	0.91	0.11	70,70,70,70	0
54	MG	1A	3113	1/1	0.91	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3745	1/1	0.91	0.10	80,80,80,80	0
54	MG	2A	3576	1/1	0.91	0.10	63,63,63,63	0
54	MG	13	102	1/1	0.91	0.11	55,55,55,55	0
54	MG	15	103	1/1	0.91	0.13	67,67,67,67	0
54	MG	1A	3129	1/1	0.91	0.17	42,42,42,42	0
54	MG	1A	3002	1/1	0.91	0.11	46,46,46,46	0
54	MG	1a	1690	1/1	0.91	0.11	62,62,62,62	0
54	MG	1A	3553	1/1	0.91	0.37	57,57,57,57	0
54	MG	2A	3162	1/1	0.91	0.10	101,101,101,101	0
54	MG	2A	3042	1/1	0.91	0.11	65,65,65,65	0
54	MG	2a	1704	1/1	0.91	0.19	84,84,84,84	0
54	MG	2A	3606	1/1	0.91	0.10	63,63,63,63	0
54	MG	2A	3608	1/1	0.91	0.22	86,86,86,86	0
54	MG	1A	3194	1/1	0.91	0.15	50,50,50,50	0
54	MG	2A	3614	1/1	0.91	0.13	64,64,64,64	0
54	MG	2A	3349	1/1	0.91	0.20	54,54,54,54	0
54	MG	1A	3556	1/1	0.91	0.12	53,53,53,53	0
54	MG	1a	1801	1/1	0.91	0.07	107,107,107,107	0
54	MG	1A	3345	1/1	0.91	0.10	60,60,60,60	0
54	MG	1A	3396	1/1	0.91	0.14	25,25,25,25	0
54	MG	1a	1699	1/1	0.91	0.12	90,90,90,90	0
54	MG	1A	3398	1/1	0.91	0.10	89,89,89,89	0
54	MG	2A	3640	1/1	0.91	0.09	58,58,58,58	0
54	MG	1A	3564	1/1	0.91	0.12	65,65,65,65	0
54	MG	1B	1003	1/1	0.91	0.15	60,60,60,60	0
54	MG	1A	3676	1/1	0.91	0.15	77,77,77,77	0
54	MG	1A	3131	1/1	0.91	0.12	39,39,39,39	0
54	MG	1a	1710	1/1	0.91	0.17	56,56,56,56	0
54	MG	1A	3411	1/1	0.91	0.09	54,54,54,54	0
54	MG	1a	1818	1/1	0.91	0.08	56,56,56,56	0
54	MG	2A	3063	1/1	0.91	0.13	52,52,52,52	0
54	MG	2A	3064	1/1	0.91	0.16	77,77,77,77	0
54	MG	2A	3389	1/1	0.91	0.10	69,69,69,69	0
54	MG	2A	3065	1/1	0.91	0.26	67,67,67,67	0
54	MG	1A	3803	1/1	0.91	0.10	70,70,70,70	0
54	MG	2A	3068	1/1	0.91	0.12	51,51,51,51	0
54	MG	1B	1010	1/1	0.91	0.07	58,58,58,58	0
54	MG	1A	3805	1/1	0.91	0.10	49,49,49,49	0
54	MG	2a	1758	1/1	0.91	0.07	102,102,102,102	0
54	MG	1A	3490	1/1	0.91	0.10	60,60,60,60	0
54	MG	1A	3414	1/1	0.91	0.07	69,69,69,69	0
54	MG	2A	3402	1/1	0.91	0.07	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1720	1/1	0.91	0.21	94,94,94,94	0
54	MG	1B	1021	1/1	0.91	0.10	54,54,54,54	0
54	MG	1B	1022	1/1	0.91	0.08	59,59,59,59	0
54	MG	2A	3406	1/1	0.91	0.09	72,72,72,72	0
54	MG	1a	1726	1/1	0.91	0.17	61,61,61,61	0
54	MG	1a	1630	1/1	0.91	0.07	54,54,54,54	0
54	MG	1a	1730	1/1	0.91	0.15	53,53,53,53	0
54	MG	2R	201	1/1	0.91	0.18	58,58,58,58	0
54	MG	1a	1837	1/1	0.91	0.09	64,64,64,64	0
54	MG	1A	3108	1/1	0.91	0.20	57,57,57,57	0
54	MG	19	103	1/1	0.92	0.27	93,93,93,93	0
54	MG	1A	3085	1/1	0.92	0.11	22,22,22,22	0
54	MG	1A	3509	1/1	0.92	0.20	52,52,52,52	0
54	MG	2A	3081	1/1	0.92	0.13	52,52,52,52	0
54	MG	1a	1826	1/1	0.92	0.07	109,109,109,109	0
54	MG	1A	3291	1/1	0.92	0.13	57,57,57,57	0
54	MG	2A	3215	1/1	0.92	0.13	65,65,65,65	0
54	MG	1A	3731	1/1	0.92	0.12	75,75,75,75	0
54	MG	1a	1606	1/1	0.92	0.13	64,64,64,64	0
54	MG	2A	3425	1/1	0.92	0.08	78,78,78,78	0
54	MG	1A	3513	1/1	0.92	0.14	63,63,63,63	0
54	MG	1a	1712	1/1	0.92	0.12	109,109,109,109	0
54	MG	1A	3053	1/1	0.92	0.11	30,30,30,30	0
54	MG	2A	3222	1/1	0.92	0.13	65,65,65,65	0
54	MG	1A	3517	1/1	0.92	0.09	71,71,71,71	0
54	MG	1A	3441	1/1	0.92	0.10	64,64,64,64	0
54	MG	2a	1607	1/1	0.92	0.07	94,94,94,94	0
54	MG	2A	3229	1/1	0.92	0.17	56,56,56,56	0
54	MG	1A	3063	1/1	0.92	0.21	41,41,41,41	0
54	MG	1A	3746	1/1	0.92	0.09	55,55,55,55	0
54	MG	1A	3525	1/1	0.92	0.08	62,62,62,62	0
54	MG	1A	3306	1/1	0.92	0.06	57,57,57,57	0
54	MG	1A	3213	1/1	0.92	0.12	60,60,60,60	0
54	MG	1A	3755	1/1	0.92	0.10	78,78,78,78	0
54	MG	1a	1623	1/1	0.92	0.10	62,62,62,62	0
54	MG	1a	1624	1/1	0.92	0.12	85,85,85,85	0
54	MG	1A	3451	1/1	0.92	0.13	72,72,72,72	0
54	MG	2A	3104	1/1	0.92	0.11	67,67,67,67	0
54	MG	2A	3251	1/1	0.92	0.14	76,76,76,76	0
54	MG	1A	3375	1/1	0.92	0.06	45,45,45,45	0
54	MG	1A	3622	1/1	0.92	0.10	51,51,51,51	0
54	MG	2A	3259	1/1	0.92	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3260	1/1	0.92	0.06	48,48,48,48	0
54	MG	1A	3533	1/1	0.92	0.35	43,43,43,43	0
54	MG	2A	3462	1/1	0.92	0.08	74,74,74,74	0
54	MG	2A	3109	1/1	0.92	0.30	57,57,57,57	0
54	MG	1A	3453	1/1	0.92	0.14	39,39,39,39	0
54	MG	2A	3111	1/1	0.92	0.13	57,57,57,57	0
54	MG	1B	1019	1/1	0.92	0.08	75,75,75,75	0
54	MG	2A	3471	1/1	0.92	0.15	58,58,58,58	0
54	MG	1A	3454	1/1	0.92	0.14	67,67,67,67	0
54	MG	2A	3476	1/1	0.92	0.09	78,78,78,78	0
54	MG	1A	3377	1/1	0.92	0.14	55,55,55,55	0
54	MG	1A	3145	1/1	0.92	0.23	45,45,45,45	0
54	MG	1B	1027	1/1	0.92	0.07	43,43,43,43	0
54	MG	1A	3069	1/1	0.92	0.10	39,39,39,39	0
54	MG	1A	3650	1/1	0.92	0.10	61,61,61,61	0
54	MG	2A	3121	1/1	0.92	0.14	82,82,82,82	0
54	MG	2A	3490	1/1	0.92	0.10	64,64,64,64	0
54	MG	1A	3545	1/1	0.92	0.09	50,50,50,50	0
54	MG	1A	3219	1/1	0.92	0.14	34,34,34,34	0
54	MG	1A	3663	1/1	0.92	0.11	51,51,51,51	0
54	MG	2A	3500	1/1	0.92	0.13	89,89,89,89	0
54	MG	1A	3550	1/1	0.92	0.13	46,46,46,46	0
54	MG	1A	3552	1/1	0.92	0.14	36,36,36,36	0
54	MG	1D	309	1/1	0.92	0.13	71,71,71,71	0
54	MG	2A	3515	1/1	0.92	0.08	45,45,45,45	0
54	MG	2A	3518	1/1	0.92	0.17	65,65,65,65	0
54	MG	1A	3020	1/1	0.92	0.09	50,50,50,50	0
54	MG	2A	3525	1/1	0.92	0.13	61,61,61,61	0
54	MG	1F	302	1/1	0.92	0.08	57,57,57,57	0
54	MG	1A	3811	1/1	0.92	0.12	58,58,58,58	0
54	MG	1a	1651	1/1	0.92	0.14	54,54,54,54	0
54	MG	2a	1665	1/1	0.92	0.17	37,37,37,37	0
54	MG	1A	3812	1/1	0.92	0.09	55,55,55,55	0
54	MG	1A	3813	1/1	0.92	0.11	75,75,75,75	0
54	MG	1A	3554	1/1	0.92	0.09	70,70,70,70	0
54	MG	1F	313	1/1	0.92	0.09	64,64,64,64	0
54	MG	2a	1670	1/1	0.92	0.10	57,57,57,57	0
54	MG	1A	3026	1/1	0.92	0.08	48,48,48,48	0
54	MG	1A	3160	1/1	0.92	0.12	37,37,37,37	0
54	MG	2A	3321	1/1	0.92	0.08	77,77,77,77	0
54	MG	1A	3325	1/1	0.92	0.10	57,57,57,57	0
54	MG	2A	3144	1/1	0.92	0.13	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3161	1/1	0.92	0.13	61,61,61,61	0
54	MG	2A	3147	1/1	0.92	0.22	69,69,69,69	0
54	MG	2A	3557	1/1	0.92	0.07	106,106,106,106	0
54	MG	1A	3560	1/1	0.92	0.08	48,48,48,48	0
54	MG	1A	3829	1/1	0.92	0.14	73,73,73,73	0
54	MG	1N	203	1/1	0.92	0.23	88,88,88,88	0
54	MG	1A	3561	1/1	0.92	0.39	70,70,70,70	0
54	MG	2A	3579	1/1	0.92	0.07	52,52,52,52	0
54	MG	2A	3335	1/1	0.92	0.08	61,61,61,61	0
54	MG	2A	3582	1/1	0.92	0.16	91,91,91,91	0
54	MG	2A	3026	1/1	0.92	0.16	42,42,42,42	0
54	MG	2a	1696	1/1	0.92	0.06	82,82,82,82	0
54	MG	2A	3027	1/1	0.92	0.20	47,47,47,47	0
54	MG	1A	3005	1/1	0.92	0.08	56,56,56,56	0
54	MG	2A	3339	1/1	0.92	0.07	68,68,68,68	0
54	MG	2A	3155	1/1	0.92	0.15	59,59,59,59	0
54	MG	2A	3600	1/1	0.92	0.14	66,66,66,66	0
54	MG	2A	3341	1/1	0.92	0.10	83,83,83,83	0
54	MG	1A	3332	1/1	0.92	0.13	36,36,36,36	0
54	MG	1A	3408	1/1	0.92	0.12	19,19,19,19	0
54	MG	1A	3486	1/1	0.92	0.08	69,69,69,69	0
54	MG	1A	3119	1/1	0.92	0.26	44,44,44,44	0
54	MG	2A	3348	1/1	0.92	0.09	37,37,37,37	0
54	MG	1A	3840	1/1	0.92	0.12	62,62,62,62	0
54	MG	1T	2005	1/1	0.92	0.11	53,53,53,53	0
54	MG	2A	3358	1/1	0.92	0.09	104,104,104,104	0
54	MG	2a	1721	1/1	0.92	0.07	86,86,86,86	0
54	MG	1A	3413	1/1	0.92	0.10	42,42,42,42	0
54	MG	1a	1792	1/1	0.92	0.13	111,111,111,111	0
54	MG	2A	3635	1/1	0.92	0.14	64,64,64,64	0
54	MG	2A	3365	1/1	0.92	0.26	70,70,70,70	0
54	MG	2A	3370	1/1	0.92	0.12	82,82,82,82	0
54	MG	2A	3043	1/1	0.92	0.12	60,60,60,60	0
54	MG	1A	3492	1/1	0.92	0.12	70,70,70,70	0
54	MG	1a	1677	1/1	0.92	0.13	66,66,66,66	0
54	MG	1a	1678	1/1	0.92	0.28	57,57,57,57	0
54	MG	1A	3263	1/1	0.92	0.13	44,44,44,44	0
54	MG	1A	3415	1/1	0.92	0.09	40,40,40,40	0
54	MG	1A	3708	1/1	0.92	0.22	49,49,49,49	0
54	MG	1A	3854	1/1	0.92	0.15	34,34,34,34	0
54	MG	1A	3587	1/1	0.92	0.07	64,64,64,64	0
54	MG	1a	1685	1/1	0.92	0.12	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	10	103	1/1	0.92	0.10	56,56,56,56	0
54	MG	10	104	1/1	0.92	0.09	54,54,54,54	0
54	MG	1a	1805	1/1	0.92	0.06	53,53,53,53	0
54	MG	1a	1688	1/1	0.92	0.21	36,36,36,36	0
54	MG	1A	3229	1/1	0.92	0.26	38,38,38,38	0
54	MG	1a	1808	1/1	0.92	0.10	63,63,63,63	0
54	MG	1A	3204	1/1	0.92	0.09	76,76,76,76	0
54	MG	1a	1692	1/1	0.92	0.08	78,78,78,78	0
54	MG	1A	3233	1/1	0.92	0.12	66,66,66,66	0
54	MG	2A	3198	1/1	0.92	0.16	72,72,72,72	0
54	MG	1a	1812	1/1	0.92	0.08	90,90,90,90	0
54	MG	1A	3107	1/1	0.92	0.15	47,47,47,47	0
54	MG	1A	3865	1/1	0.92	0.18	58,58,58,58	0
54	MG	1A	3239	1/1	0.92	0.12	50,50,50,50	0
54	MG	1a	1698	1/1	0.92	0.10	48,48,48,48	0
54	MG	1A	3596	1/1	0.92	0.07	64,64,64,64	0
54	MG	2A	3409	1/1	0.92	0.12	45,45,45,45	0
54	MG	1A	3103	1/1	0.93	0.12	25,25,25,25	0
54	MG	1A	3597	1/1	0.93	0.10	57,57,57,57	0
54	MG	1A	3024	1/1	0.93	0.09	71,71,71,71	0
54	MG	2W	202	1/1	0.93	0.10	79,79,79,79	0
54	MG	1A	3371	1/1	0.93	0.07	52,52,52,52	0
54	MG	1A	3852	1/1	0.93	0.12	85,85,85,85	0
54	MG	1A	3297	1/1	0.93	0.18	51,51,51,51	0
54	MG	2I	102	1/1	0.93	0.10	63,63,63,63	0
54	MG	1A	3140	1/1	0.93	0.17	46,46,46,46	0
54	MG	1A	3450	1/1	0.93	0.10	61,61,61,61	0
54	MG	1A	3300	1/1	0.93	0.20	75,75,75,75	0
54	MG	1A	3859	1/1	0.93	0.18	74,74,74,74	0
54	MG	1W	201	1/1	0.93	0.16	92,92,92,92	0
54	MG	2a	1602	1/1	0.93	0.12	62,62,62,62	0
54	MG	2A	3126	1/1	0.93	0.21	53,53,53,53	0
54	MG	1A	3073	1/1	0.93	0.14	75,75,75,75	0
54	MG	1a	1783	1/1	0.93	0.10	64,64,64,64	0
54	MG	2A	3267	1/1	0.93	0.09	58,58,58,58	0
54	MG	2A	3011	1/1	0.93	0.17	44,44,44,44	0
54	MG	2A	3270	1/1	0.93	0.11	56,56,56,56	0
54	MG	2A	3012	1/1	0.93	0.13	73,73,73,73	0
54	MG	1A	3304	1/1	0.93	0.09	30,30,30,30	0
54	MG	1A	3531	1/1	0.93	0.09	45,45,45,45	0
54	MG	2A	3459	1/1	0.93	0.07	64,64,64,64	0
54	MG	1A	3168	1/1	0.93	0.27	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3740	1/1	0.93	0.09	47,47,47,47	0
54	MG	1A	3456	1/1	0.93	0.07	84,84,84,84	0
54	MG	1A	3534	1/1	0.93	0.18	57,57,57,57	0
54	MG	1I	104	1/1	0.93	0.15	61,61,61,61	0
54	MG	2A	3289	1/1	0.93	0.10	49,49,49,49	0
54	MG	1A	3620	1/1	0.93	0.13	47,47,47,47	0
54	MG	2a	1624	1/1	0.93	0.12	55,55,55,55	0
54	MG	2A	3295	1/1	0.93	0.12	84,84,84,84	0
54	MG	2A	3029	1/1	0.93	0.06	48,48,48,48	0
54	MG	2a	1628	1/1	0.93	0.15	94,94,94,94	0
54	MG	2A	3030	1/1	0.93	0.20	64,64,64,64	0
54	MG	1A	3067	1/1	0.93	0.19	46,46,46,46	0
54	MG	1A	3463	1/1	0.93	0.12	54,54,54,54	0
54	MG	1A	3094	1/1	0.93	0.10	58,58,58,58	0
54	MG	1A	3889	1/1	0.93	0.09	50,50,50,50	0
54	MG	2A	3484	1/1	0.93	0.07	64,64,64,64	0
54	MG	1A	3316	1/1	0.93	0.08	99,99,99,99	0
54	MG	2A	3488	1/1	0.93	0.16	97,97,97,97	0
54	MG	2A	3039	1/1	0.93	0.26	48,48,48,48	0
54	MG	1A	3891	1/1	0.93	0.17	48,48,48,48	0
54	MG	2A	3308	1/1	0.93	0.25	52,52,52,52	0
54	MG	1A	3218	1/1	0.93	0.11	50,50,50,50	0
54	MG	1A	3896	1/1	0.93	0.24	51,51,51,51	0
54	MG	2A	3311	1/1	0.93	0.14	66,66,66,66	0
54	MG	1A	3636	1/1	0.93	0.06	81,81,81,81	0
54	MG	1A	3900	1/1	0.93	0.14	54,54,54,54	0
54	MG	1A	3097	1/1	0.93	0.19	38,38,38,38	0
54	MG	1A	3111	1/1	0.93	0.07	69,69,69,69	0
54	MG	2A	3159	1/1	0.93	0.10	50,50,50,50	0
54	MG	1A	3175	1/1	0.93	0.17	51,51,51,51	0
54	MG	1a	1612	1/1	0.93	0.05	32,32,32,32	0
54	MG	1A	3773	1/1	0.93	0.11	79,79,79,79	0
54	MG	1A	3775	1/1	0.93	0.08	72,72,72,72	0
54	MG	1A	3776	1/1	0.93	0.07	40,40,40,40	0
54	MG	2A	3168	1/1	0.93	0.09	51,51,51,51	0
54	MG	2A	3536	1/1	0.93	0.12	71,71,71,71	0
54	MG	1A	3177	1/1	0.93	0.16	49,49,49,49	0
54	MG	1A	3654	1/1	0.93	0.07	59,59,59,59	0
54	MG	1a	1816	1/1	0.93	0.06	79,79,79,79	0
54	MG	2a	1661	1/1	0.93	0.10	84,84,84,84	0
54	MG	1a	1817	1/1	0.93	0.10	57,57,57,57	0
54	MG	2A	3059	1/1	0.93	0.08	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3175	1/1	0.93	0.10	63,63,63,63	0
54	MG	1A	3785	1/1	0.93	0.13	63,63,63,63	0
54	MG	2A	3545	1/1	0.93	0.06	110,110,110,110	0
54	MG	2A	3177	1/1	0.93	0.23	60,60,60,60	0
54	MG	2A	3549	1/1	0.93	0.17	60,60,60,60	0
54	MG	2A	3550	1/1	0.93	0.13	105,105,105,105	0
54	MG	1a	1621	1/1	0.93	0.08	59,59,59,59	0
54	MG	1A	3794	1/1	0.93	0.19	67,67,67,67	0
54	MG	2A	3561	1/1	0.93	0.08	97,97,97,97	0
54	MG	1A	3400	1/1	0.93	0.09	50,50,50,50	0
54	MG	1A	3080	1/1	0.93	0.21	59,59,59,59	0
54	MG	1A	3407	1/1	0.93	0.13	41,41,41,41	0
54	MG	1a	1825	1/1	0.93	0.16	61,61,61,61	0
54	MG	2A	3069	1/1	0.93	0.08	60,60,60,60	0
54	MG	1A	3482	1/1	0.93	0.07	52,52,52,52	0
54	MG	2A	3581	1/1	0.93	0.12	77,77,77,77	0
54	MG	2A	3362	1/1	0.93	0.20	75,75,75,75	0
54	MG	1A	3099	1/1	0.93	0.22	51,51,51,51	0
54	MG	2a	1689	1/1	0.93	0.16	102,102,102,102	0
54	MG	2A	3587	1/1	0.93	0.09	83,83,83,83	0
54	MG	1A	3158	1/1	0.93	0.10	66,66,66,66	0
54	MG	2A	3591	1/1	0.93	0.05	85,85,85,85	0
54	MG	2A	3369	1/1	0.93	0.08	53,53,53,53	0
54	MG	2A	3190	1/1	0.93	0.12	76,76,76,76	0
54	MG	2A	3371	1/1	0.93	0.11	48,48,48,48	0
54	MG	2A	3191	1/1	0.93	0.09	40,40,40,40	0
54	MG	1A	3674	1/1	0.93	0.07	57,57,57,57	0
54	MG	1A	3675	1/1	0.93	0.08	53,53,53,53	0
54	MG	1A	3228	1/1	0.93	0.07	62,62,62,62	0
54	MG	2A	3376	1/1	0.93	0.07	64,64,64,64	0
54	MG	1A	3266	1/1	0.93	0.10	46,46,46,46	0
54	MG	2A	3612	1/1	0.93	0.18	72,72,72,72	0
54	MG	2A	3079	1/1	0.93	0.10	67,67,67,67	0
54	MG	1D	305	1/1	0.93	0.11	55,55,55,55	0
54	MG	2A	3617	1/1	0.93	0.11	66,66,66,66	0
54	MG	1A	3678	1/1	0.93	0.11	115,115,115,115	0
54	MG	2a	1711	1/1	0.93	0.07	80,80,80,80	0
54	MG	2A	3621	1/1	0.93	0.09	73,73,73,73	0
54	MG	1a	1841	1/1	0.93	0.23	72,72,72,72	0
54	MG	2a	1719	1/1	0.93	0.06	110,110,110,110	0
54	MG	2A	3626	1/1	0.93	0.13	44,44,44,44	0
54	MG	1A	3344	1/1	0.93	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	2A	3084	1/1	0.93	0.10	71,71,71,71	0
54	MG	1a	1637	1/1	0.93	0.37	79,79,79,79	0
54	MG	1A	3048	1/1	0.93	0.23	60,60,60,60	0
54	MG	2A	3390	1/1	0.93	0.10	71,71,71,71	0
54	MG	1A	3420	1/1	0.93	0.07	35,35,35,35	0
54	MG	1E	304	1/1	0.93	0.25	80,80,80,80	0
54	MG	1A	3688	1/1	0.93	0.07	47,47,47,47	0
54	MG	1a	1642	1/1	0.93	0.15	84,84,84,84	0
54	MG	1A	3422	1/1	0.93	0.09	45,45,45,45	0
54	MG	1a	1644	1/1	0.93	0.16	55,55,55,55	0
54	MG	2A	3216	1/1	0.93	0.09	42,42,42,42	0
54	MG	2A	3400	1/1	0.93	0.10	55,55,55,55	0
54	MG	1A	3573	1/1	0.93	0.10	30,30,30,30	0
54	MG	1A	3498	1/1	0.93	0.07	55,55,55,55	0
54	MG	1A	3499	1/1	0.93	0.15	53,53,53,53	0
54	MG	1A	3134	1/1	0.93	0.07	38,38,38,38	0
54	MG	2a	1752	1/1	0.93	0.06	103,103,103,103	0
54	MG	1A	3116	1/1	0.93	0.08	28,28,28,28	0
54	MG	1A	3504	1/1	0.93	0.10	25,25,25,25	0
54	MG	2A	3223	1/1	0.93	0.09	48,48,48,48	0
54	MG	1A	3276	1/1	0.93	0.15	46,46,46,46	0
54	MG	2A	3227	1/1	0.93	0.12	72,72,72,72	0
54	MG	1A	3205	1/1	0.93	0.12	58,58,58,58	0
54	MG	2a	1763	1/1	0.93	0.09	96,96,96,96	0
54	MG	1A	3278	1/1	0.93	0.07	45,45,45,45	0
54	MG	1a	1758	1/1	0.93	0.05	48,48,48,48	0
54	MG	2A	3232	1/1	0.93	0.16	69,69,69,69	0
54	MG	1A	3508	1/1	0.93	0.11	51,51,51,51	0
54	MG	1A	3434	1/1	0.93	0.07	67,67,67,67	0
54	MG	1A	3843	1/1	0.93	0.13	54,54,54,54	0
54	MG	2A	3237	1/1	0.93	0.21	71,71,71,71	0
54	MG	2A	3426	1/1	0.93	0.09	55,55,55,55	0
54	MG	1P	204	1/1	0.93	0.08	50,50,50,50	0
54	MG	1A	3280	1/1	0.93	0.13	46,46,46,46	0
54	MG	1A	3193	1/1	0.94	0.23	61,61,61,61	0
54	MG	1A	3093	1/1	0.94	0.14	43,43,43,43	0
54	MG	1A	3541	1/1	0.94	0.11	66,66,66,66	0
54	MG	2T	204	1/1	0.94	0.07	71,71,71,71	0
54	MG	1X	101	1/1	0.94	0.09	66,66,66,66	0
54	MG	1A	3036	1/1	0.94	0.19	56,56,56,56	0
54	MG	2A	3278	1/1	0.94	0.12	65,65,65,65	0
54	MG	1A	3631	1/1	0.94	0.10	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	1A	3201	1/1	0.94	0.21	49,49,49,49	0
54	MG	1A	3231	1/1	0.94	0.12	55,55,55,55	0
54	MG	2A	3453	1/1	0.94	0.08	43,43,43,43	0
54	MG	1A	3082	1/1	0.94	0.25	47,47,47,47	0
54	MG	2A	3286	1/1	0.94	0.08	53,53,53,53	0
54	MG	1I	101	1/1	0.94	0.20	66,66,66,66	0
54	MG	2A	3146	1/1	0.94	0.07	70,70,70,70	0
54	MG	2A	3458	1/1	0.94	0.10	59,59,59,59	0
54	MG	2A	3291	1/1	0.94	0.15	64,64,64,64	0
54	MG	1A	3549	1/1	0.94	0.11	59,59,59,59	0
54	MG	1A	3762	1/1	0.94	0.14	49,49,49,49	0
54	MG	2A	3033	1/1	0.94	0.15	76,76,76,76	0
54	MG	1A	3146	1/1	0.94	0.12	46,46,46,46	0
54	MG	15	101	1/1	0.94	0.13	44,44,44,44	0
54	MG	2A	3037	1/1	0.94	0.12	52,52,52,52	0
54	MG	1A	3646	1/1	0.94	0.07	71,71,71,71	0
54	MG	2a	1611	1/1	0.94	0.09	76,76,76,76	0
54	MG	1A	3410	1/1	0.94	0.11	20,20,20,20	0
54	MG	1A	3236	1/1	0.94	0.15	52,52,52,52	0
54	MG	19	101	1/1	0.94	0.13	42,42,42,42	0
54	MG	1a	1689	1/1	0.94	0.18	61,61,61,61	0
54	MG	2A	3158	1/1	0.94	0.08	68,68,68,68	0
54	MG	1A	3483	1/1	0.94	0.11	39,39,39,39	0
54	MG	1A	3237	1/1	0.94	0.06	61,61,61,61	0
54	MG	1A	3780	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3781	1/1	0.94	0.11	55,55,55,55	0
54	MG	2A	3487	1/1	0.94	0.07	75,75,75,75	0
54	MG	1A	3782	1/1	0.94	0.08	35,35,35,35	0
54	MG	2A	3319	1/1	0.94	0.13	60,60,60,60	0
54	MG	2A	3320	1/1	0.94	0.07	72,72,72,72	0
54	MG	2A	3492	1/1	0.94	0.09	51,51,51,51	0
54	MG	2a	1630	1/1	0.94	0.21	55,55,55,55	0
54	MG	1A	3485	1/1	0.94	0.07	54,54,54,54	0
54	MG	1A	3279	1/1	0.94	0.10	67,67,67,67	0
54	MG	2A	3324	1/1	0.94	0.07	46,46,46,46	0
54	MG	1a	1697	1/1	0.94	0.20	63,63,63,63	0
54	MG	1A	3790	1/1	0.94	0.13	34,34,34,34	0
54	MG	1A	3021	1/1	0.94	0.06	60,60,60,60	0
54	MG	2A	3054	1/1	0.94	0.14	38,38,38,38	0
54	MG	1a	1611	1/1	0.94	0.07	90,90,90,90	0
54	MG	2A	3520	1/1	0.94	0.17	91,91,91,91	0
54	MG	2A	3521	1/1	0.94	0.07	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3667	1/1	0.94	0.07	32,32,32,32	0
54	MG	2A	3524	1/1	0.94	0.12	47,47,47,47	0
54	MG	1a	1704	1/1	0.94	0.07	45,45,45,45	0
54	MG	1B	1012	1/1	0.94	0.06	79,79,79,79	0
54	MG	1A	3669	1/1	0.94	0.13	34,34,34,34	0
54	MG	1A	3416	1/1	0.94	0.14	41,41,41,41	0
54	MG	1A	3352	1/1	0.94	0.12	62,62,62,62	0
54	MG	1A	3353	1/1	0.94	0.09	38,38,38,38	0
54	MG	2A	3534	1/1	0.94	0.10	68,68,68,68	0
54	MG	2a	1651	1/1	0.94	0.15	68,68,68,68	0
54	MG	1A	3034	1/1	0.94	0.14	60,60,60,60	0
54	MG	2A	3066	1/1	0.94	0.07	50,50,50,50	0
54	MG	1A	3565	1/1	0.94	0.21	69,69,69,69	0
54	MG	1A	3287	1/1	0.94	0.10	47,47,47,47	0
54	MG	1A	3680	1/1	0.94	0.12	64,64,64,64	0
54	MG	2A	3070	1/1	0.94	0.20	59,59,59,59	0
54	MG	2A	3347	1/1	0.94	0.07	45,45,45,45	0
54	MG	1A	3171	1/1	0.94	0.11	56,56,56,56	0
54	MG	1A	3360	1/1	0.94	0.09	30,30,30,30	0
54	MG	2A	3353	1/1	0.94	0.12	42,42,42,42	0
54	MG	2A	3192	1/1	0.94	0.07	45,45,45,45	0
54	MG	1a	1829	1/1	0.94	0.08	76,76,76,76	0
54	MG	1A	3362	1/1	0.94	0.08	48,48,48,48	0
54	MG	2A	3195	1/1	0.94	0.21	66,66,66,66	0
54	MG	1a	1721	1/1	0.94	0.08	53,53,53,53	0
54	MG	2A	3562	1/1	0.94	0.09	64,64,64,64	0
54	MG	2A	3364	1/1	0.94	0.07	55,55,55,55	0
54	MG	1a	1627	1/1	0.94	0.05	72,72,72,72	0
54	MG	2A	3567	1/1	0.94	0.06	63,63,63,63	0
54	MG	2A	3572	1/1	0.94	0.08	57,57,57,57	0
54	MG	2A	3367	1/1	0.94	0.09	93,93,93,93	0
54	MG	2A	3368	1/1	0.94	0.12	57,57,57,57	0
54	MG	2A	3577	1/1	0.94	0.08	54,54,54,54	0
54	MG	1A	3135	1/1	0.94	0.08	72,72,72,72	0
54	MG	1A	3298	1/1	0.94	0.06	55,55,55,55	0
54	MG	2a	1678	1/1	0.94	0.16	53,53,53,53	0
54	MG	2a	1679	1/1	0.94	0.07	68,68,68,68	0
54	MG	1A	3816	1/1	0.94	0.14	34,34,34,34	0
54	MG	1A	3157	1/1	0.94	0.11	42,42,42,42	0
54	MG	1a	1842	1/1	0.94	0.08	73,73,73,73	0
54	MG	2A	3205	1/1	0.94	0.13	53,53,53,53	0
54	MG	1A	3245	1/1	0.94	0.07	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3174	1/1	0.94	0.13	53,53,53,53	0
54	MG	2A	3592	1/1	0.94	0.08	63,63,63,63	0
54	MG	1E	303	1/1	0.94	0.13	31,31,31,31	0
54	MG	2A	3595	1/1	0.94	0.08	68,68,68,68	0
54	MG	1A	3442	1/1	0.94	0.08	35,35,35,35	0
54	MG	1A	3827	1/1	0.94	0.05	57,57,57,57	0
54	MG	1A	3444	1/1	0.94	0.06	34,34,34,34	0
54	MG	1A	3120	1/1	0.94	0.25	39,39,39,39	0
54	MG	1F	306	1/1	0.94	0.16	41,41,41,41	0
54	MG	1A	3121	1/1	0.94	0.25	43,43,43,43	0
54	MG	1A	3832	1/1	0.94	0.19	60,60,60,60	0
54	MG	1a	1744	1/1	0.94	0.12	63,63,63,63	0
54	MG	2A	3611	1/1	0.94	0.10	63,63,63,63	0
54	MG	1A	3514	1/1	0.94	0.18	58,58,58,58	0
54	MG	1A	3515	1/1	0.94	0.07	57,57,57,57	0
54	MG	1A	3012	1/1	0.94	0.12	58,58,58,58	0
54	MG	1d	506	1/1	0.94	0.08	98,98,98,98	0
54	MG	1A	3598	1/1	0.94	0.06	82,82,82,82	0
54	MG	1A	3184	1/1	0.94	0.22	65,65,65,65	0
54	MG	2A	3224	1/1	0.94	0.11	51,51,51,51	0
54	MG	2A	3623	1/1	0.94	0.18	76,76,76,76	0
54	MG	1A	3381	1/1	0.94	0.09	58,58,58,58	0
54	MG	2A	3399	1/1	0.94	0.08	68,68,68,68	0
54	MG	2A	3629	1/1	0.94	0.07	67,67,67,67	0
54	MG	1N	201	1/1	0.94	0.17	49,49,49,49	0
54	MG	1A	3312	1/1	0.94	0.10	62,62,62,62	0
54	MG	1A	3313	1/1	0.94	0.10	31,31,31,31	0
54	MG	1a	1755	1/1	0.94	0.15	57,57,57,57	0
54	MG	1A	3526	1/1	0.94	0.14	83,83,83,83	0
54	MG	2a	1734	1/1	0.94	0.09	62,62,62,62	0
54	MG	2a	1735	1/1	0.94	0.11	76,76,76,76	0
54	MG	1a	1757	1/1	0.94	0.08	62,62,62,62	0
54	MG	1l	201	1/1	0.94	0.12	65,65,65,65	0
54	MG	1A	3723	1/1	0.94	0.11	59,59,59,59	0
54	MG	1A	3102	1/1	0.94	0.11	42,42,42,42	0
54	MG	2A	3411	1/1	0.94	0.06	78,78,78,78	0
54	MG	2a	1742	1/1	0.94	0.07	96,96,96,96	0
54	MG	2A	3240	1/1	0.94	0.09	39,39,39,39	0
54	MG	1a	1655	1/1	0.94	0.15	61,61,61,61	0
54	MG	1A	3609	1/1	0.94	0.15	52,52,52,52	0
54	MG	1R	201	1/1	0.94	0.17	46,46,46,46	0
54	MG	1y	201	1/1	0.94	0.06	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1658	1/1	0.94	0.10	55,55,55,55	0
54	MG	1y	203	1/1	0.94	0.10	57,57,57,57	0
54	MG	2A	3423	1/1	0.94	0.10	94,94,94,94	0
54	MG	1A	3611	1/1	0.94	0.14	59,59,59,59	0
54	MG	1A	3385	1/1	0.94	0.08	70,70,70,70	0
54	MG	1A	3457	1/1	0.94	0.07	46,46,46,46	0
54	MG	2D	301	1/1	0.94	0.17	63,63,63,63	0
54	MG	2D	302	1/1	0.94	0.13	56,56,56,56	0
54	MG	2A	3428	1/1	0.94	0.07	61,61,61,61	0
54	MG	2E	302	1/1	0.94	0.17	66,66,66,66	0
54	MG	1A	3187	1/1	0.94	0.04	51,51,51,51	0
54	MG	1A	3189	1/1	0.94	0.12	43,43,43,43	0
54	MG	2A	3128	1/1	0.94	0.27	58,58,58,58	0
54	MG	2A	3262	1/1	0.94	0.04	46,46,46,46	0
54	MG	1A	3064	1/1	0.94	0.14	43,43,43,43	0
54	MG	2I	201	1/1	0.94	0.07	89,89,89,89	0
54	MG	1A	3860	1/1	0.94	0.16	65,65,65,65	0
54	MG	1a	1773	1/1	0.94	0.12	77,77,77,77	0
54	MG	1A	3393	1/1	0.94	0.08	60,60,60,60	0
54	MG	1A	3469	1/1	0.94	0.08	73,73,73,73	0
54	MG	1a	1674	1/1	0.95	0.06	52,52,52,52	0
54	MG	1U	203	1/1	0.95	0.24	58,58,58,58	0
54	MG	1A	3753	1/1	0.95	0.07	43,43,43,43	0
54	MG	2A	3167	1/1	0.95	0.21	56,56,56,56	0
54	MG	1A	3226	1/1	0.95	0.06	53,53,53,53	0
54	MG	1A	3315	1/1	0.95	0.09	48,48,48,48	0
54	MG	1A	3081	1/1	0.95	0.06	61,61,61,61	0
54	MG	2A	3485	1/1	0.95	0.11	66,66,66,66	0
54	MG	1W	203	1/1	0.95	0.13	45,45,45,45	0
54	MG	1A	3875	1/1	0.95	0.11	78,78,78,78	0
54	MG	2A	3325	1/1	0.95	0.08	96,96,96,96	0
54	MG	2A	3489	1/1	0.95	0.08	74,74,74,74	0
54	MG	1a	1682	1/1	0.95	0.06	69,69,69,69	0
54	MG	1A	3761	1/1	0.95	0.10	38,38,38,38	0
54	MG	1Z	301	1/1	0.95	0.04	51,51,51,51	0
54	MG	1A	3446	1/1	0.95	0.08	60,60,60,60	0
54	MG	1A	3566	1/1	0.95	0.12	69,69,69,69	0
54	MG	1A	3883	1/1	0.95	0.21	51,51,51,51	0
54	MG	1A	3885	1/1	0.95	0.10	53,53,53,53	0
54	MG	2a	1613	1/1	0.95	0.14	71,71,71,71	0
54	MG	2A	3502	1/1	0.95	0.09	57,57,57,57	0
54	MG	2A	3504	1/1	0.95	0.08	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3886	1/1	0.95	0.17	46,46,46,46	0
54	MG	1A	3569	1/1	0.95	0.07	46,46,46,46	0
54	MG	2A	3511	1/1	0.95	0.07	89,89,89,89	0
54	MG	2A	3512	1/1	0.95	0.06	67,67,67,67	0
54	MG	11	103	1/1	0.95	0.22	48,48,48,48	0
54	MG	2A	3516	1/1	0.95	0.15	85,85,85,85	0
54	MG	2A	3185	1/1	0.95	0.14	39,39,39,39	0
54	MG	2A	3062	1/1	0.95	0.10	51,51,51,51	0
54	MG	2a	1626	1/1	0.95	0.18	57,57,57,57	0
54	MG	1A	3141	1/1	0.95	0.33	45,45,45,45	0
54	MG	1A	3031	1/1	0.95	0.04	31,31,31,31	0
54	MG	1A	3050	1/1	0.95	0.18	22,22,22,22	0
54	MG	1A	3032	1/1	0.95	0.06	45,45,45,45	0
54	MG	2a	1631	1/1	0.95	0.14	60,60,60,60	0
54	MG	2A	3344	1/1	0.95	0.07	55,55,55,55	0
54	MG	1A	3893	1/1	0.95	0.15	44,44,44,44	0
54	MG	1A	3203	1/1	0.95	0.11	60,60,60,60	0
54	MG	17	101	1/1	0.95	0.19	44,44,44,44	0
54	MG	1A	3016	1/1	0.95	0.06	33,33,33,33	0
54	MG	1A	3040	1/1	0.95	0.19	32,32,32,32	0
54	MG	1A	3007	1/1	0.95	0.11	35,35,35,35	0
54	MG	2A	3354	1/1	0.95	0.14	92,92,92,92	0
54	MG	1a	1703	1/1	0.95	0.07	54,54,54,54	0
54	MG	1A	3238	1/1	0.95	0.09	31,31,31,31	0
54	MG	1A	3459	1/1	0.95	0.16	58,58,58,58	0
54	MG	2A	3360	1/1	0.95	0.09	47,47,47,47	0
54	MG	2A	3201	1/1	0.95	0.12	51,51,51,51	0
54	MG	1A	3523	1/1	0.95	0.09	67,67,67,67	0
54	MG	1B	1005	1/1	0.95	0.06	71,71,71,71	0
54	MG	1A	3334	1/1	0.95	0.11	40,40,40,40	0
54	MG	2A	3548	1/1	0.95	0.08	62,62,62,62	0
54	MG	2A	3366	1/1	0.95	0.20	47,47,47,47	0
54	MG	1B	1007	1/1	0.95	0.25	67,67,67,67	0
54	MG	1A	3797	1/1	0.95	0.08	82,82,82,82	0
54	MG	1A	3055	1/1	0.95	0.07	40,40,40,40	0
54	MG	1a	1610	1/1	0.95	0.07	85,85,85,85	0
54	MG	1A	3685	1/1	0.95	0.08	51,51,51,51	0
54	MG	1A	3802	1/1	0.95	0.16	75,75,75,75	0
54	MG	1A	3095	1/1	0.95	0.21	41,41,41,41	0
54	MG	1B	1015	1/1	0.95	0.12	79,79,79,79	0
54	MG	2A	3570	1/1	0.95	0.19	69,69,69,69	0
54	MG	1a	1615	1/1	0.95	0.14	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	3405	1/1	0.95	0.16	54,54,54,54	0
54	MG	1A	3406	1/1	0.95	0.06	67,67,67,67	0
54	MG	1A	3691	1/1	0.95	0.16	61,61,61,61	0
54	MG	1A	3529	1/1	0.95	0.12	52,52,52,52	0
54	MG	1A	3282	1/1	0.95	0.07	64,64,64,64	0
54	MG	1a	1731	1/1	0.95	0.07	73,73,73,73	0
54	MG	1B	1023	1/1	0.95	0.09	66,66,66,66	0
54	MG	1A	3153	1/1	0.95	0.07	56,56,56,56	0
54	MG	1A	3284	1/1	0.95	0.09	60,60,60,60	0
54	MG	2A	3588	1/1	0.95	0.06	93,93,93,93	0
54	MG	1A	3156	1/1	0.95	0.11	39,39,39,39	0
54	MG	1A	3289	1/1	0.95	0.07	47,47,47,47	0
54	MG	2A	3226	1/1	0.95	0.15	52,52,52,52	0
54	MG	1A	3606	1/1	0.95	0.06	55,55,55,55	0
54	MG	1A	3176	1/1	0.95	0.10	42,42,42,42	0
54	MG	1D	302	1/1	0.95	0.16	55,55,55,55	0
54	MG	1A	3074	1/1	0.95	0.13	47,47,47,47	0
54	MG	1A	3819	1/1	0.95	0.08	71,71,71,71	0
54	MG	2A	3233	1/1	0.95	0.07	57,57,57,57	0
54	MG	2A	3602	1/1	0.95	0.09	99,99,99,99	0
54	MG	2A	3603	1/1	0.95	0.07	78,78,78,78	0
54	MG	2a	1682	1/1	0.95	0.15	71,71,71,71	0
54	MG	1A	3538	1/1	0.95	0.08	37,37,37,37	0
54	MG	1A	3357	1/1	0.95	0.09	26,26,26,26	0
54	MG	2A	3607	1/1	0.95	0.10	52,52,52,52	0
54	MG	2a	1688	1/1	0.95	0.08	64,64,64,64	0
54	MG	1A	3246	1/1	0.95	0.08	41,41,41,41	0
54	MG	2A	3112	1/1	0.95	0.06	54,54,54,54	0
54	MG	1A	3826	1/1	0.95	0.06	90,90,90,90	0
54	MG	1E	301	1/1	0.95	0.07	25,25,25,25	0
54	MG	1h	201	1/1	0.95	0.17	64,64,64,64	0
54	MG	1A	3713	1/1	0.95	0.15	60,60,60,60	0
54	MG	2A	3408	1/1	0.95	0.14	81,81,81,81	0
54	MG	1A	3075	1/1	0.95	0.17	48,48,48,48	0
54	MG	2A	3247	1/1	0.95	0.13	64,64,64,64	0
54	MG	1E	305	1/1	0.95	0.15	59,59,59,59	0
54	MG	1A	3361	1/1	0.95	0.09	49,49,49,49	0
54	MG	2a	1703	1/1	0.95	0.17	81,81,81,81	0
54	MG	2A	3624	1/1	0.95	0.13	39,39,39,39	0
54	MG	1A	3830	1/1	0.95	0.07	59,59,59,59	0
54	MG	2A	3253	1/1	0.95	0.08	51,51,51,51	0
54	MG	2A	3254	1/1	0.95	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3255	1/1	0.95	0.07	50,50,50,50	0
54	MG	2A	3633	1/1	0.95	0.19	46,46,46,46	0
54	MG	1A	3716	1/1	0.95	0.06	50,50,50,50	0
54	MG	1A	3182	1/1	0.95	0.20	44,44,44,44	0
54	MG	1F	307	1/1	0.95	0.09	38,38,38,38	0
54	MG	2a	1717	1/1	0.95	0.07	83,83,83,83	0
54	MG	2A	3639	1/1	0.95	0.10	67,67,67,67	0
54	MG	1A	3547	1/1	0.95	0.11	60,60,60,60	0
54	MG	1A	3159	1/1	0.95	0.22	46,46,46,46	0
54	MG	1a	1647	1/1	0.95	0.24	62,62,62,62	0
54	MG	2a	1724	1/1	0.95	0.06	108,108,108,108	0
54	MG	1A	3429	1/1	0.95	0.12	41,41,41,41	0
54	MG	1A	3726	1/1	0.95	0.17	52,52,52,52	0
54	MG	1A	3303	1/1	0.95	0.07	60,60,60,60	0
54	MG	1A	3623	1/1	0.95	0.08	65,65,65,65	0
54	MG	1A	3009	1/1	0.95	0.23	59,59,59,59	0
54	MG	1a	1766	1/1	0.95	0.06	83,83,83,83	0
54	MG	1A	3844	1/1	0.95	0.12	63,63,63,63	0
54	MG	1A	3626	1/1	0.95	0.10	58,58,58,58	0
54	MG	2A	3013	1/1	0.95	0.13	59,59,59,59	0
54	MG	2A	3274	1/1	0.95	0.08	45,45,45,45	0
54	MG	2B	212	1/1	0.95	0.10	111,111,111,111	0
54	MG	1A	3305	1/1	0.95	0.09	23,23,23,23	0
54	MG	1A	3630	1/1	0.95	0.05	50,50,50,50	0
54	MG	2a	1744	1/1	0.95	0.05	73,73,73,73	0
54	MG	2A	3020	1/1	0.95	0.05	60,60,60,60	0
54	MG	2B	216	1/1	0.95	0.05	106,106,106,106	0
54	MG	1A	3849	1/1	0.95	0.08	78,78,78,78	0
54	MG	1P	203	1/1	0.95	0.07	52,52,52,52	0
54	MG	1A	3734	1/1	0.95	0.06	82,82,82,82	0
54	MG	2A	3024	1/1	0.95	0.11	68,68,68,68	0
54	MG	1A	3494	1/1	0.95	0.05	53,53,53,53	0
54	MG	2A	3288	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3737	1/1	0.95	0.08	74,74,74,74	0
54	MG	1Q	203	1/1	0.95	0.08	51,51,51,51	0
54	MG	1A	3186	1/1	0.95	0.36	60,60,60,60	0
54	MG	1A	3635	1/1	0.95	0.11	62,62,62,62	0
54	MG	1A	3079	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3637	1/1	0.95	0.11	86,86,86,86	0
54	MG	1a	1787	1/1	0.95	0.08	74,74,74,74	0
54	MG	1R	207	1/1	0.95	0.09	35,35,35,35	0
54	MG	1A	3257	1/1	0.95	0.06	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	1A	3440	1/1	0.95	0.11	59,59,59,59	0
54	MG	1a	1791	1/1	0.95	0.10	70,70,70,70	0
54	MG	2T	203	1/1	0.95	0.11	73,73,73,73	0
53	MPD	18	101	8/8	0.95	0.17	47,49,54,59	0
54	MG	2A	3160	1/1	0.95	0.14	37,37,37,37	0
54	MG	2W	201	1/1	0.95	0.18	65,65,65,65	0
54	MG	1U	201	1/1	0.95	0.05	29,29,29,29	0
54	MG	1A	3643	1/1	0.95	0.08	65,65,65,65	0
56	ZN	24	101	1/1	0.95	0.05	154,154,154,154	0
54	MG	2P	202	1/1	0.96	0.06	90,90,90,90	0
54	MG	1A	3059	1/1	0.96	0.04	24,24,24,24	0
54	MG	1A	3580	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3271	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3214	1/1	0.96	0.14	40,40,40,40	0
54	MG	1A	3376	1/1	0.96	0.11	30,30,30,30	0
54	MG	2A	3294	1/1	0.96	0.14	60,60,60,60	0
54	MG	2A	3142	1/1	0.96	0.17	28,28,28,28	0
54	MG	1A	3681	1/1	0.96	0.06	99,99,99,99	0
54	MG	1a	1753	1/1	0.96	0.20	84,84,84,84	0
54	MG	1A	3586	1/1	0.96	0.10	81,81,81,81	0
54	MG	2A	3474	1/1	0.96	0.06	84,84,84,84	0
54	MG	2A	3475	1/1	0.96	0.05	88,88,88,88	0
54	MG	1A	3320	1/1	0.96	0.06	52,52,52,52	0
54	MG	1D	306	1/1	0.96	0.08	53,53,53,53	0
54	MG	1A	3100	1/1	0.96	0.17	49,49,49,49	0
54	MG	2A	3479	1/1	0.96	0.10	52,52,52,52	0
54	MG	2A	3480	1/1	0.96	0.08	61,61,61,61	0
54	MG	2A	3303	1/1	0.96	0.12	75,75,75,75	0
54	MG	1A	3110	1/1	0.96	0.05	64,64,64,64	0
54	MG	1A	3155	1/1	0.96	0.17	53,53,53,53	0
54	MG	1D	311	1/1	0.96	0.08	47,47,47,47	0
54	MG	1A	3689	1/1	0.96	0.08	99,99,99,99	0
54	MG	1A	3091	1/1	0.96	0.11	57,57,57,57	0
54	MG	1A	3326	1/1	0.96	0.09	44,44,44,44	0
54	MG	2A	3019	1/1	0.96	0.15	80,80,80,80	0
54	MG	1A	3521	1/1	0.96	0.08	60,60,60,60	0
54	MG	1A	3695	1/1	0.96	0.06	57,57,57,57	0
54	MG	2A	3318	1/1	0.96	0.06	38,38,38,38	0
54	MG	1F	301	1/1	0.96	0.08	43,43,43,43	0
54	MG	1A	3696	1/1	0.96	0.05	30,30,30,30	0
54	MG	1A	3192	1/1	0.96	0.15	65,65,65,65	0
54	MG	1A	3699	1/1	0.96	0.08	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	2A	3323	1/1	0.96	0.06	65,65,65,65	0
54	MG	1A	3061	1/1	0.96	0.11	48,48,48,48	0
54	MG	2A	3503	1/1	0.96	0.06	69,69,69,69	0
54	MG	1A	3390	1/1	0.96	0.09	65,65,65,65	0
54	MG	2A	3505	1/1	0.96	0.06	73,73,73,73	0
54	MG	1A	3247	1/1	0.96	0.13	27,27,27,27	0
54	MG	2A	3507	1/1	0.96	0.07	50,50,50,50	0
54	MG	2a	1623	1/1	0.96	0.03	60,60,60,60	0
54	MG	1A	3248	1/1	0.96	0.09	42,42,42,42	0
54	MG	2A	3509	1/1	0.96	0.07	65,65,65,65	0
54	MG	1a	1775	1/1	0.96	0.05	98,98,98,98	0
54	MG	1a	1776	1/1	0.96	0.06	91,91,91,91	0
54	MG	1a	1777	1/1	0.96	0.07	99,99,99,99	0
54	MG	1A	3336	1/1	0.96	0.09	44,44,44,44	0
54	MG	2A	3517	1/1	0.96	0.07	57,57,57,57	0
54	MG	2A	3035	1/1	0.96	0.11	68,68,68,68	0
54	MG	2A	3519	1/1	0.96	0.07	64,64,64,64	0
54	MG	1A	3340	1/1	0.96	0.07	31,31,31,31	0
54	MG	1A	3397	1/1	0.96	0.12	67,67,67,67	0
54	MG	1a	1781	1/1	0.96	0.06	83,83,83,83	0
54	MG	1A	3285	1/1	0.96	0.11	67,67,67,67	0
54	MG	1A	3399	1/1	0.96	0.07	78,78,78,78	0
54	MG	1H	201	1/1	0.96	0.10	64,64,64,64	0
54	MG	1A	3466	1/1	0.96	0.15	95,95,95,95	0
54	MG	2A	3530	1/1	0.96	0.10	62,62,62,62	0
54	MG	1A	3710	1/1	0.96	0.06	61,61,61,61	0
54	MG	1A	3712	1/1	0.96	0.05	46,46,46,46	0
54	MG	1A	3014	1/1	0.96	0.07	31,31,31,31	0
54	MG	1a	1663	1/1	0.96	0.24	68,68,68,68	0
54	MG	2A	3535	1/1	0.96	0.06	88,88,88,88	0
54	MG	1O	201	1/1	0.96	0.06	58,58,58,58	0
54	MG	1A	3195	1/1	0.96	0.10	58,58,58,58	0
54	MG	1A	3197	1/1	0.96	0.09	49,49,49,49	0
54	MG	1A	3349	1/1	0.96	0.11	62,62,62,62	0
54	MG	2A	3540	1/1	0.96	0.05	77,77,77,77	0
54	MG	2A	3350	1/1	0.96	0.08	43,43,43,43	0
54	MG	2A	3352	1/1	0.96	0.10	51,51,51,51	0
54	MG	1A	3617	1/1	0.96	0.10	100,100,100,100	0
54	MG	1A	3350	1/1	0.96	0.08	55,55,55,55	0
54	MG	1A	3721	1/1	0.96	0.04	43,43,43,43	0
54	MG	1A	3198	1/1	0.96	0.13	64,64,64,64	0
54	MG	2A	3056	1/1	0.96	0.11	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3542	1/1	0.96	0.13	49,49,49,49	0
54	MG	2A	3361	1/1	0.96	0.12	53,53,53,53	0
54	MG	1A	3853	1/1	0.96	0.06	33,33,33,33	0
54	MG	2A	3556	1/1	0.96	0.05	90,90,90,90	0
54	MG	1R	204	1/1	0.96	0.19	53,53,53,53	0
54	MG	1A	3475	1/1	0.96	0.09	44,44,44,44	0
54	MG	1A	3104	1/1	0.96	0.07	33,33,33,33	0
54	MG	1A	3128	1/1	0.96	0.09	44,44,44,44	0
54	MG	1T	2003	1/1	0.96	0.09	83,83,83,83	0
54	MG	1A	3546	1/1	0.96	0.09	43,43,43,43	0
54	MG	2A	3569	1/1	0.96	0.07	87,87,87,87	0
54	MG	1A	3412	1/1	0.96	0.08	28,28,28,28	0
54	MG	1A	3072	1/1	0.96	0.13	60,60,60,60	0
54	MG	2A	3574	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3355	1/1	0.96	0.10	20,20,20,20	0
54	MG	1A	3733	1/1	0.96	0.08	35,35,35,35	0
54	MG	1A	3043	1/1	0.96	0.10	50,50,50,50	0
54	MG	2A	3578	1/1	0.96	0.06	52,52,52,52	0
54	MG	1V	202	1/1	0.96	0.12	67,67,67,67	0
54	MG	2a	1677	1/1	0.96	0.05	98,98,98,98	0
54	MG	1A	3866	1/1	0.96	0.09	102,102,102,102	0
54	MG	1A	3867	1/1	0.96	0.17	46,46,46,46	0
54	MG	1A	3868	1/1	0.96	0.09	34,34,34,34	0
54	MG	2A	3583	1/1	0.96	0.05	96,96,96,96	0
54	MG	1A	3632	1/1	0.96	0.09	57,57,57,57	0
54	MG	1A	3870	1/1	0.96	0.13	55,55,55,55	0
54	MG	2a	1684	1/1	0.96	0.07	73,73,73,73	0
54	MG	1A	3871	1/1	0.96	0.12	83,83,83,83	0
54	MG	2A	3383	1/1	0.96	0.08	81,81,81,81	0
54	MG	1A	3178	1/1	0.96	0.08	50,50,50,50	0
54	MG	1A	3873	1/1	0.96	0.08	56,56,56,56	0
54	MG	10	102	1/1	0.96	0.10	76,76,76,76	0
54	MG	2a	1691	1/1	0.96	0.09	91,91,91,91	0
54	MG	1A	3739	1/1	0.96	0.12	72,72,72,72	0
54	MG	1A	3634	1/1	0.96	0.12	43,43,43,43	0
54	MG	1A	3741	1/1	0.96	0.14	51,51,51,51	0
54	MG	1A	3417	1/1	0.96	0.10	34,34,34,34	0
54	MG	2A	3085	1/1	0.96	0.07	73,73,73,73	0
54	MG	1A	3358	1/1	0.96	0.09	54,54,54,54	0
54	MG	1A	3088	1/1	0.96	0.08	52,52,52,52	0
54	MG	1A	3261	1/1	0.96	0.07	30,30,30,30	0
54	MG	2a	1700	1/1	0.96	0.06	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3262	1/1	0.96	0.08	45,45,45,45	0
54	MG	2a	1702	1/1	0.96	0.08	83,83,83,83	0
54	MG	1A	3640	1/1	0.96	0.07	48,48,48,48	0
54	MG	1a	1836	1/1	0.96	0.06	85,85,85,85	0
54	MG	2A	3092	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3424	1/1	0.96	0.07	38,38,38,38	0
54	MG	1a	1838	1/1	0.96	0.07	90,90,90,90	0
54	MG	1A	3642	1/1	0.96	0.06	50,50,50,50	0
54	MG	1a	1840	1/1	0.96	0.06	61,61,61,61	0
54	MG	1A	3754	1/1	0.96	0.07	29,29,29,29	0
54	MG	2A	3618	1/1	0.96	0.09	104,104,104,104	0
54	MG	2a	1712	1/1	0.96	0.14	75,75,75,75	0
54	MG	2a	1713	1/1	0.96	0.06	85,85,85,85	0
54	MG	1A	3559	1/1	0.96	0.17	61,61,61,61	0
54	MG	2a	1716	1/1	0.96	0.06	89,89,89,89	0
54	MG	2A	3099	1/1	0.96	0.16	42,42,42,42	0
54	MG	1A	3892	1/1	0.96	0.10	35,35,35,35	0
54	MG	1a	1844	1/1	0.96	0.11	76,76,76,76	0
54	MG	1A	3180	1/1	0.96	0.09	37,37,37,37	0
54	MG	1A	3758	1/1	0.96	0.09	84,84,84,84	0
54	MG	2a	1722	1/1	0.96	0.05	109,109,109,109	0
54	MG	2A	3627	1/1	0.96	0.06	55,55,55,55	0
54	MG	1a	1848	1/1	0.96	0.05	90,90,90,90	0
54	MG	2a	1727	1/1	0.96	0.06	88,88,88,88	0
54	MG	2a	1728	1/1	0.96	0.06	87,87,87,87	0
54	MG	2a	1729	1/1	0.96	0.06	93,93,93,93	0
54	MG	1A	3647	1/1	0.96	0.13	58,58,58,58	0
54	MG	2A	3249	1/1	0.96	0.13	74,74,74,74	0
54	MG	2A	3632	1/1	0.96	0.09	75,75,75,75	0
54	MG	1A	3648	1/1	0.96	0.06	47,47,47,47	0
54	MG	1A	3308	1/1	0.96	0.07	40,40,40,40	0
54	MG	2A	3252	1/1	0.96	0.06	49,49,49,49	0
54	MG	2A	3421	1/1	0.96	0.06	68,68,68,68	0
54	MG	1A	3901	1/1	0.96	0.09	64,64,64,64	0
54	MG	1A	3651	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3653	1/1	0.96	0.09	52,52,52,52	0
54	MG	2a	1740	1/1	0.96	0.05	98,98,98,98	0
54	MG	1A	3235	1/1	0.96	0.07	53,53,53,53	0
54	MG	2A	3427	1/1	0.96	0.07	68,68,68,68	0
54	MG	2a	1743	1/1	0.96	0.08	84,84,84,84	0
54	MG	1A	3655	1/1	0.96	0.10	67,67,67,67	0
54	MG	1A	3657	1/1	0.96	0.11	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1728	1/1	0.96	0.10	65,65,65,65	0
54	MG	1d	504	1/1	0.96	0.15	70,70,70,70	0
54	MG	2A	3434	1/1	0.96	0.10	47,47,47,47	0
54	MG	1A	3658	1/1	0.96	0.11	69,69,69,69	0
54	MG	1A	3367	1/1	0.96	0.11	46,46,46,46	0
54	MG	1A	3132	1/1	0.96	0.11	39,39,39,39	0
54	MG	2a	1753	1/1	0.96	0.08	73,73,73,73	0
54	MG	1A	3133	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3664	1/1	0.96	0.09	32,32,32,32	0
54	MG	1A	3567	1/1	0.96	0.12	71,71,71,71	0
54	MG	1A	3788	1/1	0.96	0.17	58,58,58,58	0
54	MG	2a	1760	1/1	0.96	0.06	102,102,102,102	0
54	MG	1A	3268	1/1	0.96	0.11	42,42,42,42	0
54	MG	1a	1619	1/1	0.96	0.06	102,102,102,102	0
54	MG	1A	3503	1/1	0.96	0.07	66,66,66,66	0
54	MG	2A	3129	1/1	0.96	0.08	37,37,37,37	0
54	MG	2A	3448	1/1	0.96	0.05	69,69,69,69	0
54	MG	1A	3668	1/1	0.96	0.06	41,41,41,41	0
54	MG	2A	3277	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3436	1/1	0.96	0.07	68,68,68,68	0
54	MG	1a	1742	1/1	0.96	0.17	95,95,95,95	0
54	MG	1A	3437	1/1	0.96	0.08	53,53,53,53	0
54	MG	2l	202	1/1	0.96	0.06	55,55,55,55	0
54	MG	1A	3438	1/1	0.96	0.08	27,27,27,27	0
54	MG	2A	3282	1/1	0.96	0.11	41,41,41,41	0
54	MG	1B	1025	1/1	0.96	0.13	70,70,70,70	0
54	MG	1A	3801	1/1	0.96	0.10	58,58,58,58	0
54	MG	2P	201	1/1	0.96	0.15	83,83,83,83	0
54	MG	2A	3170	1/1	0.97	0.09	55,55,55,55	0
54	MG	1A	3348	1/1	0.97	0.07	37,37,37,37	0
54	MG	2A	3290	1/1	0.97	0.10	57,57,57,57	0
54	MG	1A	3625	1/1	0.97	0.16	54,54,54,54	0
54	MG	1A	3391	1/1	0.97	0.07	53,53,53,53	0
54	MG	1A	3628	1/1	0.97	0.07	47,47,47,47	0
54	MG	1A	3496	1/1	0.97	0.06	35,35,35,35	0
54	MG	1a	1853	1/1	0.97	0.10	65,65,65,65	0
54	MG	2A	3584	1/1	0.97	0.08	60,60,60,60	0
54	MG	2A	3072	1/1	0.97	0.04	51,51,51,51	0
54	MG	1A	3070	1/1	0.97	0.11	47,47,47,47	0
54	MG	1A	3232	1/1	0.97	0.09	68,68,68,68	0
54	MG	1a	1857	1/1	0.97	0.08	92,92,92,92	0
54	MG	2A	3437	1/1	0.97	0.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1X	102	1/1	0.97	0.07	62,62,62,62	0
54	MG	2A	3182	1/1	0.97	0.11	53,53,53,53	0
54	MG	1A	3008	1/1	0.97	0.12	39,39,39,39	0
54	MG	1A	3062	1/1	0.97	0.33	41,41,41,41	0
54	MG	1A	3501	1/1	0.97	0.06	32,32,32,32	0
54	MG	1A	3264	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3183	1/1	0.97	0.04	28,28,28,28	0
54	MG	1A	3208	1/1	0.97	0.08	40,40,40,40	0
54	MG	1a	1767	1/1	0.97	0.05	46,46,46,46	0
54	MG	2A	3604	1/1	0.97	0.05	66,66,66,66	0
54	MG	1A	3448	1/1	0.97	0.17	24,24,24,24	0
54	MG	1A	3084	1/1	0.97	0.13	40,40,40,40	0
54	MG	1l	102	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3401	1/1	0.97	0.04	53,53,53,53	0
54	MG	1A	3147	1/1	0.97	0.09	35,35,35,35	0
54	MG	2A	3610	1/1	0.97	0.08	61,61,61,61	0
54	MG	1A	3568	1/1	0.97	0.19	51,51,51,51	0
54	MG	1A	3166	1/1	0.97	0.14	45,45,45,45	0
54	MG	2A	3613	1/1	0.97	0.07	102,102,102,102	0
54	MG	1B	1024	1/1	0.97	0.06	61,61,61,61	0
54	MG	1A	3240	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3571	1/1	0.97	0.05	42,42,42,42	0
54	MG	2A	3200	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3511	1/1	0.97	0.09	52,52,52,52	0
54	MG	2A	3460	1/1	0.97	0.04	73,73,73,73	0
54	MG	1A	3649	1/1	0.97	0.10	52,52,52,52	0
54	MG	1A	3512	1/1	0.97	0.10	63,63,63,63	0
54	MG	2A	3331	1/1	0.97	0.06	98,98,98,98	0
54	MG	1o	101	1/1	0.97	0.08	42,42,42,42	0
54	MG	1A	3576	1/1	0.97	0.07	71,71,71,71	0
54	MG	1A	3652	1/1	0.97	0.05	54,54,54,54	0
54	MG	2A	3468	1/1	0.97	0.11	45,45,45,45	0
54	MG	2A	3470	1/1	0.97	0.05	46,46,46,46	0
54	MG	2A	3631	1/1	0.97	0.08	82,82,82,82	0
54	MG	1A	3045	1/1	0.97	0.11	41,41,41,41	0
54	MG	1A	3841	1/1	0.97	0.05	49,49,49,49	0
54	MG	1D	304	1/1	0.97	0.11	47,47,47,47	0
54	MG	1a	1786	1/1	0.97	0.06	82,82,82,82	0
54	MG	1A	3215	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3579	1/1	0.97	0.11	49,49,49,49	0
54	MG	2A	3106	1/1	0.97	0.05	51,51,51,51	0
54	MG	1A	3656	1/1	0.97	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3006	1/1	0.97	0.05	64,64,64,64	0
54	MG	1A	3188	1/1	0.97	0.07	38,38,38,38	0
54	MG	1A	3742	1/1	0.97	0.05	59,59,59,59	0
54	MG	1A	3149	1/1	0.97	0.07	43,43,43,43	0
54	MG	1A	3583	1/1	0.97	0.07	60,60,60,60	0
54	MG	1A	3460	1/1	0.97	0.09	46,46,46,46	0
54	MG	1A	3190	1/1	0.97	0.05	84,84,84,84	0
54	MG	1A	3519	1/1	0.97	0.10	39,39,39,39	0
54	MG	2A	3116	1/1	0.97	0.14	45,45,45,45	0
54	MG	2B	209	1/1	0.97	0.17	64,64,64,64	0
54	MG	1A	3046	1/1	0.97	0.18	46,46,46,46	0
54	MG	2A	3015	1/1	0.97	0.09	53,53,53,53	0
54	MG	2A	3016	1/1	0.97	0.06	71,71,71,71	0
54	MG	2A	3357	1/1	0.97	0.07	53,53,53,53	0
54	MG	1a	1798	1/1	0.97	0.05	107,107,107,107	0
54	MG	2A	3018	1/1	0.97	0.26	45,45,45,45	0
54	MG	2A	3498	1/1	0.97	0.11	67,67,67,67	0
54	MG	1A	3522	1/1	0.97	0.05	59,59,59,59	0
54	MG	2A	3231	1/1	0.97	0.10	72,72,72,72	0
54	MG	2A	3123	1/1	0.97	0.06	47,47,47,47	0
54	MG	2D	304	1/1	0.97	0.15	51,51,51,51	0
54	MG	1A	3368	1/1	0.97	0.05	54,54,54,54	0
54	MG	1A	3857	1/1	0.97	0.05	81,81,81,81	0
54	MG	1A	3151	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3467	1/1	0.97	0.15	67,67,67,67	0
54	MG	2a	1714	1/1	0.97	0.05	84,84,84,84	0
54	MG	1A	3756	1/1	0.97	0.05	67,67,67,67	0
54	MG	2A	3238	1/1	0.97	0.06	46,46,46,46	0
54	MG	2A	3239	1/1	0.97	0.11	38,38,38,38	0
54	MG	2A	3025	1/1	0.97	0.09	50,50,50,50	0
54	MG	1F	310	1/1	0.97	0.06	32,32,32,32	0
54	MG	2A	3243	1/1	0.97	0.05	67,67,67,67	0
54	MG	1A	3065	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3066	1/1	0.97	0.13	66,66,66,66	0
54	MG	2a	1723	1/1	0.97	0.05	79,79,79,79	0
54	MG	1A	3327	1/1	0.97	0.06	26,26,26,26	0
54	MG	1A	3223	1/1	0.97	0.08	55,55,55,55	0
54	MG	2R	203	1/1	0.97	0.07	53,53,53,53	0
54	MG	1A	3421	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3473	1/1	0.97	0.12	45,45,45,45	0
54	MG	1A	3679	1/1	0.97	0.09	73,73,73,73	0
54	MG	1A	3022	1/1	0.97	0.09	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	3382	1/1	0.97	0.07	59,59,59,59	0
54	MG	1A	3288	1/1	0.97	0.05	39,39,39,39	0
54	MG	1a	1724	1/1	0.97	0.04	72,72,72,72	0
54	MG	1A	3114	1/1	0.97	0.06	40,40,40,40	0
54	MG	1A	3477	1/1	0.97	0.04	48,48,48,48	0
54	MG	1a	1727	1/1	0.97	0.08	67,67,67,67	0
54	MG	1A	3425	1/1	0.97	0.06	36,36,36,36	0
54	MG	2A	3258	1/1	0.97	0.09	58,58,58,58	0
54	MG	1A	3686	1/1	0.97	0.08	51,51,51,51	0
54	MG	1A	3878	1/1	0.97	0.13	50,50,50,50	0
54	MG	1P	202	1/1	0.97	0.17	34,34,34,34	0
54	MG	1a	1824	1/1	0.97	0.15	82,82,82,82	0
54	MG	1A	3378	1/1	0.97	0.06	71,71,71,71	0
54	MG	1A	3480	1/1	0.97	0.21	50,50,50,50	0
54	MG	1A	3427	1/1	0.97	0.09	46,46,46,46	0
54	MG	2A	3398	1/1	0.97	0.10	78,78,78,78	0
54	MG	1A	3882	1/1	0.97	0.16	42,42,42,42	0
54	MG	1Q	202	1/1	0.97	0.09	48,48,48,48	0
54	MG	1A	3786	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3428	1/1	0.97	0.09	67,67,67,67	0
54	MG	2A	3547	1/1	0.97	0.09	72,72,72,72	0
54	MG	1A	3379	1/1	0.97	0.06	55,55,55,55	0
54	MG	1A	3692	1/1	0.97	0.10	41,41,41,41	0
54	MG	2A	3273	1/1	0.97	0.05	73,73,73,73	0
54	MG	1A	3795	1/1	0.97	0.06	60,60,60,60	0
54	MG	2A	3554	1/1	0.97	0.04	72,72,72,72	0
54	MG	1A	3139	1/1	0.97	0.18	42,42,42,42	0
54	MG	1A	3616	1/1	0.97	0.07	61,61,61,61	0
54	MG	1A	3293	1/1	0.97	0.07	36,36,36,36	0
54	MG	2a	1619	1/1	0.97	0.07	81,81,81,81	0
54	MG	1A	3126	1/1	0.97	0.13	42,42,42,42	0
54	MG	2A	3563	1/1	0.97	0.05	67,67,67,67	0
54	MG	1A	3200	1/1	0.97	0.12	40,40,40,40	0
54	MG	1A	3127	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3346	1/1	0.97	0.11	48,48,48,48	0
54	MG	2A	3568	1/1	0.97	0.07	78,78,78,78	0
54	MG	2A	3283	1/1	0.97	0.10	50,50,50,50	0
54	MG	2A	3284	1/1	0.97	0.07	43,43,43,43	0
54	MG	1A	3897	1/1	0.97	0.17	48,48,48,48	0
54	MG	2A	3573	1/1	0.97	0.06	52,52,52,52	0
54	MG	1A	3060	1/1	0.97	0.09	34,34,34,34	0
54	MG	1A	3551	1/1	0.97	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3337	1/1	0.98	0.03	70,70,70,70	0
54	MG	2A	3590	1/1	0.98	0.05	52,52,52,52	0
54	MG	1A	3607	1/1	0.98	0.07	50,50,50,50	0
54	MG	1A	3419	1/1	0.98	0.07	64,64,64,64	0
54	MG	1A	3339	1/1	0.98	0.12	34,34,34,34	0
54	MG	2A	3594	1/1	0.98	0.05	88,88,88,88	0
54	MG	1A	3671	1/1	0.98	0.06	39,39,39,39	0
54	MG	2A	3596	1/1	0.98	0.05	52,52,52,52	0
54	MG	1A	3610	1/1	0.98	0.12	42,42,42,42	0
54	MG	1A	3673	1/1	0.98	0.05	55,55,55,55	0
54	MG	1A	3464	1/1	0.98	0.03	53,53,53,53	0
54	MG	1A	3041	1/1	0.98	0.06	32,32,32,32	0
54	MG	1A	3202	1/1	0.98	0.15	33,33,33,33	0
54	MG	1a	1702	1/1	0.98	0.08	47,47,47,47	0
54	MG	1A	3342	1/1	0.98	0.04	28,28,28,28	0
54	MG	1A	3838	1/1	0.98	0.10	42,42,42,42	0
54	MG	1A	3343	1/1	0.98	0.06	32,32,32,32	0
54	MG	1a	1706	1/1	0.98	0.05	72,72,72,72	0
54	MG	1a	1707	1/1	0.98	0.04	57,57,57,57	0
54	MG	1A	3087	1/1	0.98	0.06	32,32,32,32	0
54	MG	1A	3019	1/1	0.98	0.08	45,45,45,45	0
54	MG	2A	3469	1/1	0.98	0.07	64,64,64,64	0
54	MG	1A	3181	1/1	0.98	0.15	46,46,46,46	0
54	MG	1A	3750	1/1	0.98	0.11	84,84,84,84	0
54	MG	1D	310	1/1	0.98	0.03	53,53,53,53	0
54	MG	2A	3473	1/1	0.98	0.03	104,104,104,104	0
54	MG	2A	3616	1/1	0.98	0.04	67,67,67,67	0
54	MG	1a	1814	1/1	0.98	0.05	65,65,65,65	0
54	MG	1A	3310	1/1	0.98	0.12	44,44,44,44	0
54	MG	2A	3619	1/1	0.98	0.07	65,65,65,65	0
54	MG	2A	3355	1/1	0.98	0.05	54,54,54,54	0
54	MG	2A	3241	1/1	0.98	0.04	86,86,86,86	0
54	MG	1A	3683	1/1	0.98	0.09	34,34,34,34	0
54	MG	1a	1715	1/1	0.98	0.05	54,54,54,54	0
54	MG	1A	3563	1/1	0.98	0.12	66,66,66,66	0
54	MG	2A	3625	1/1	0.98	0.18	56,56,56,56	0
54	MG	1A	3311	1/1	0.98	0.04	74,74,74,74	0
54	MG	1A	3286	1/1	0.98	0.08	32,32,32,32	0
54	MG	1A	3431	1/1	0.98	0.04	36,36,36,36	0
54	MG	1A	3520	1/1	0.98	0.05	51,51,51,51	0
54	MG	1A	3760	1/1	0.98	0.05	71,71,71,71	0
54	MG	1A	3015	1/1	0.98	0.20	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	3314	1/1	0.98	0.11	35,35,35,35	0
54	MG	1A	3090	1/1	0.98	0.20	36,36,36,36	0
54	MG	2A	3634	1/1	0.98	0.08	56,56,56,56	0
54	MG	1A	3764	1/1	0.98	0.07	62,62,62,62	0
54	MG	2A	3636	1/1	0.98	0.04	51,51,51,51	0
54	MG	1F	308	1/1	0.98	0.06	32,32,32,32	0
54	MG	1F	309	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3766	1/1	0.98	0.06	69,69,69,69	0
54	MG	1A	3767	1/1	0.98	0.04	53,53,53,53	0
54	MG	2A	3494	1/1	0.98	0.04	71,71,71,71	0
54	MG	2A	3495	1/1	0.98	0.06	36,36,36,36	0
54	MG	1A	3044	1/1	0.98	0.07	41,41,41,41	0
54	MG	2a	1686	1/1	0.98	0.07	67,67,67,67	0
54	MG	2A	3497	1/1	0.98	0.04	67,67,67,67	0
54	MG	1A	3771	1/1	0.98	0.06	48,48,48,48	0
54	MG	2A	3499	1/1	0.98	0.04	64,64,64,64	0
54	MG	1a	1834	1/1	0.98	0.08	74,74,74,74	0
54	MG	1A	3863	1/1	0.98	0.09	50,50,50,50	0
54	MG	1A	3693	1/1	0.98	0.24	56,56,56,56	0
54	MG	1A	3290	1/1	0.98	0.03	37,37,37,37	0
54	MG	2A	3379	1/1	0.98	0.10	73,73,73,73	0
54	MG	1A	3318	1/1	0.98	0.06	32,32,32,32	0
54	MG	1A	3574	1/1	0.98	0.07	69,69,69,69	0
54	MG	1A	3778	1/1	0.98	0.05	44,44,44,44	0
54	MG	1A	3575	1/1	0.98	0.07	41,41,41,41	0
54	MG	1A	3698	1/1	0.98	0.05	69,69,69,69	0
54	MG	1A	3196	1/1	0.98	0.05	37,37,37,37	0
54	MG	2A	3166	1/1	0.98	0.08	52,52,52,52	0
54	MG	2A	3387	1/1	0.98	0.04	63,63,63,63	0
54	MG	1A	3292	1/1	0.98	0.04	45,45,45,45	0
54	MG	1A	3784	1/1	0.98	0.10	35,35,35,35	0
54	MG	2D	303	1/1	0.98	0.07	52,52,52,52	0
54	MG	1A	3092	1/1	0.98	0.05	29,29,29,29	0
54	MG	2D	305	1/1	0.98	0.08	48,48,48,48	0
54	MG	1A	3294	1/1	0.98	0.06	31,31,31,31	0
54	MG	2E	301	1/1	0.98	0.06	39,39,39,39	0
54	MG	1A	3877	1/1	0.98	0.09	46,46,46,46	0
54	MG	1A	3787	1/1	0.98	0.11	82,82,82,82	0
54	MG	1A	3296	1/1	0.98	0.10	38,38,38,38	0
54	MG	1A	3487	1/1	0.98	0.05	56,56,56,56	0
54	MG	1A	3791	1/1	0.98	0.08	48,48,48,48	0
54	MG	2A	3526	1/1	0.98	0.11	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1855	1/1	0.98	0.05	74,74,74,74	0
54	MG	2O	201	1/1	0.98	0.05	69,69,69,69	0
54	MG	1A	3792	1/1	0.98	0.05	67,67,67,67	0
54	MG	1A	3793	1/1	0.98	0.07	67,67,67,67	0
54	MG	1A	3582	1/1	0.98	0.16	84,84,84,84	0
54	MG	2A	3401	1/1	0.98	0.06	75,75,75,75	0
54	MG	1A	3212	1/1	0.98	0.08	43,43,43,43	0
54	MG	1A	3403	1/1	0.98	0.07	71,71,71,71	0
54	MG	1R	206	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3491	1/1	0.98	0.04	66,66,66,66	0
54	MG	1A	3644	1/1	0.98	0.13	45,45,45,45	0
54	MG	1A	3536	1/1	0.98	0.04	42,42,42,42	0
54	MG	1T	2004	1/1	0.98	0.07	69,69,69,69	0
54	MG	2T	205	1/1	0.98	0.10	43,43,43,43	0
54	MG	1A	3800	1/1	0.98	0.09	61,61,61,61	0
54	MG	1A	3711	1/1	0.98	0.04	72,72,72,72	0
54	MG	2A	3296	1/1	0.98	0.06	47,47,47,47	0
54	MG	1A	3273	1/1	0.98	0.06	52,52,52,52	0
54	MG	1A	3894	1/1	0.98	0.03	46,46,46,46	0
54	MG	1A	3255	1/1	0.98	0.08	42,42,42,42	0
54	MG	2I	101	1/1	0.98	0.05	54,54,54,54	0
54	MG	1A	3804	1/1	0.98	0.07	81,81,81,81	0
54	MG	2A	3416	1/1	0.98	0.04	48,48,48,48	0
54	MG	2A	3417	1/1	0.98	0.09	60,60,60,60	0
54	MG	1A	3539	1/1	0.98	0.04	26,26,26,26	0
54	MG	1A	3898	1/1	0.98	0.04	34,34,34,34	0
54	MG	2A	3551	1/1	0.98	0.07	86,86,86,86	0
54	MG	2A	3552	1/1	0.98	0.05	66,66,66,66	0
54	MG	1A	3364	1/1	0.98	0.08	24,24,24,24	0
54	MG	1A	3365	1/1	0.98	0.07	22,22,22,22	0
54	MG	2A	3422	1/1	0.98	0.05	65,65,65,65	0
54	MG	1A	3328	1/1	0.98	0.05	35,35,35,35	0
54	MG	2a	1749	1/1	0.98	0.12	79,79,79,79	0
54	MG	2A	3306	1/1	0.98	0.07	34,34,34,34	0
54	MG	1A	3719	1/1	0.98	0.04	51,51,51,51	0
54	MG	1A	3595	1/1	0.98	0.07	50,50,50,50	0
54	MG	1A	3256	1/1	0.98	0.10	48,48,48,48	0
54	MG	1A	3076	1/1	0.98	0.07	46,46,46,46	0
54	MG	2a	1755	1/1	0.98	0.09	79,79,79,79	0
54	MG	2A	3429	1/1	0.98	0.05	81,81,81,81	0
54	MG	1A	3302	1/1	0.98	0.07	43,43,43,43	0
54	MG	2A	3312	1/1	0.98	0.04	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3814	1/1	0.98	0.10	51,51,51,51	0
54	MG	2A	3433	1/1	0.98	0.08	43,43,43,43	0
54	MG	2A	3314	1/1	0.98	0.03	81,81,81,81	0
54	MG	1A	3333	1/1	0.98	0.08	21,21,21,21	0
54	MG	1A	3455	1/1	0.98	0.05	38,38,38,38	0
54	MG	1A	3817	1/1	0.98	0.07	32,32,32,32	0
54	MG	1A	3601	1/1	0.98	0.07	39,39,39,39	0
54	MG	1A	3003	1/1	0.98	0.07	58,58,58,58	0
54	MG	1A	3820	1/1	0.98	0.08	59,59,59,59	0
54	MG	1B	1016	1/1	0.98	0.04	55,55,55,55	0
54	MG	1A	3603	1/1	0.98	0.10	51,51,51,51	0
54	MG	1A	3822	1/1	0.98	0.05	65,65,65,65	0
54	MG	1A	3823	1/1	0.98	0.05	82,82,82,82	0
54	MG	2A	3327	1/1	0.98	0.05	77,77,77,77	0
54	MG	1B	1020	1/1	0.98	0.05	50,50,50,50	0
54	MG	1A	3335	1/1	0.98	0.10	38,38,38,38	0
56	ZN	14	101	1/1	0.98	0.04	135,135,135,135	0
54	MG	1A	3078	1/1	0.98	0.10	51,51,51,51	0
56	ZN	2n	101	1/1	0.98	0.04	120,120,120,120	0
57	SF4	1d	501	8/8	0.98	0.05	77,92,105,112	0
57	SF4	2d	501	8/8	0.98	0.05	71,89,97,104	0
54	MG	1A	3269	1/1	0.99	0.16	30,30,30,30	0
54	MG	1A	3789	1/1	0.99	0.05	58,58,58,58	0
54	MG	1A	3209	1/1	0.99	0.07	35,35,35,35	0
54	MG	1A	3752	1/1	0.99	0.03	37,37,37,37	0
54	MG	1B	1013	1/1	0.99	0.05	49,49,49,49	0
54	MG	2A	3523	1/1	0.99	0.07	50,50,50,50	0
54	MG	1A	3323	1/1	0.99	0.12	67,67,67,67	0
54	MG	1A	3660	1/1	0.99	0.03	52,52,52,52	0
54	MG	1A	3661	1/1	0.99	0.07	32,32,32,32	0
54	MG	1a	1717	1/1	0.99	0.06	46,46,46,46	0
54	MG	2A	3528	1/1	0.99	0.05	60,60,60,60	0
54	MG	1A	3833	1/1	0.99	0.08	53,53,53,53	0
54	MG	1A	3876	1/1	0.99	0.04	29,29,29,29	0
54	MG	1A	3154	1/1	0.99	0.04	35,35,35,35	0
54	MG	2A	3467	1/1	0.99	0.03	83,83,83,83	0
54	MG	2A	3293	1/1	0.99	0.04	44,44,44,44	0
54	MG	2A	3351	1/1	0.99	0.09	74,74,74,74	0
54	MG	2Q	202	1/1	0.99	0.10	70,70,70,70	0
54	MG	1A	3338	1/1	0.99	0.10	18,18,18,18	0
54	MG	2a	1726	1/1	0.99	0.04	83,83,83,83	0
54	MG	1A	3281	1/1	0.99	0.05	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1723	1/1	0.99	0.12	75,75,75,75	0
54	MG	1A	3725	1/1	0.99	0.10	76,76,76,76	0
54	MG	1A	3272	1/1	0.99	0.04	23,23,23,23	0
54	MG	1A	3458	1/1	0.99	0.05	41,41,41,41	0
54	MG	1A	3590	1/1	0.99	0.04	61,61,61,61	0
54	MG	1A	3884	1/1	0.99	0.04	37,37,37,37	0
54	MG	1A	3029	1/1	0.99	0.04	44,44,44,44	0
54	MG	1A	3404	1/1	0.99	0.06	55,55,55,55	0
54	MG	1A	3765	1/1	0.99	0.05	38,38,38,38	0
54	MG	1A	3670	1/1	0.99	0.13	56,56,56,56	0
54	MG	16	102	1/1	0.99	0.06	54,54,54,54	0
54	MG	1A	3370	1/1	0.99	0.04	25,25,25,25	0
54	MG	2A	3048	1/1	0.99	0.06	80,80,80,80	0
54	MG	17	102	1/1	0.99	0.12	53,53,53,53	0
54	MG	1a	1736	1/1	0.99	0.03	76,76,76,76	0
54	MG	1A	3594	1/1	0.99	0.07	31,31,31,31	0
54	MG	1A	3769	1/1	0.99	0.04	69,69,69,69	0
54	MG	1a	1835	1/1	0.99	0.04	80,80,80,80	0
54	MG	2A	3555	1/1	0.99	0.06	71,71,71,71	0
54	MG	1A	3462	1/1	0.99	0.07	33,33,33,33	0
54	MG	2A	3315	1/1	0.99	0.04	50,50,50,50	0
54	MG	2A	3558	1/1	0.99	0.05	70,70,70,70	0
54	MG	2A	3559	1/1	0.99	0.10	50,50,50,50	0
54	MG	2A	3316	1/1	0.99	0.03	58,58,58,58	0
54	MG	2A	3208	1/1	0.99	0.07	68,68,68,68	0
54	MG	1A	3772	1/1	0.99	0.09	57,57,57,57	0
54	MG	2A	3564	1/1	0.99	0.04	53,53,53,53	0
54	MG	1A	3645	1/1	0.99	0.04	52,52,52,52	0
54	MG	2a	1756	1/1	0.99	0.03	73,73,73,73	0
54	MG	1A	3774	1/1	0.99	0.06	65,65,65,65	0
54	MG	1A	3068	1/1	0.99	0.06	36,36,36,36	0
54	MG	1A	3738	1/1	0.99	0.10	43,43,43,43	0
54	MG	1A	3443	1/1	0.99	0.04	36,36,36,36	0
54	MG	1A	3295	1/1	0.99	0.04	26,26,26,26	0
54	MG	2A	3571	1/1	0.99	0.04	68,68,68,68	0
54	MG	2A	3268	1/1	0.99	0.08	58,58,58,58	0
54	MG	1A	3779	1/1	0.99	0.06	68,68,68,68	0
54	MG	1E	302	1/1	0.99	0.07	24,24,24,24	0
54	MG	1a	1846	1/1	0.99	0.04	43,43,43,43	0
54	MG	1A	3330	1/1	0.99	0.07	45,45,45,45	0
54	MG	2A	3446	1/1	0.99	0.06	53,53,53,53	0
54	MG	1A	3488	1/1	0.99	0.06	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3409	1/1	0.99	0.05	50,50,50,50	0
54	MG	1A	3275	1/1	0.99	0.03	50,50,50,50	0
54	MG	2A	3510	1/1	0.99	0.04	45,45,45,45	0
54	MG	2A	3276	1/1	0.99	0.06	47,47,47,47	0
54	MG	1A	3627	1/1	0.99	0.07	67,67,67,67	0
54	MG	2A	3513	1/1	0.99	0.04	81,81,81,81	0
56	ZN	1Y	201	1/1	0.99	0.03	83,83,83,83	0
54	MG	2A	3585	1/1	0.99	0.07	81,81,81,81	0
56	ZN	1n	102	1/1	0.99	0.02	94,94,94,94	0
56	ZN	2Y	202	1/1	0.99	0.03	95,95,95,95	0
54	MG	2A	3514	1/1	0.99	0.09	69,69,69,69	0
56	ZN	25	101	1/1	0.99	0.02	83,83,83,83	0
56	ZN	26	101	1/1	0.99	0.04	72,72,72,72	0
56	ZN	29	101	1/1	0.99	0.03	101,101,101,101	0
54	MG	1A	3096	1/1	0.99	0.09	47,47,47,47	0
54	MG	1A	3394	1/1	0.99	0.03	78,78,78,78	0
54	MG	1A	3004	1/1	0.99	0.08	48,48,48,48	0
54	MG	1A	3722	1/1	1.00	0.02	35,35,35,35	0
54	MG	1A	3846	1/1	1.00	0.04	43,43,43,43	0
54	MG	1A	3751	1/1	1.00	0.02	47,47,47,47	0
54	MG	1A	3387	1/1	1.00	0.02	33,33,33,33	0
54	MG	1B	1014	1/1	1.00	0.02	50,50,50,50	0
56	ZN	15	102	1/1	1.00	0.02	53,53,53,53	0
56	ZN	16	101	1/1	1.00	0.02	52,52,52,52	0
56	ZN	19	102	1/1	1.00	0.02	50,50,50,50	0
54	MG	1A	3388	1/1	1.00	0.02	23,23,23,23	0
54	MG	1A	3380	1/1	1.00	0.02	23,23,23,23	0
54	MG	2A	3599	1/1	1.00	0.03	48,48,48,48	0
54	MG	2A	3560	1/1	1.00	0.05	51,51,51,51	0
54	MG	1A	3736	1/1	1.00	0.02	37,37,37,37	0
54	MG	1A	3862	1/1	1.00	0.03	35,35,35,35	0
54	MG	1A	3842	1/1	1.00	0.03	35,35,35,35	0
54	MG	1A	3770	1/1	1.00	0.02	37,37,37,37	0
54	MG	1A	3717	1/1	1.00	0.05	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.