



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 03:38 AM EDT

PDB ID : 8FC2 / pdb_00008fc2
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with protein Y, hygromycin A, and azithromycin at 2.50Å resolution
Authors : Chen, C.-W.; Syroegin, E.A.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on : 2022-12-01
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

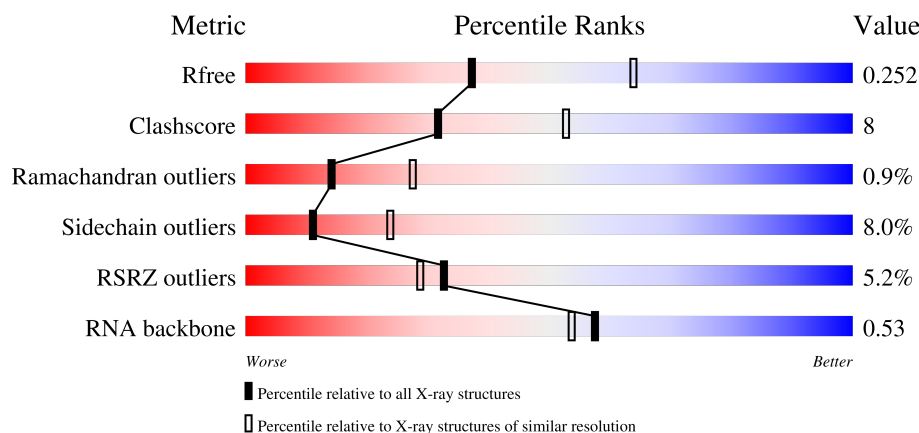
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



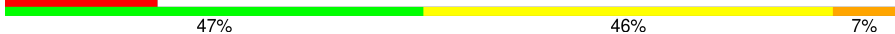
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 68% 25% 6%
1	2A	2915	4% 62% 29% 7%
2	1B	121	% 71% 23% 5%
2	2B	121	2% 59% 35% 6%

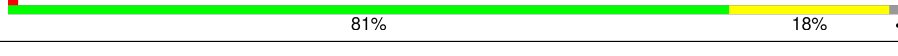
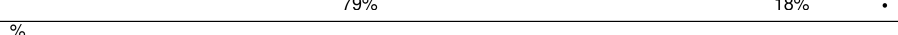
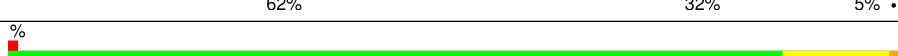
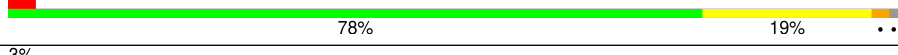
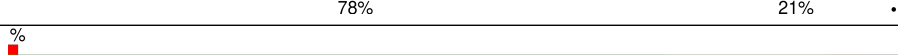
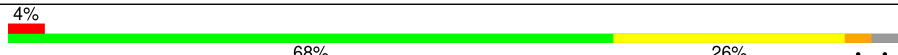
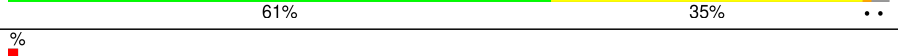
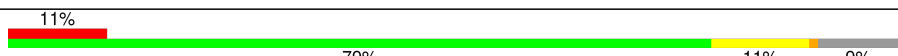
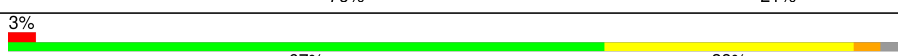
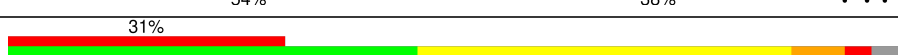
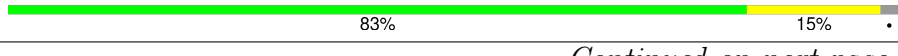
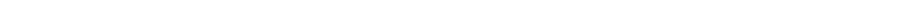
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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118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

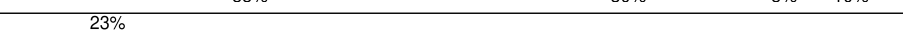
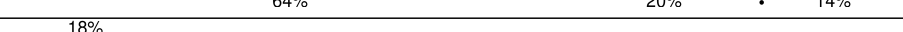
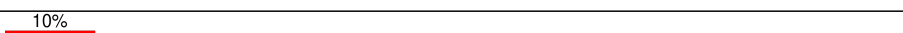
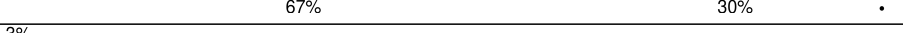
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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25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

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Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

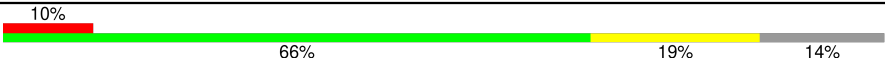
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Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50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

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Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	SF4	1d	305	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296715 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1021	Total	Mg	0	0
			1021	1021		
54	1B	29	Total	Mg	0	0
			29	29		
54	1D	20	Total	Mg	0	0
			20	20		
54	1E	10	Total	Mg	0	0
			10	10		
54	1F	17	Total	Mg	0	0
			17	17		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	4	Total	Mg	0	0
			4	4		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	5	Total	Mg	0	0
			5	5		
54	1Q	5	Total	Mg	0	0
			5	5		
54	1R	8	Total	Mg	0	0
			8	8		
54	1T	3	Total	Mg	0	0
			3	3		
54	1U	6	Total	Mg	0	0
			6	6		
54	1V	6	Total	Mg	0	0
			6	6		
54	1W	4	Total	Mg	0	0
			4	4		
54	1Y	1	Total	Mg	0	0
			1	1		
54	1Z	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	10	8	Total 8	Mg 8	0	0
54	11	5	Total 5	Mg 5	0	0
54	13	3	Total 3	Mg 3	0	0
54	14	1	Total 1	Mg 1	0	0
54	15	8	Total 8	Mg 8	0	0
54	17	6	Total 6	Mg 6	0	0
54	18	2	Total 2	Mg 2	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	281	Total 281	Mg 281	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	4	Total 4	Mg 4	0	0
54	1e	4	Total 4	Mg 4	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1g	2	Total 2	Mg 2	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	1k	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1m	1	Total 1	Mg 1	0	0
54	1n	2	Total 2	Mg 2	0	0
54	1o	2	Total 2	Mg 2	0	0

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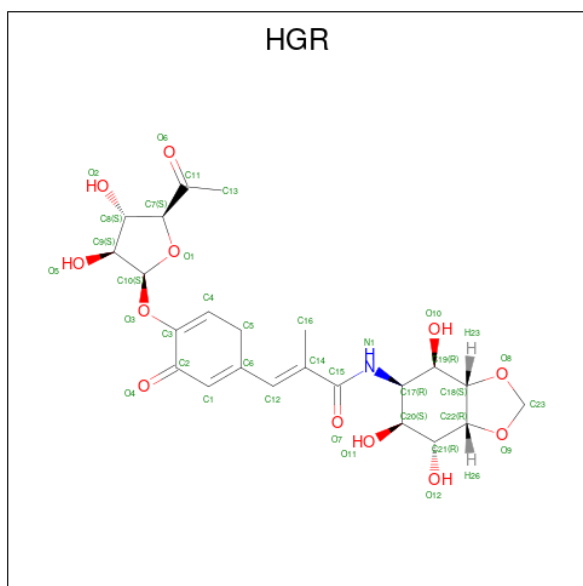
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1t	1	Total 1	Mg 1	0	0
54	1y	3	Total 3	Mg 3	0	0
54	2A	729	Total 729	Mg 729	0	0
54	2B	16	Total 16	Mg 16	0	0
54	2D	12	Total 12	Mg 12	0	0
54	2E	7	Total 7	Mg 7	0	0
54	2F	4	Total 4	Mg 4	0	0
54	2G	2	Total 2	Mg 2	0	0
54	2I	2	Total 2	Mg 2	0	0
54	2O	2	Total 2	Mg 2	0	0
54	2P	2	Total 2	Mg 2	0	0
54	2Q	3	Total 3	Mg 3	0	0
54	2R	2	Total 2	Mg 2	0	0
54	2T	4	Total 4	Mg 4	0	0
54	2U	1	Total 1	Mg 1	0	0
54	2V	3	Total 3	Mg 3	0	0
54	2W	3	Total 3	Mg 3	0	0
54	2X	1	Total 1	Mg 1	0	0
54	2Y	1	Total 1	Mg 1	0	0
54	20	3	Total 3	Mg 3	0	0
54	21	1	Total 1	Mg 1	0	0

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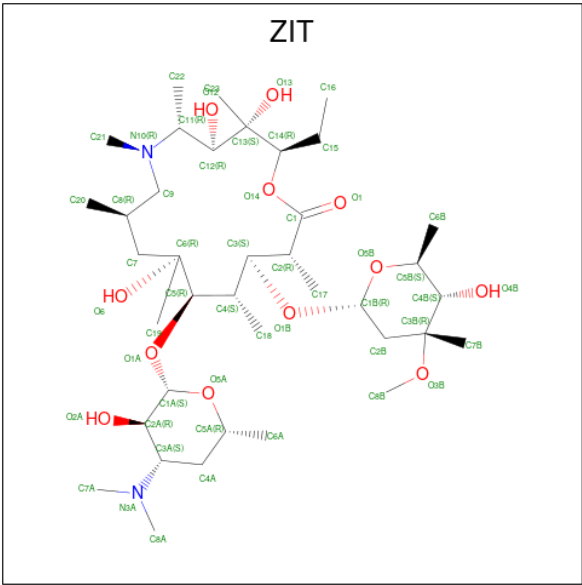
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	23	1	Total	Mg	0	0
			1	1		
54	25	3	Total	Mg	0	0
			3	3		
54	27	3	Total	Mg	0	0
			3	3		
54	28	3	Total	Mg	0	0
			3	3		
54	2a	193	Total	Mg	0	0
			193	193		
54	2e	1	Total	Mg	0	0
			1	1		
54	2f	1	Total	Mg	0	0
			1	1		
54	2j	1	Total	Mg	0	0
			1	1		
54	2k	1	Total	Mg	0	0
			1	1		
54	2o	1	Total	Mg	0	0
			1	1		
54	2t	1	Total	Mg	0	0
			1	1		

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



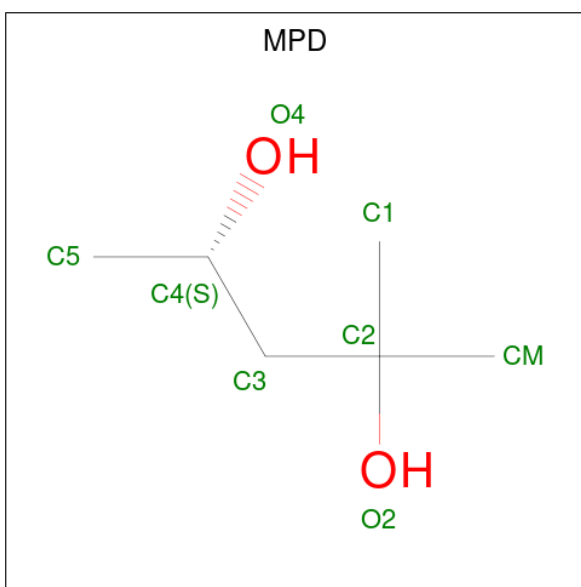
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	1A	1	Total	C	N	O	0	0
			36	23	1	12		
55	2A	1	Total	C	N	O	0	0
			36	23	1	12		

- Molecule 56 is AZITHROMYCIN (CCD ID: ZIT) (formula: C₃₈H₇₂N₂O₁₂) (labeled as "Ligand of Interest" by depositor).



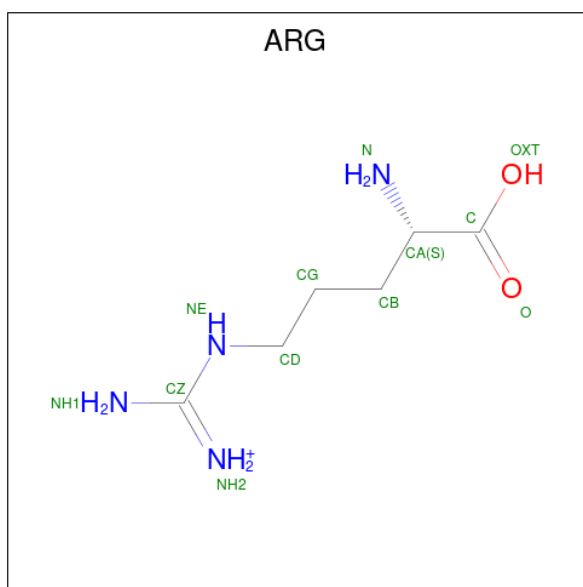
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	1A	1	Total	C	N	O	0	0
			52	38	2	12		
56	2A	1	Total	C	N	O	0	0
			52	38	2	12		

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



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

- Molecule 58 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



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

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

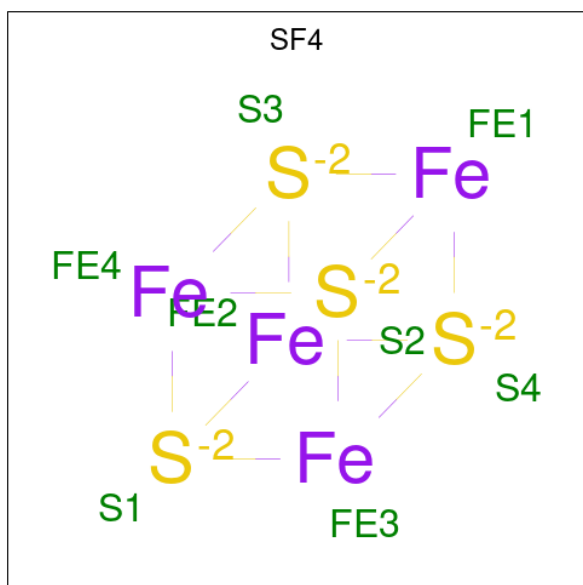
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0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

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

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	3943	Total	O	0	0
			3943	3943		
61	1B	106	Total	O	0	0
			106	106		
61	1D	106	Total	O	0	0
			106	106		
61	1E	75	Total	O	0	0
			75	75		
61	1F	62	Total	O	0	0
			62	62		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	15	Total 15	O 15	0	0
61	1H	13	Total 13	O 13	0	0
61	1I	6	Total 6	O 6	0	0
61	1N	50	Total 50	O 50	0	0
61	1O	23	Total 23	O 23	0	0
61	1P	56	Total 56	O 56	0	0
61	1Q	38	Total 38	O 38	0	0
61	1R	37	Total 37	O 37	0	0
61	1S	11	Total 11	O 11	0	0
61	1T	39	Total 39	O 39	0	0
61	1U	43	Total 43	O 43	0	0
61	1V	36	Total 36	O 36	0	0
61	1W	29	Total 29	O 29	0	0
61	1X	26	Total 26	O 26	0	0
61	1Y	16	Total 16	O 16	0	0
61	1Z	12	Total 12	O 12	0	0
61	10	21	Total 21	O 21	0	0
61	11	24	Total 24	O 24	0	0
61	12	12	Total 12	O 12	0	0
61	13	19	Total 19	O 19	0	0
61	14	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	15	24	Total 24	O 24	0	0
61	16	19	Total 19	O 19	0	0
61	17	14	Total 14	O 14	0	0
61	18	25	Total 25	O 25	0	0
61	19	2	Total 2	O 2	0	0
61	1a	465	Total 465	O 465	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	8	Total 8	O 8	0	0
61	1e	4	Total 4	O 4	0	0
61	1f	1	Total 1	O 1	0	0
61	1h	1	Total 1	O 1	0	0
61	1i	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	4	Total 4	O 4	0	0
61	1o	4	Total 4	O 4	0	0
61	1t	1	Total 1	O 1	0	0
61	1u	1	Total 1	O 1	0	0
61	1y	3	Total 3	O 3	0	0
61	2A	1664	Total 1664	O 1664	0	0
61	2B	25	Total 25	O 25	0	0
61	2D	38	Total 38	O 38	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2E	18	Total 18	O 18	0	0
61	2F	18	Total 18	O 18	0	0
61	2G	4	Total 4	O 4	0	0
61	2H	1	Total 1	O 1	0	0
61	2I	1	Total 1	O 1	0	0
61	2N	2	Total 2	O 2	0	0
61	2O	11	Total 11	O 11	0	0
61	2P	11	Total 11	O 11	0	0
61	2Q	10	Total 10	O 10	0	0
61	2R	16	Total 16	O 16	0	0
61	2T	7	Total 7	O 7	0	0
61	2U	8	Total 8	O 8	0	0
61	2V	5	Total 5	O 5	0	0
61	2W	17	Total 17	O 17	0	0
61	2X	3	Total 3	O 3	0	0
61	2Y	3	Total 3	O 3	0	0
61	2Z	3	Total 3	O 3	0	0
61	20	6	Total 6	O 6	0	0
61	21	12	Total 12	O 12	0	0
61	23	1	Total 1	O 1	0	0
61	25	6	Total 6	O 6	0	0

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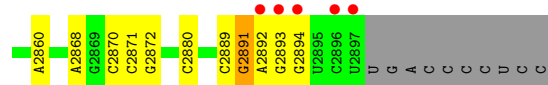
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	26	5	Total 5	O 5	0	0
61	27	5	Total 5	O 5	0	0
61	28	8	Total 8	O 8	0	0
61	2a	245	Total 245	O 245	0	0
61	2d	2	Total 2	O 2	0	0
61	2e	1	Total 1	O 1	0	0
61	2f	3	Total 3	O 3	0	0
61	2l	3	Total 3	O 3	0	0
61	2m	1	Total 1	O 1	0	0
61	2o	2	Total 2	O 2	0	0
61	2q	2	Total 2	O 2	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	2	Total 2	O 2	0	0
61	2y	2	Total 2	O 2	0	0

U097	U098	U099	G100	U101	G102	A103	C104	U105	G106	C109	G110	A111	U112	U113	G114	G115	C116	A118	A119	G135	G136	U141	U142	A143	A155	U165	C166	U167	G171	G173	A174	U175	G176	A177	C178	C179	C180	U188	A190	U191	G192	C193	A194	G195	U196	U197	U198	U199	U200	U201	U202	U203	U204	U205	U206	U207	U208	U209	U210	U211	U212	U213	U214	U215	U216	U217	U218	U219	U220	U221	U222	U223	U224	U225	U226	U227	U228	U229	U230	U231	U232	U233	U234	U235	U236	U237	U238	U239	U240	U241	U242	U243	U244	U245	U246	U247	U248	U249	U250	U251	U252	U253	U254	U255	U256	U257	U258	U259	U260	U261	U262	U263	U264	U265	U266	U267	U268	U269	U270	U271	U272	U273	U274	U275	U276	U277	U278	U279	U280	U281	U282	U283	U284	U285	U286	U287	U288	U289	U290	U291	U292	U293	U294	U295	U296	U297	U298	U299	U300	U301	U302	U303	U304	U305	U306	U307	U308	U309	U310	U311	U312	U313	U314	U315	U316	U317	U318	U319	U320	U321	U322	U323	U324	U325	U326	U327	U328	U329	U330	U331	U332	U333	U334	U335	U336	U337	U338	U339	U340	U341	U342	U343	U344	U345	U346	U347	U348	U349	U350	U351	U352	U353	U354	U355	U356	U357	U358	U359	U360	U361	U362	U363	U364	U365	U366	U367	U368	U369	U370	U371	U372	U373	U374	U375	U376	U377	U378	U379	U380	U381	U382	U383	U384	U385	U386	U387	U388	U389	U390	U391	U392	U393	U394	U395	U396	U397	U398	U399	U400	U401	U402	U403	U404	U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125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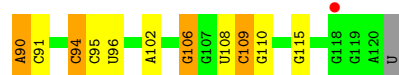
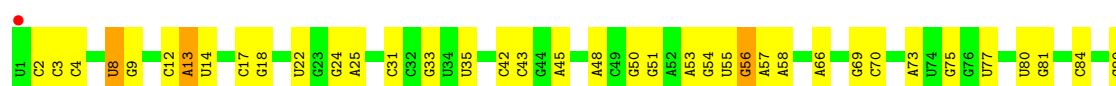
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C	G2445	A2448	C2342	A2267	G2160	U2099	U1991	U1576	G1456	G1459	G1456	G1325
U2792	G2570	A2448	C2343	A2268	C2161	G2100	C1992	C1577	G1459	U1577	U1340	U1340
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C2811	U2606	C2477	A2376	G2289	C2177	U2022	G2023	A1587	A1587	G1482	A1372	A1372
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C2610	C2610	A2478	A2377	C2294	C2179	A2119	U2028	A1587	A1587	G1482	A1374	A1374
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U2615	U2615	U2491	C2380	U2296	G2182	U2122	A2030	A1587	A1587	G1482	A1377	A1377
C2616	C2616	U2492	C2381	C2297	C2183	G2123	G2031	A1587	A1587	G1482	A1378	A1378
C2617	C2617	C2498	G2382	A2298	G2184	G2124	G2032	A1587	A1587	G1482	A1379	A1379
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C2627	C2627	C2507	C2395	A2311	G2193	U2133	C2043	A1587	A1587	G1482	A1389	A1389
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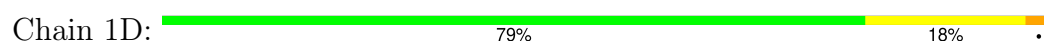
• Molecule 2: 5S Ribosomal RNA



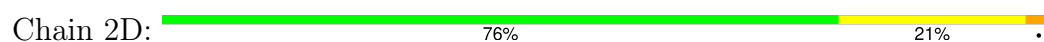
• Molecule 2: 5S Ribosomal RNA



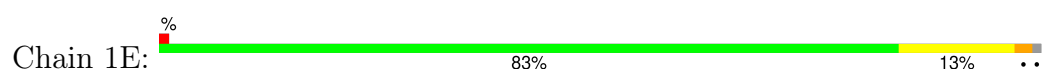
• Molecule 3: 50S ribosomal protein L2



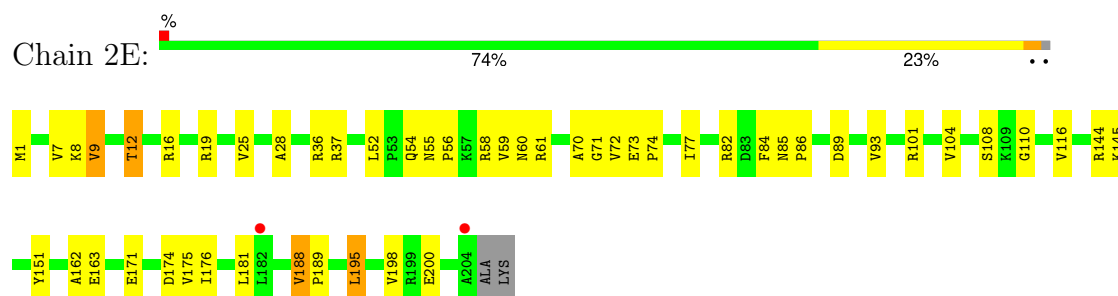
• Molecule 3: 50S ribosomal protein L2



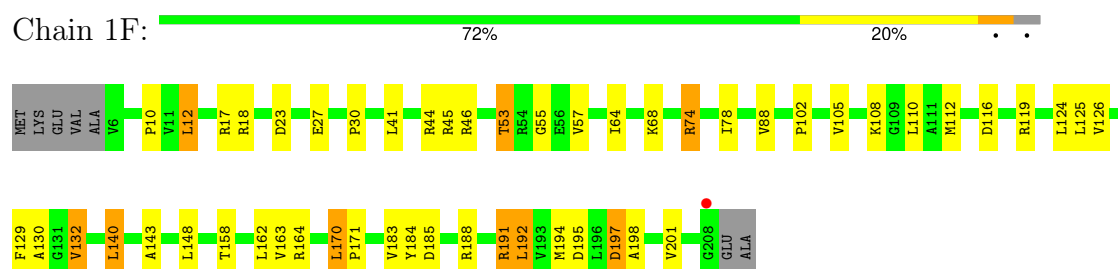
• Molecule 4: 50S ribosomal protein L3



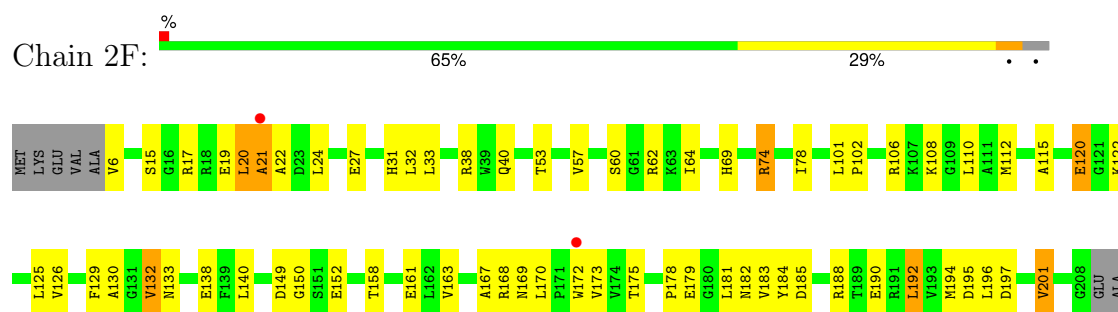
- Molecule 4: 50S ribosomal protein L3



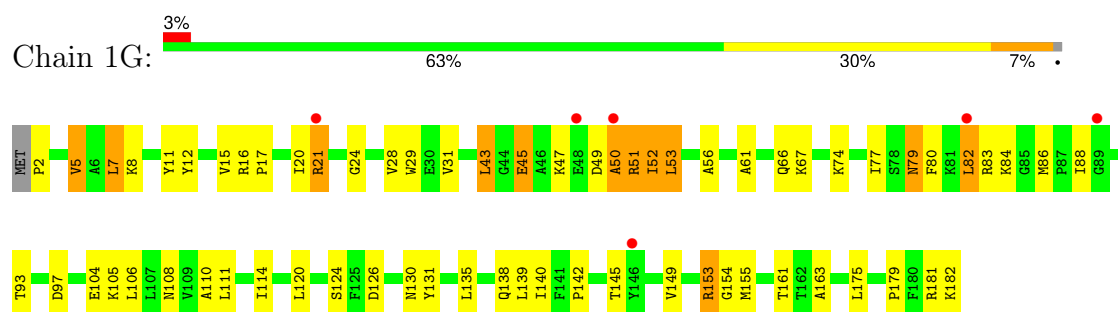
- Molecule 5: 50S ribosomal protein L4



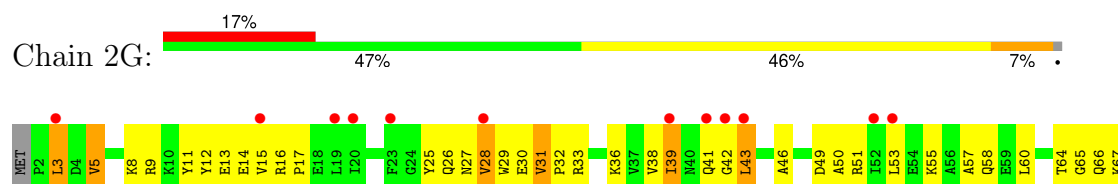
- Molecule 5: 50S ribosomal protein L4

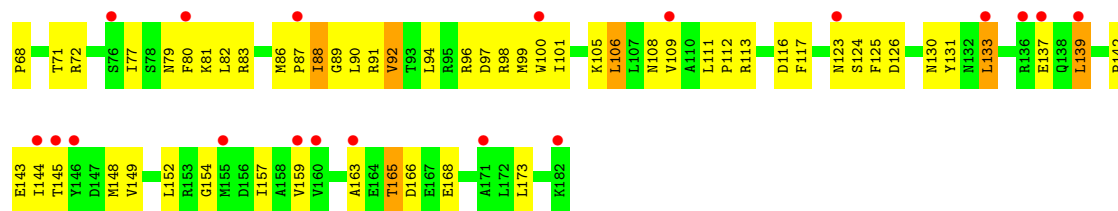


- Molecule 6: 50S ribosomal protein L5

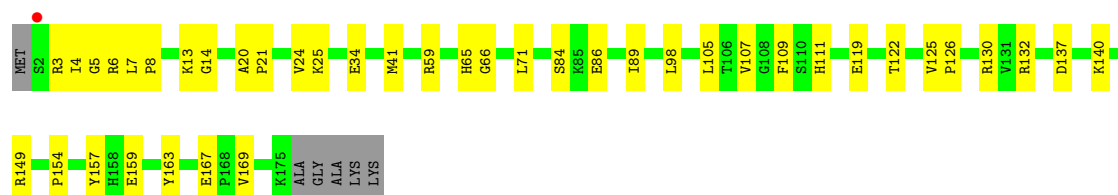
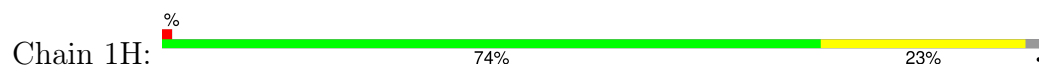


- Molecule 6: 50S ribosomal protein L5

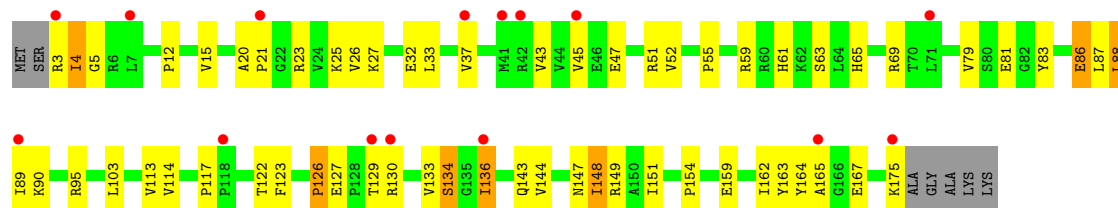




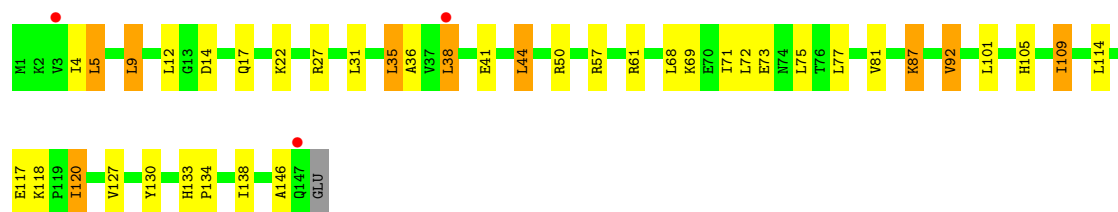
• Molecule 7: 50S ribosomal protein L6



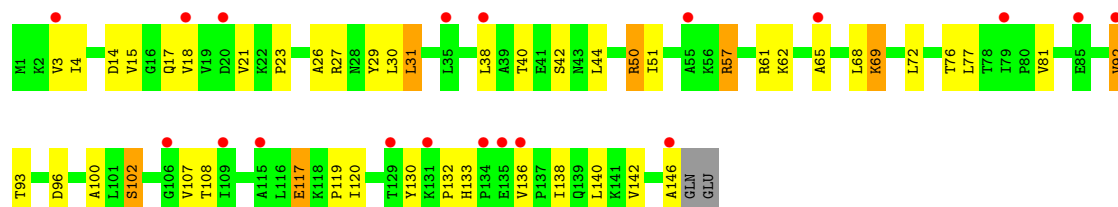
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L9



• Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13

Chain 1N:  79% 19% .



- Molecule 9: 50S ribosomal protein L13

Chain 2N:  75% 23% .



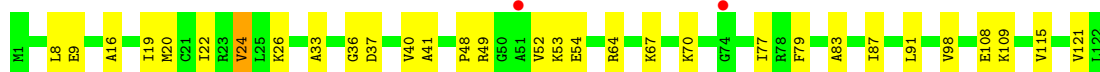
- Molecule 10: 50S ribosomal protein L14

Chain 1O:  82% 16% .



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  75% 25% .



- Molecule 11: 50S ribosomal protein L15

Chain 1P:  77% 21% ..



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  78% 20% ..



- Molecule 12: 50S ribosomal protein L16

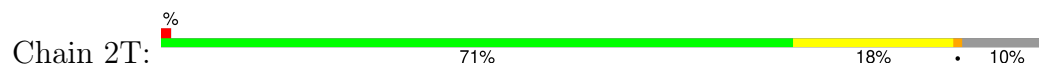
Chain 1Q:  84% 13% .



-
- | Category | Count |
|----------|-------|
| M1 | 100 |
| N2 | 100 |
| R3 | 100 |
| E11 | 100 |
| R23 | 100 |
| P24 | 100 |
| V28 | 100 |
| K33 | 100 |
| V34 | 100 |
| G37 | 100 |
| N38 | 100 |
| V49 | 100 |
| F50 | 100 |
| R51 | 100 |
| F52 | 100 |
| R53 | 100 |
| R54 | 100 |
| F57 | 100 |
| N58 | 100 |
| T59 | 100 |
| R64 | 100 |
| E73 | 100 |
| L82 | 100 |
| R86 | 100 |
| R95 | 100 |
| R96 | 100 |
| A97 | 100 |
| K98 | 100 |
| R118 | 100 |
| R119 | 100 |
| R120 | 100 |
| A126 | 100 |
| A127 | 100 |
| E128 | 100 |
| R129 | 100 |
| A130 | 100 |
| A131 | 100 |
| LYS | 100 |
| GLU | 100 |
| GLU | 100 |
| ALA | 100 |
| ALA | 100 |
| GLN | 100 |
| LYS | 100 |
| LYS | 100 |
| ALA | 100 |
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| GLN | 100 |
| GLU | 100 |

PRO
LYS
ALA
SER
GLN
GLU

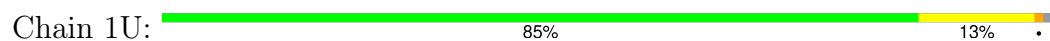
• Molecule 15: 50S ribosomal protein L19



M1 M2 R3 E11 R16 T17 R23 V28 R29 V30 V34 R39 T40 R53 T60 K65 Y66 S67 V72 E73 R74 P77 I83 I86 V89 R96 R108 E109 R112 D117 R120 A127 A130 A131 LYS GLU GLU ALA GLN

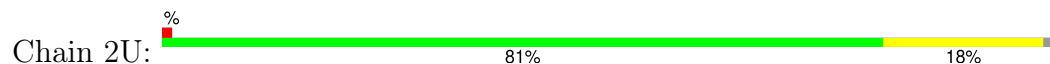
LYS
ALA
GLN
GLU
PRO
LYS
ALA
SER
GLN
GLU

• Molecule 16: 50S ribosomal protein L20



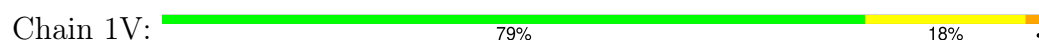
MET F2 K5 R11 K16 K16 S31 F32 R33 H49 R50 R53 L74 S77 A86 V100 R101 E108 Q117 GLY

• Molecule 16: 50S ribosomal protein L20



MET F2 K5 R10 K13 L27 S31 K34 H49 R50 K51 R52 R53 R54 R55 N66 R70 L74 S77 V90 D91 R92 K93 N94 D97 V100 R101 Q117 GLY

• Molecule 17: 50S ribosomal protein L21



M1 R21 T32 L40 E43 K44 T45 V46 T49 P50 V51 V61 R66 V72 S73 K74 K78 V79 Q80 Y81 R82 R83 K84 K85 Y91 G101

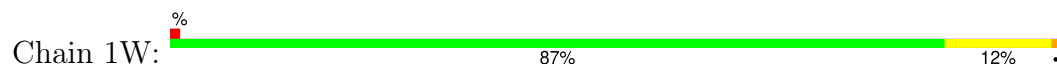
• Molecule 17: 50S ribosomal protein L21



M1 F2 V5 K6 Y12 R13 V14 E15 P16 G17 L18 E23 R24 L25 E28 L35 L38 L39 L40 G41 G42 E43 K44 T45 V46 V51 V52 A55 S56 V57 E60 V61 L62 L63 K74 F75 K76 Y79 Q80 Y81 R82 R83 T92 L95 I96 K97 E98

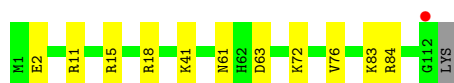
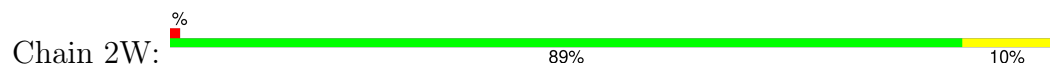
I99 R100 G101

• Molecule 18: 50S ribosomal protein L22

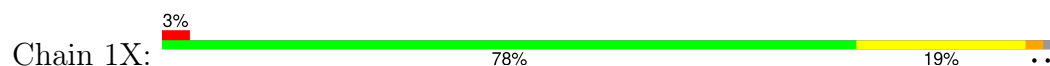




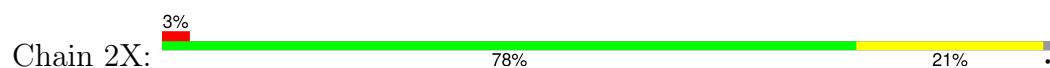
- Molecule 18: 50S ribosomal protein L22



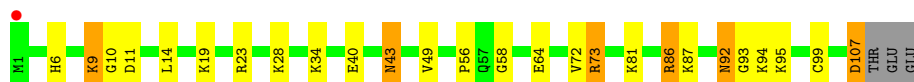
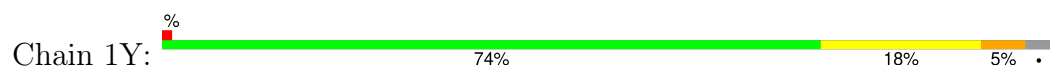
- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



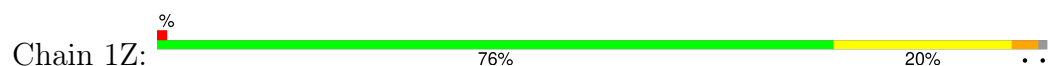
- Molecule 20: 50S ribosomal protein L24

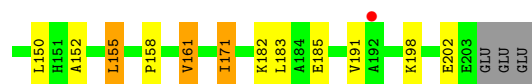


- Molecule 20: 50S ribosomal protein L24

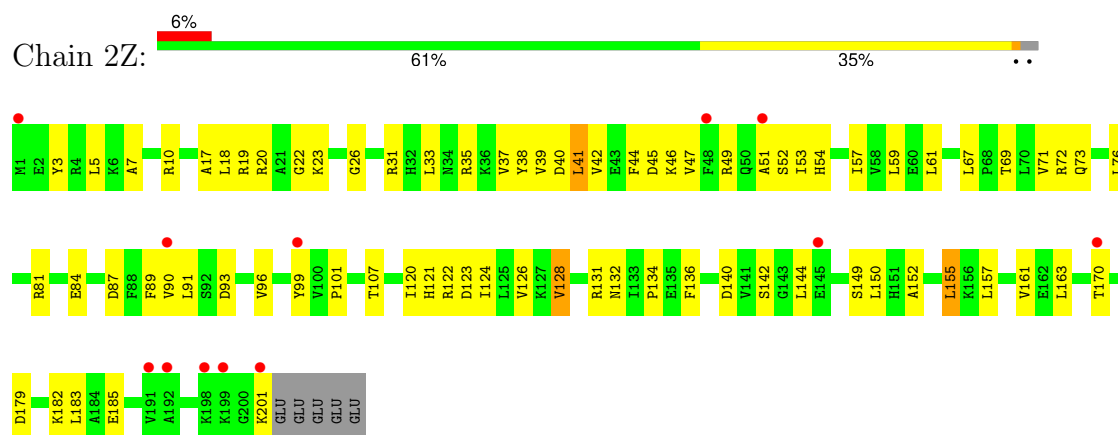


- Molecule 21: 50S ribosomal protein L25

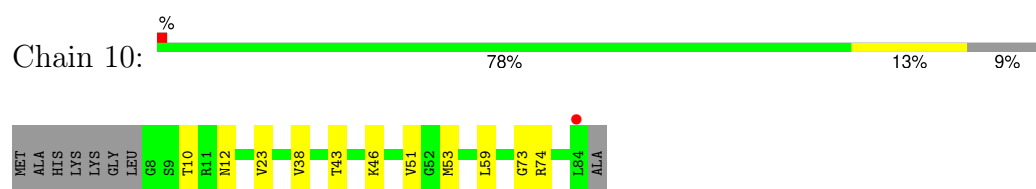




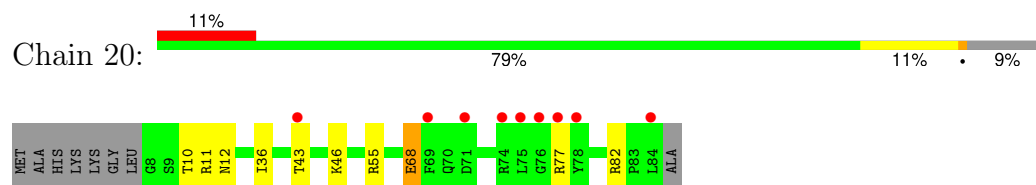
- Molecule 21: 50S ribosomal protein L25



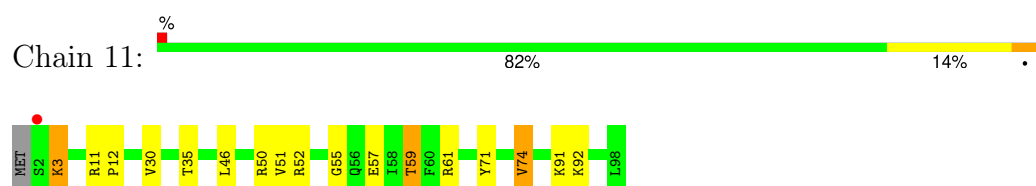
- Molecule 22: 50S ribosomal protein L27



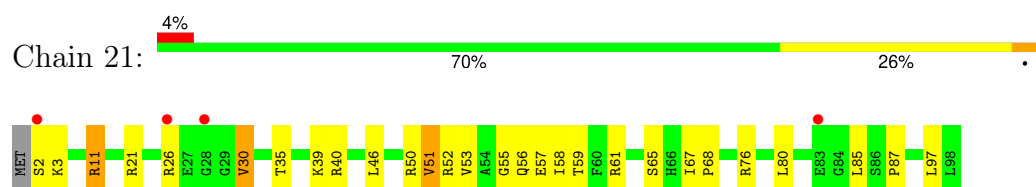
- Molecule 22: 50S ribosomal protein L27



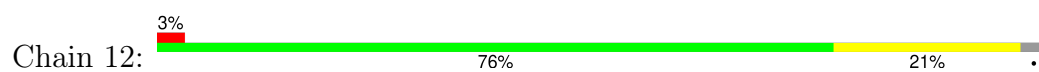
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



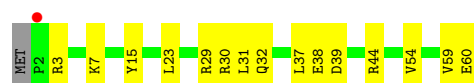
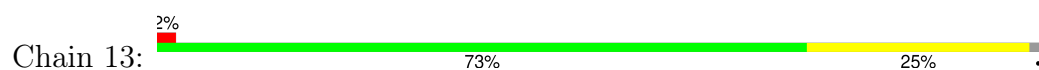
- Molecule 24: 50S ribosomal protein L29



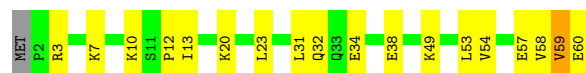
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



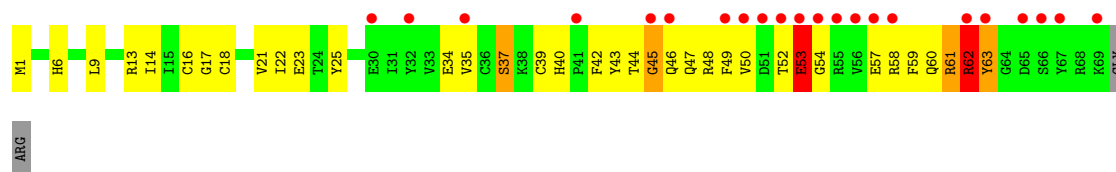
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31

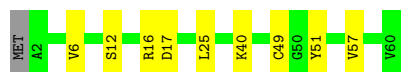
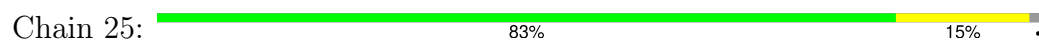


- Molecule 27: 50S ribosomal protein L32

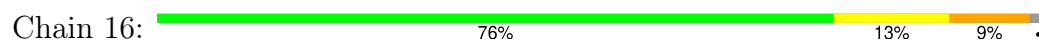




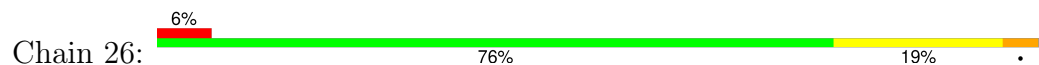
- Molecule 27: 50S ribosomal protein L32



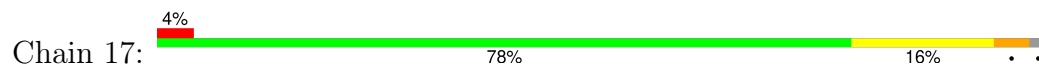
- Molecule 28: 50S ribosomal protein L33



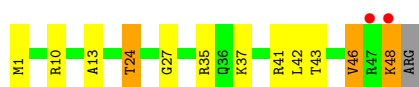
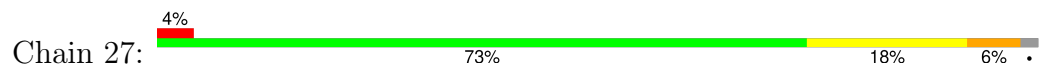
- Molecule 28: 50S ribosomal protein L33



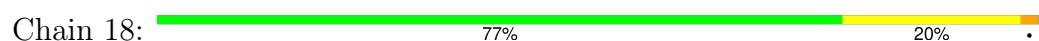
- Molecule 29: 50S ribosomal protein L34



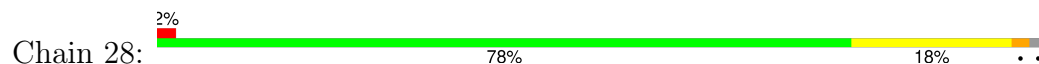
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35

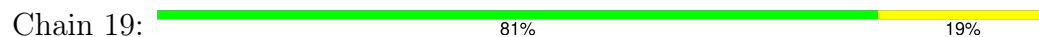


- Molecule 30: 50S ribosomal protein L35

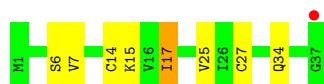
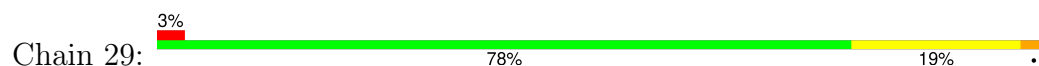




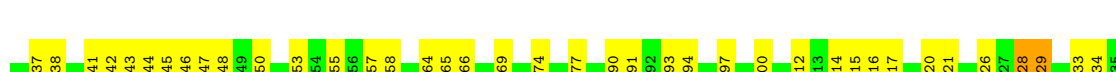
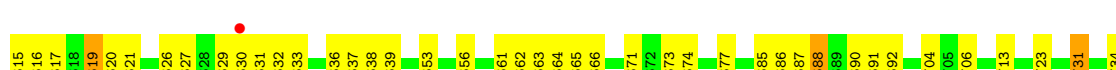
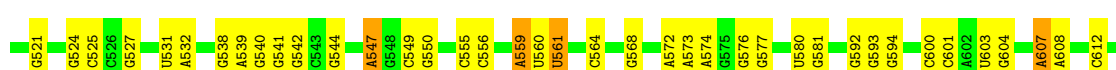
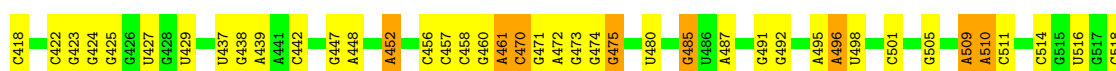
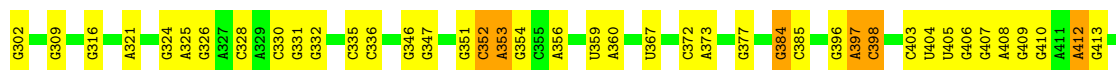
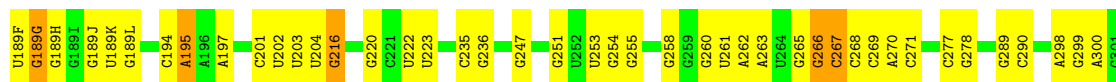
- Molecule 31: 50S ribosomal protein L36

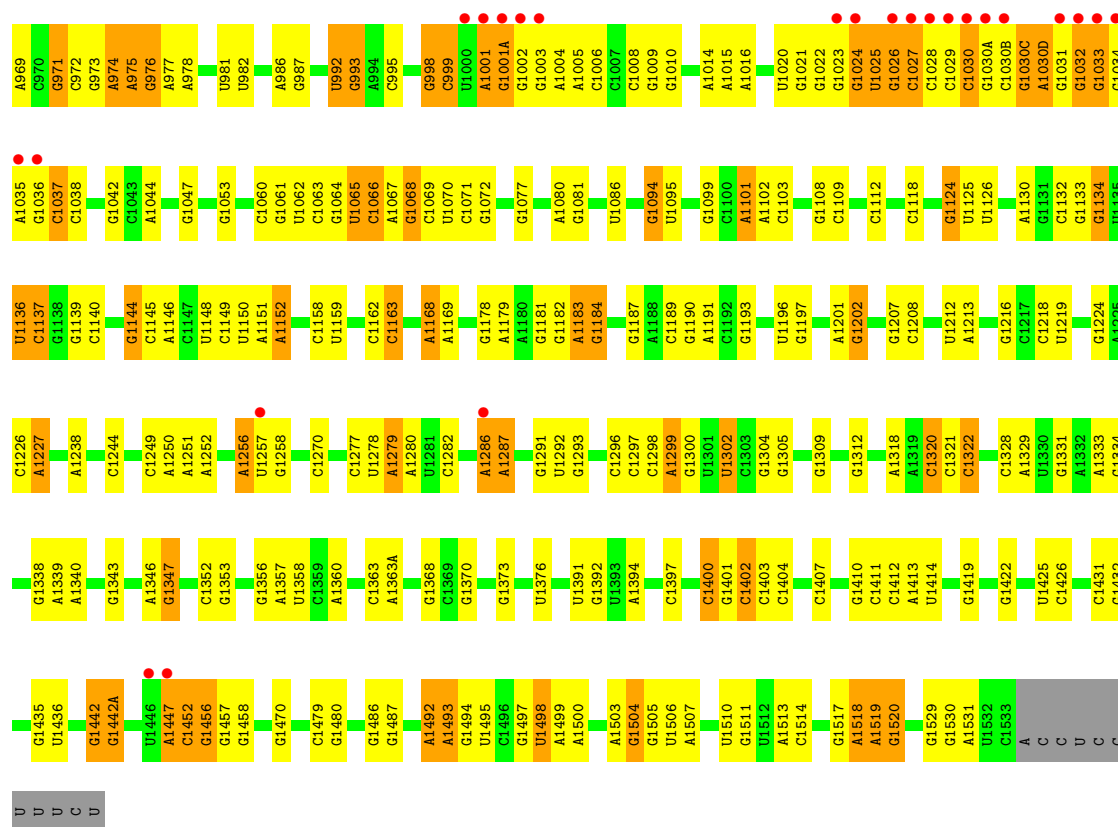


- Molecule 31: 50S ribosomal protein L36

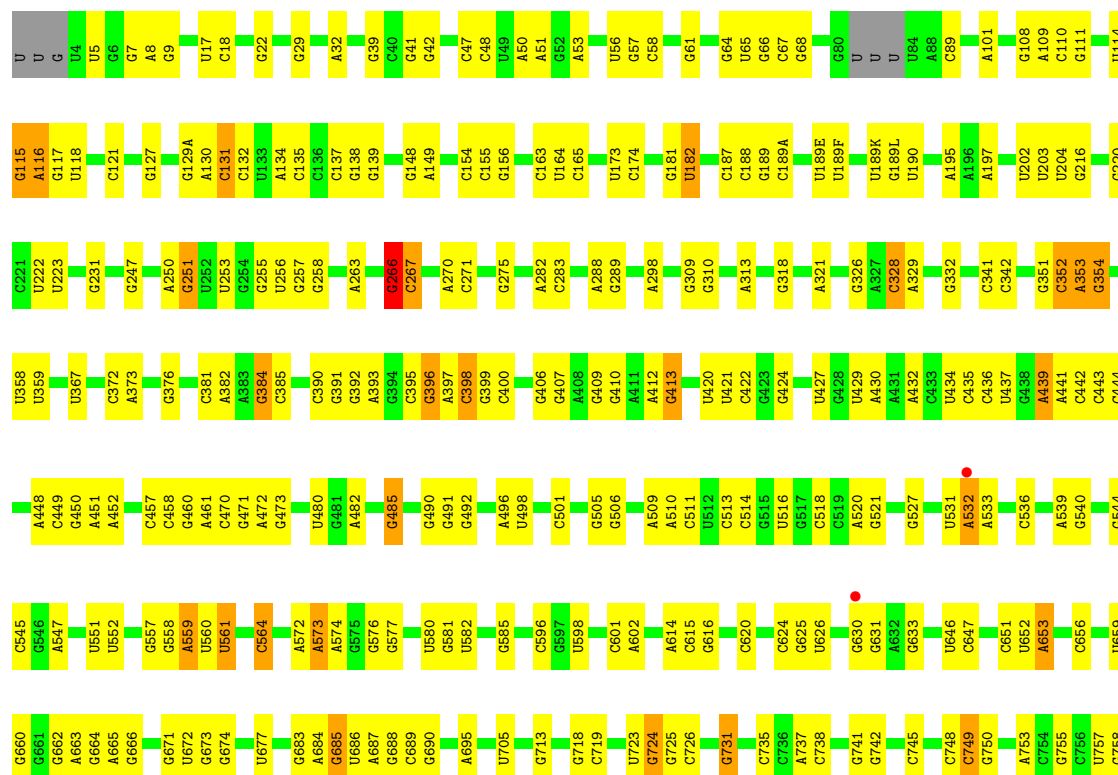


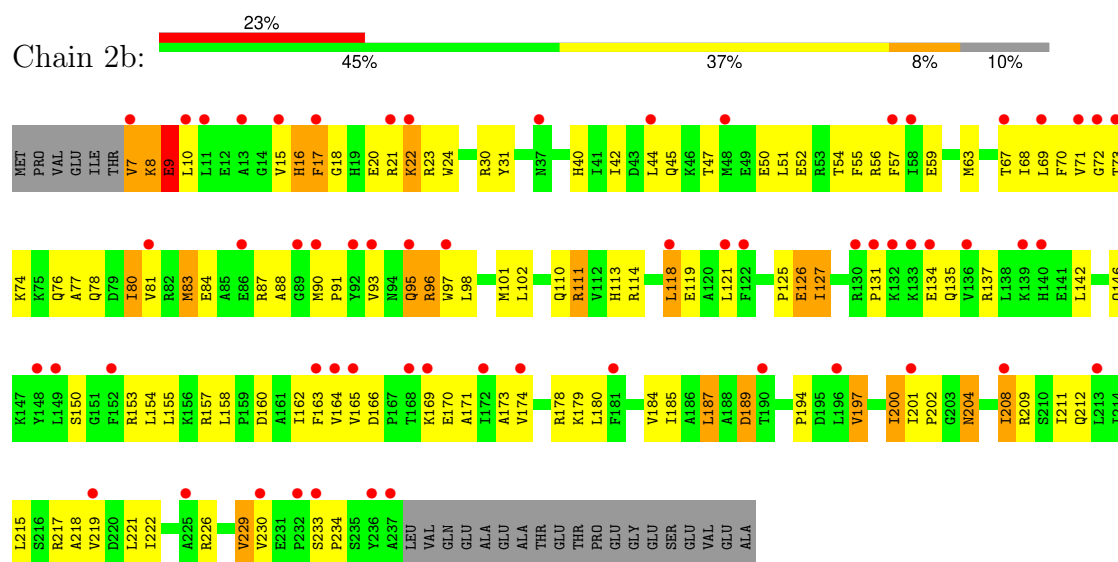
- Molecule 32: 16S Ribosomal RNA



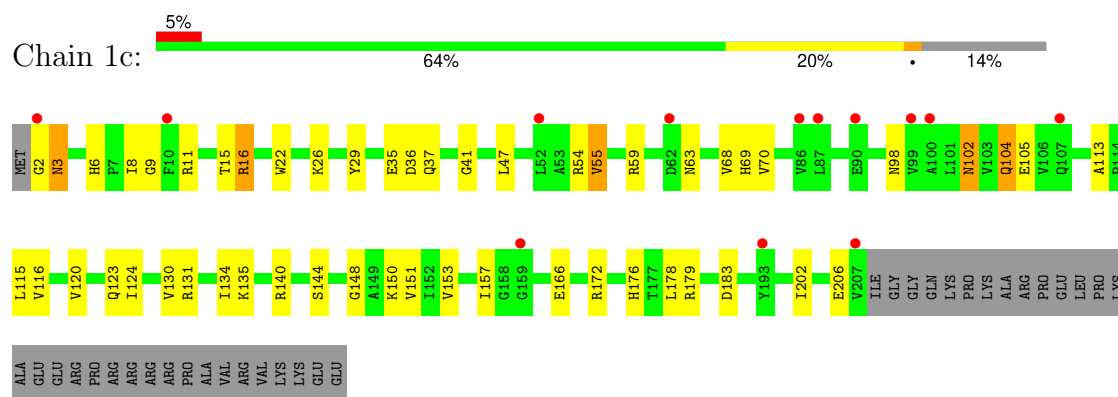


• Molecule 32: 16S Ribosomal RNA

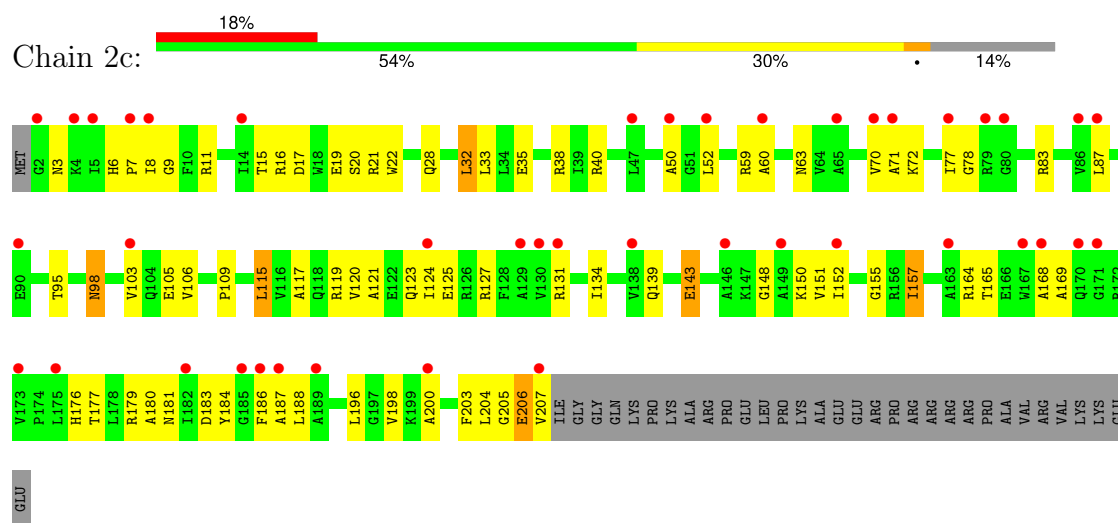




- Molecule 34: 30S ribosomal protein S3

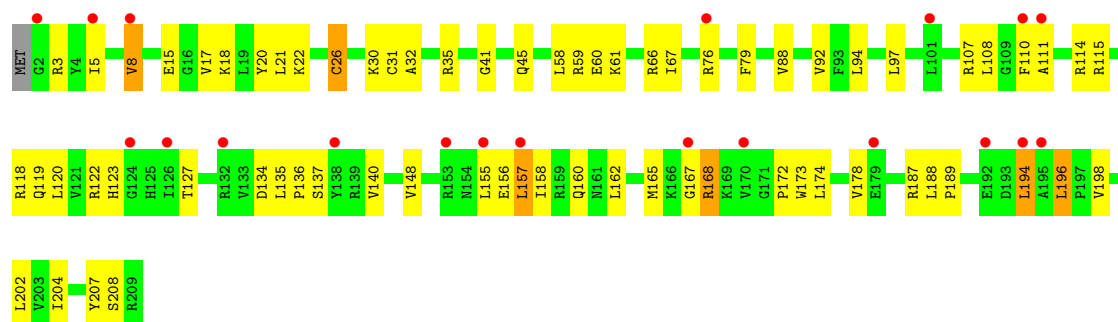


- Molecule 34: 30S ribosomal protein S3

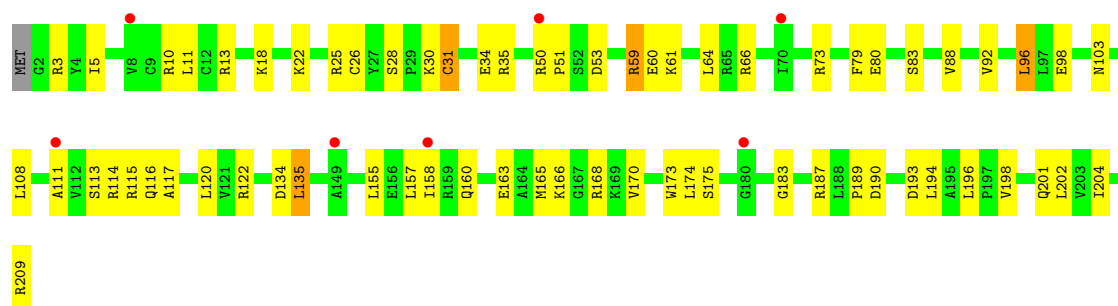


- Molecule 35: 30S ribosomal protein S4

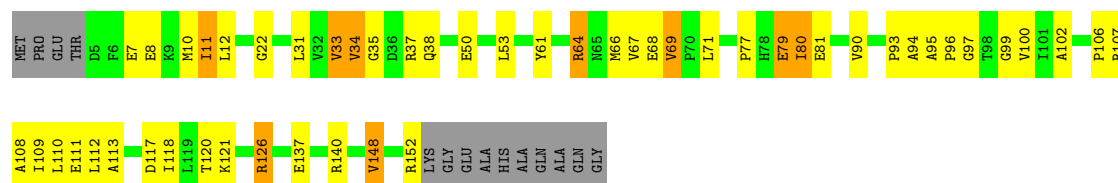




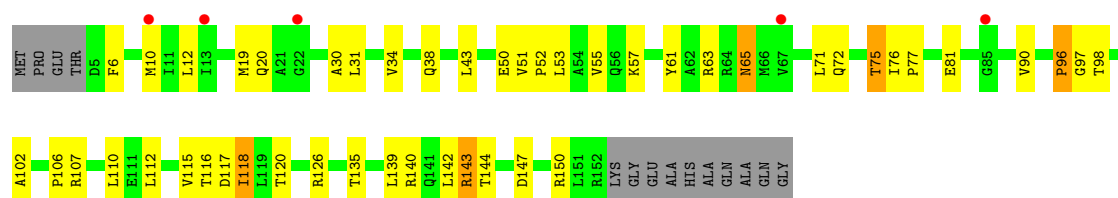
• Molecule 35: 30S ribosomal protein S4



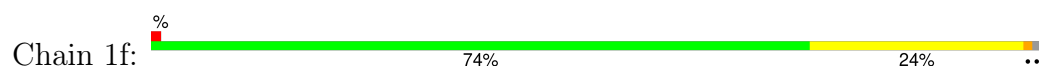
• Molecule 36: 30S ribosomal protein S5



• Molecule 36: 30S ribosomal protein S5



• Molecule 37: 30S ribosomal protein S6

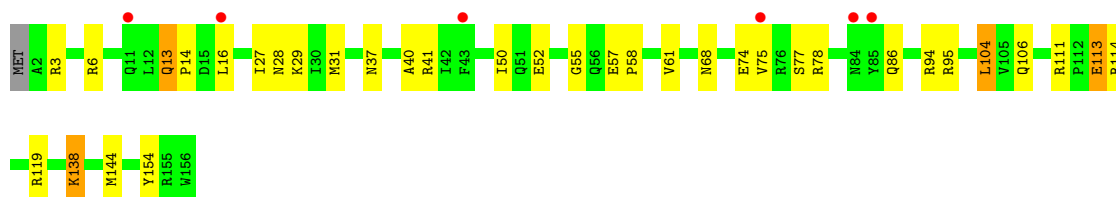
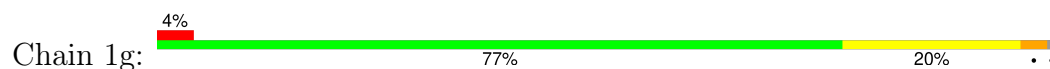




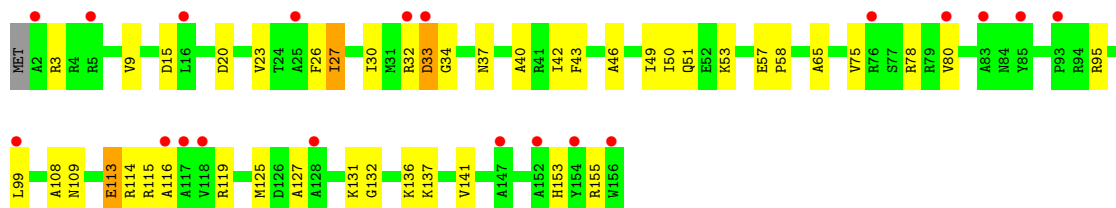
- Molecule 37: 30S ribosomal protein S6



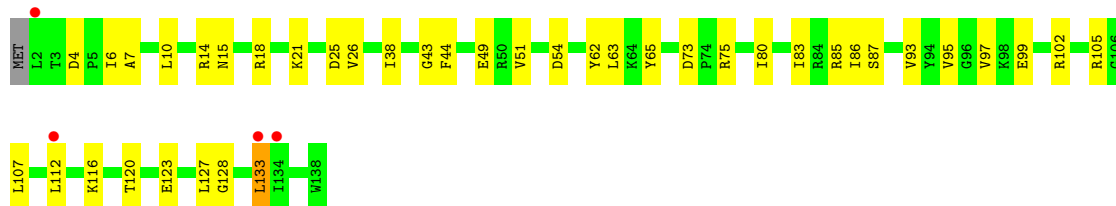
- Molecule 38: 30S ribosomal protein S7



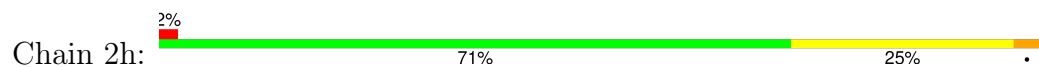
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

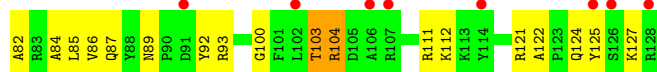
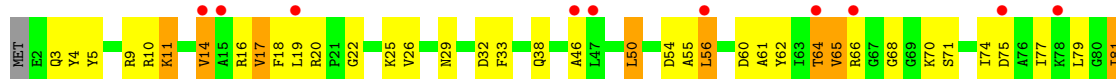


- Molecule 39: 30S ribosomal protein S8

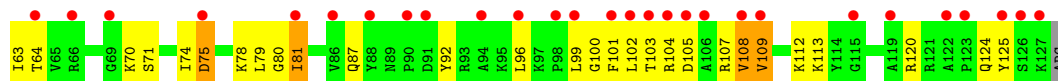
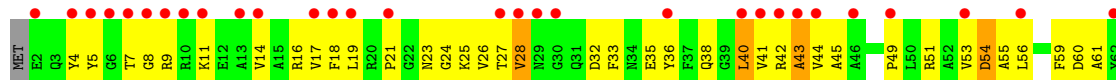




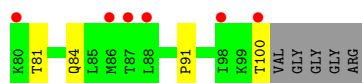
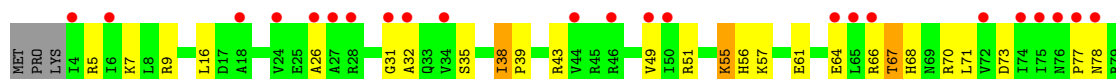
- Molecule 40: 30S ribosomal protein S9



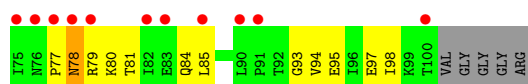
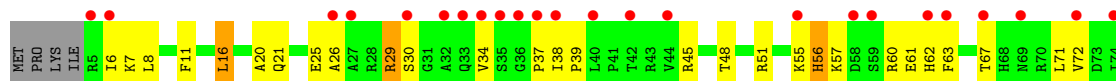
- Molecule 40: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S10

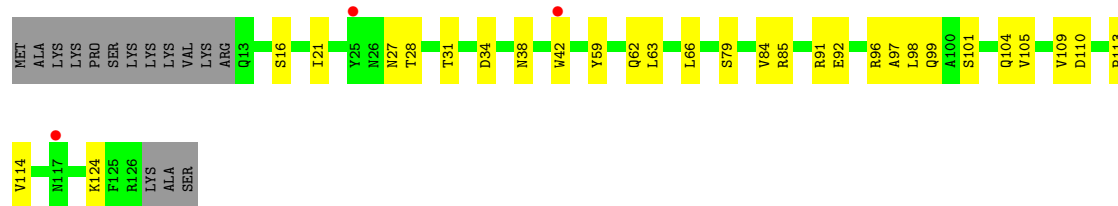


- Molecule 41: 30S ribosomal protein S10

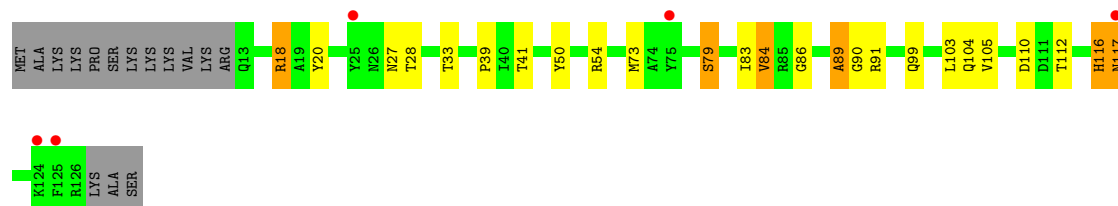


- Molecule 42: 30S ribosomal protein S11

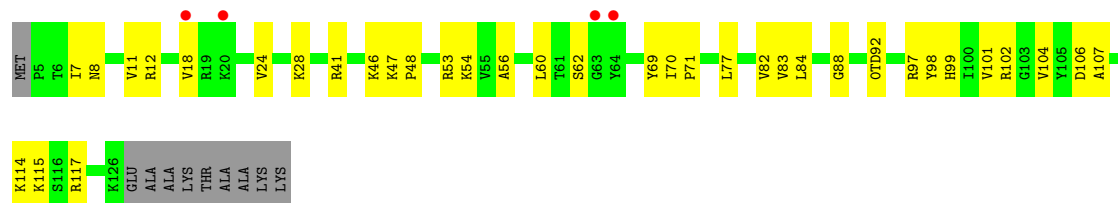




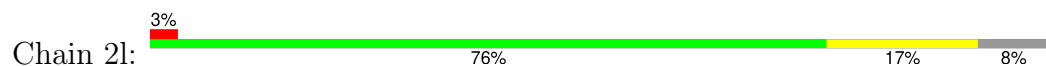
- Molecule 42: 30S ribosomal protein S11



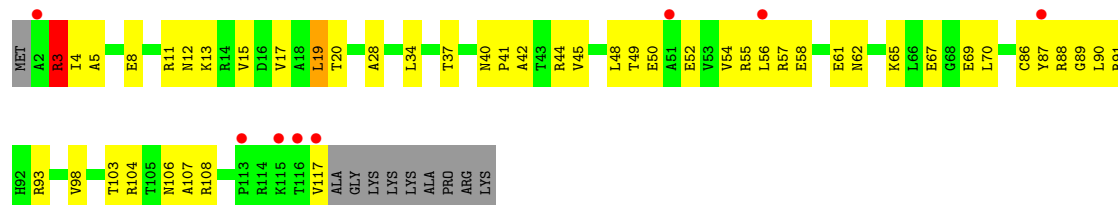
- Molecule 43: 30S ribosomal protein S12



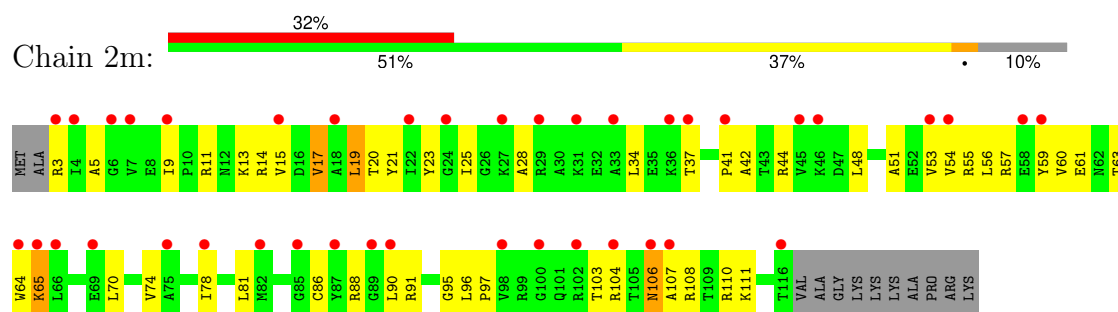
- Molecule 43: 30S ribosomal protein S12



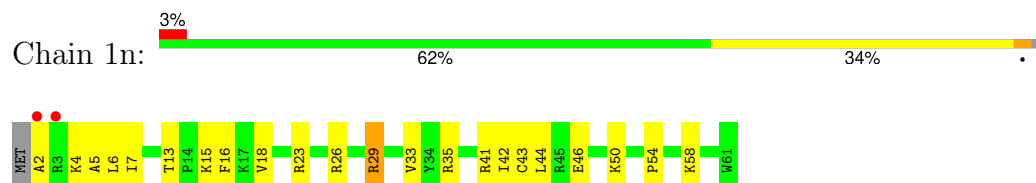
- Molecule 44: 30S ribosomal protein S13



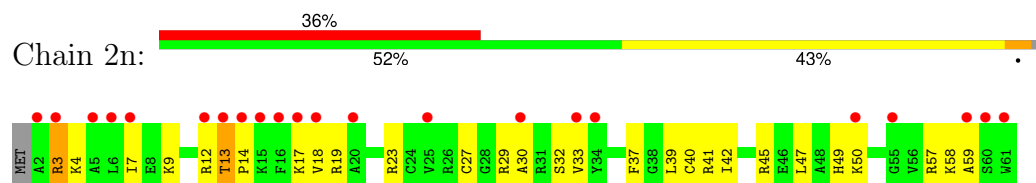
- Molecule 44: 30S ribosomal protein S13



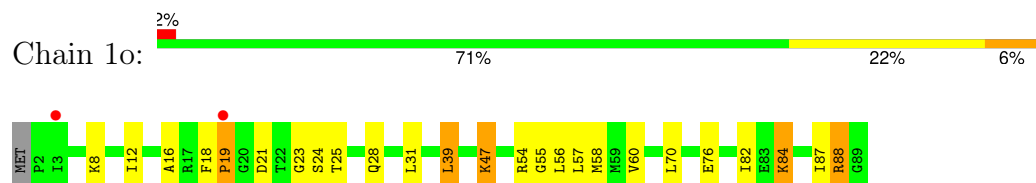
- Molecule 45: 30S ribosomal protein S14 type Z



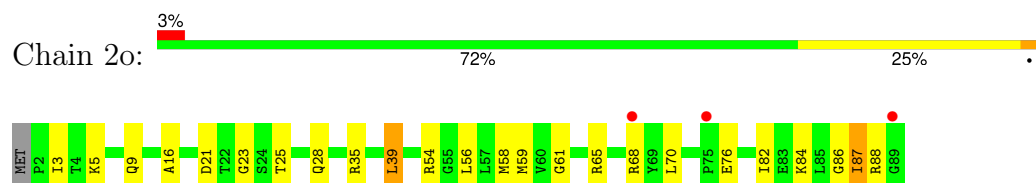
- Molecule 45: 30S ribosomal protein S14 type Z



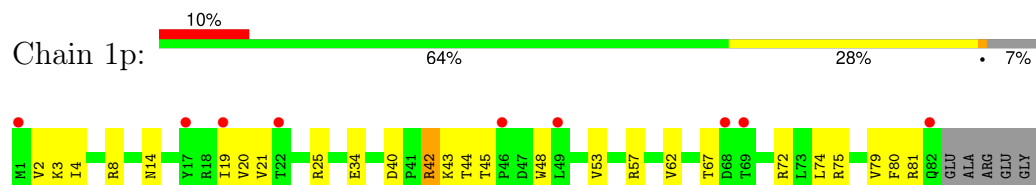
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15

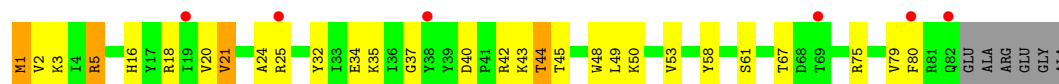


- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16





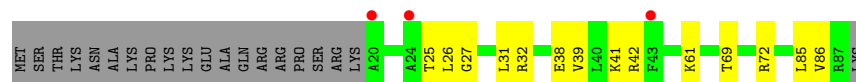
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



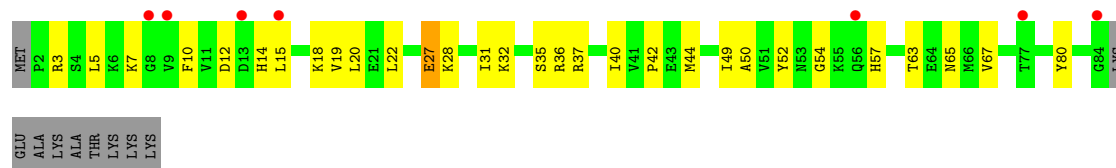
- Molecule 49: 30S ribosomal protein S18



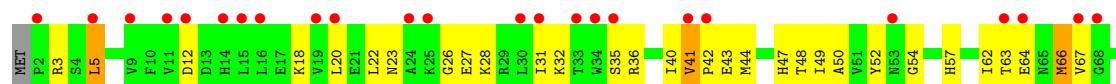
- Molecule 49: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S19

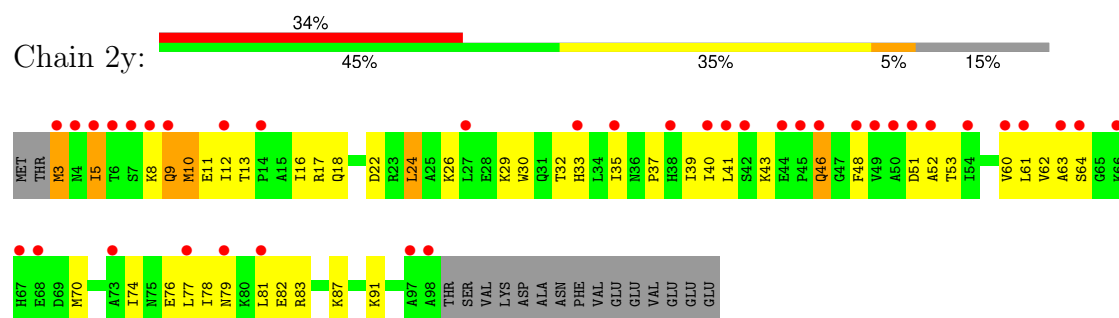


- Molecule 50: 30S ribosomal protein S19





Chain 2y:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.90Å 450.73Å 622.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	174.04 – 2.50 174.04 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (174.04-2.50) 99.8 (174.04-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.207 , 0.250 0.209 , 0.252	Depositor DCC
R_{free} test set	100475 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	296715	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, UR3, MA6, 2MU, 2MA, MPD, MG, ZN, M2G, ZIT, HGR, 2MG, G7M, SF4, OMC, 4OC, PSU, 5MC, 5MU, 0TD

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	0.29	0/69030	0.49	5/107750 (0.0%)
1	2A	0.23	0/68902	0.43	2/107548 (0.0%)
2	1B	0.24	0/2876	0.44	0/4486
2	2B	0.20	0/2878	0.39	0/4490
3	1D	0.28	0/2181	0.53	0/2940
3	2D	0.24	0/2186	0.50	0/2944
4	1E	0.27	0/1592	0.49	0/2149
4	2E	0.22	0/1592	0.45	0/2149
5	1F	0.27	0/1619	0.49	0/2193
5	2F	0.21	0/1615	0.47	2/2188 (0.1%)
6	1G	0.22	0/1451	0.43	0/1961
6	2G	0.21	0/1449	0.41	0/1957
7	1H	0.22	0/1356	0.44	0/1834
7	2H	0.19	0/1350	0.42	0/1826
8	1I	0.20	0/1109	0.43	0/1512
8	2I	0.18	0/1091	0.38	0/1490
9	1N	0.25	0/1148	0.46	0/1547
9	2N	0.21	0/1144	0.39	0/1543
10	1O	0.27	0/943	0.51	0/1269
10	2O	0.22	0/943	0.43	0/1269
11	1P	0.27	0/1152	0.51	0/1533
11	2P	0.24	0/1152	0.51	2/1533 (0.1%)
12	1Q	0.27	0/1143	0.50	0/1527
12	2Q	0.21	0/1143	0.42	0/1527
13	1R	0.30	0/982	0.53	0/1312
13	2R	0.23	0/982	0.47	0/1312
14	1S	0.23	0/887	0.47	0/1180
14	2S	0.21	0/880	0.42	0/1172
15	1T	0.27	0/1105	0.52	0/1477
15	2T	0.22	0/1097	0.44	0/1468
16	1U	0.29	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.39	0/1301
17	1V	0.27	0/786	0.48	0/1053
17	2V	0.20	0/782	0.42	0/1049
18	1W	0.29	0/897	0.48	0/1205
18	2W	0.22	0/897	0.43	0/1205
19	1X	0.27	0/764	0.52	0/1025
19	2X	0.22	0/764	0.43	0/1025
20	1Y	0.26	0/823	0.55	0/1099
20	2Y	0.20	0/823	0.48	0/1100
21	1Z	0.23	0/1620	0.45	0/2200
21	2Z	0.19	0/1590	0.41	0/2162
22	10	0.27	0/616	0.48	0/821
22	20	0.21	0/616	0.46	0/821
23	11	0.26	0/761	0.47	0/1013
23	21	0.25	0/766	0.43	0/1018
24	12	0.25	0/590	0.43	0/781
24	22	0.20	0/594	0.38	0/785
25	13	0.29	0/474	0.51	0/635
25	23	0.21	0/469	0.46	0/630
26	14	0.26	0/559	0.66	0/754
26	24	0.29	0/549	0.63	0/741
27	15	0.31	0/473	0.55	0/639
27	25	0.22	0/469	0.46	0/635
28	16	0.26	0/460	0.50	0/613
28	26	0.22	0/456	0.40	0/608
29	17	0.31	0/426	0.55	0/561
29	27	0.27	0/426	0.48	0/561
30	18	0.28	0/525	0.50	0/691
30	28	0.20	0/525	0.38	0/691
31	19	0.28	0/310	0.51	0/407
31	29	0.22	0/310	0.45	0/407
32	1a	0.21	0/35795	0.39	1/55864 (0.0%)
32	2a	0.20	0/35890	0.38	2/56012 (0.0%)
33	1b	0.22	0/1876	0.48	0/2533
33	2b	0.23	0/1860	0.47	0/2518
34	1c	0.20	0/1582	0.41	0/2137
34	2c	0.21	0/1566	0.41	0/2119
35	1d	0.21	0/1695	0.44	0/2274
35	2d	0.19	0/1698	0.41	0/2277
36	1e	0.22	0/1149	0.45	0/1548
36	2e	0.20	0/1149	0.45	0/1548
37	1f	0.20	0/827	0.39	0/1120
37	2f	0.19	0/829	0.42	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1254	0.38	0/1683
38	2g	0.20	0/1248	0.39	0/1676
39	1h	0.20	0/1118	0.43	0/1506
39	2h	0.18	0/1108	0.45	0/1494
40	1i	0.21	0/1005	0.47	0/1351
40	2i	0.22	0/985	0.50	0/1329
41	1j	0.29	0/732	0.44	0/993
41	2j	0.21	0/723	0.47	0/984
42	1k	0.18	0/849	0.39	0/1150
42	2k	0.19	0/848	0.45	0/1149
43	1l	0.20	0/937	0.43	0/1260
43	2l	0.18	0/937	0.39	0/1260
44	1m	0.20	0/924	0.50	0/1242
44	2m	0.21	0/905	0.48	0/1217
45	1n	0.21	0/501	0.46	0/664
45	2n	0.20	0/501	0.44	0/664
46	1o	0.20	0/739	0.40	0/985
46	2o	0.20	0/739	0.38	0/985
47	1p	0.20	0/697	0.49	0/939
47	2p	0.21	0/693	0.45	0/935
48	1q	0.21	0/836	0.42	0/1117
48	2q	0.21	0/836	0.43	0/1117
49	1r	0.19	0/560	0.40	0/746
49	2r	0.20	0/560	0.39	0/746
50	1s	0.21	0/663	0.44	0/895
50	2s	0.20	0/660	0.42	0/893
51	1t	0.20	0/734	0.45	0/969
51	2t	0.20	0/736	0.43	0/976
52	1u	0.19	0/203	0.41	0/266
52	2u	0.21	0/203	0.49	0/266
53	1y	0.19	0/776	0.38	0/1048
53	2y	0.19	0/761	0.36	0/1030
All	All	0.24	0/309939	0.44	14/463231 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
15	1T	0	1
21	2Z	0	1
26	14	0	1
33	1b	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1042	G	OP1-P-O3'	-9.62	79.13	108.00
1	2A	1992	G	C2'-C3'-O3'	6.32	118.99	109.50
1	1A	1042	G	OP2-P-O3'	-6.13	89.60	108.00
1	1A	1653	G	C2'-C3'-O3'	5.56	117.84	109.50
11	2P	36	LYS	CA-C-N	-5.54	116.60	122.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	52	THR	Peptide
11	1P	35	HIS	Peptide
15	1T	95	ARG	Peptide
33	1b	231	GLU	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31206	540	0
1	2A	61758	0	31152	675	0
2	1B	2572	0	1305	26	0
2	2B	2573	0	1306	33	0
3	1D	2131	0	2207	38	0
3	2D	2136	0	2218	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1E	1559	0	1618	17	0
4	2E	1559	0	1618	31	0
5	1F	1584	0	1625	33	0
5	2F	1580	0	1619	42	0
6	1G	1426	0	1445	51	0
6	2G	1424	0	1441	71	0
7	1H	1330	0	1407	26	0
7	2H	1324	0	1402	34	0
8	1I	1094	0	1127	32	0
8	2I	1076	0	1094	27	0
9	1N	1121	0	1195	15	0
9	2N	1117	0	1184	20	0
10	1O	933	0	996	15	0
10	2O	933	0	996	18	0
11	1P	1135	0	1212	26	0
11	2P	1135	0	1212	19	0
12	1Q	1122	0	1179	12	0
12	2Q	1122	0	1179	22	0
13	1R	968	0	1033	17	0
13	2R	968	0	1033	14	0
14	1S	877	0	938	13	0
14	2S	870	0	923	17	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	17	0
16	1U	959	0	1019	11	0
16	2U	959	0	1019	16	0
17	1V	775	0	841	16	0
17	2V	771	0	830	23	0
18	1W	886	0	940	8	0
18	2W	886	0	940	7	0
19	1X	750	0	814	15	0
19	2X	750	0	814	12	0
20	1Y	810	0	892	20	0
20	2Y	810	0	887	20	0
21	1Z	1587	0	1598	28	0
21	2Z	1557	0	1564	54	0
22	10	608	0	622	9	0
22	20	608	0	622	5	0
23	11	754	0	823	12	0
23	21	759	0	837	19	0
24	12	588	0	643	8	0
24	22	592	0	654	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	13	469	0	518	7	0
25	23	464	0	514	11	0
26	14	546	0	522	19	0
26	24	536	0	514	39	0
27	15	459	0	476	10	0
27	25	455	0	465	6	0
28	16	453	0	473	6	0
28	26	449	0	469	8	0
29	17	418	0	467	6	0
29	27	418	0	467	9	0
30	18	517	0	582	14	0
30	28	517	0	582	12	0
31	19	307	0	335	4	0
31	29	307	0	335	6	0
32	1a	32246	0	16294	401	0
32	2a	32331	0	16338	414	0
33	1b	1842	0	1862	58	0
33	2b	1825	0	1828	80	0
34	1c	1558	0	1557	32	0
34	2c	1542	0	1517	62	0
35	1d	1665	0	1687	52	0
35	2d	1668	0	1703	38	0
36	1e	1133	0	1191	35	0
36	2e	1133	0	1191	31	0
37	1f	814	0	808	11	0
37	2f	816	0	808	11	0
38	1g	1235	0	1249	20	0
38	2g	1229	0	1238	25	0
39	1h	1098	0	1143	22	0
39	2h	1088	0	1126	24	0
40	1i	986	0	990	52	0
40	2i	966	0	953	51	0
41	1j	719	0	672	18	0
41	2j	710	0	661	26	0
42	1k	834	0	838	16	0
42	2k	833	0	836	17	0
43	1l	932	0	981	18	0
43	2l	932	0	981	11	0
44	1m	914	0	954	30	0
44	2m	895	0	920	38	0
45	1n	492	0	529	18	0
45	2n	492	0	529	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1o	728	0	760	16	0
46	2o	728	0	760	15	0
47	1p	681	0	697	13	0
47	2p	677	0	686	20	0
48	1q	823	0	891	16	0
48	2q	823	0	891	15	0
49	1r	555	0	618	8	0
49	2r	555	0	618	9	0
50	1s	648	0	658	26	0
50	2s	645	0	635	33	0
51	1t	732	0	809	22	0
51	2t	733	0	795	14	0
52	1u	199	0	208	3	0
52	2u	199	0	208	5	0
53	1y	764	0	786	16	0
53	2y	749	0	757	34	0
54	10	8	0	0	0	0
54	11	5	0	0	0	0
54	13	3	0	0	0	0
54	14	1	0	0	0	0
54	15	8	0	0	0	0
54	17	6	0	0	0	0
54	18	2	0	0	0	0
54	19	2	0	0	0	0
54	1A	1021	0	0	0	0
54	1B	29	0	0	0	0
54	1D	20	0	0	0	0
54	1E	10	0	0	0	0
54	1F	17	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	4	0	0	0	0
54	1O	1	0	0	0	0
54	1P	5	0	0	0	0
54	1Q	5	0	0	0	0
54	1R	8	0	0	0	0
54	1T	3	0	0	0	0
54	1U	6	0	0	0	0
54	1V	6	0	0	0	0
54	1W	4	0	0	0	0
54	1Y	1	0	0	0	0
54	1Z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1a	281	0	0	0	0
54	1b	1	0	0	0	0
54	1d	4	0	0	0	0
54	1e	4	0	0	0	0
54	1f	2	0	0	0	0
54	1g	2	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1k	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	1	0	0	0	0
54	1n	2	0	0	0	0
54	1o	2	0	0	0	0
54	1t	1	0	0	0	0
54	1y	3	0	0	0	0
54	20	3	0	0	0	0
54	21	1	0	0	0	0
54	23	1	0	0	0	0
54	25	3	0	0	0	0
54	27	3	0	0	0	0
54	28	3	0	0	0	0
54	2A	729	0	0	0	0
54	2B	16	0	0	0	0
54	2D	12	0	0	0	0
54	2E	7	0	0	0	0
54	2F	4	0	0	0	0
54	2G	2	0	0	0	0
54	2I	2	0	0	0	0
54	2O	2	0	0	0	0
54	2P	2	0	0	0	0
54	2Q	3	0	0	0	0
54	2R	2	0	0	0	0
54	2T	4	0	0	0	0
54	2U	1	0	0	0	0
54	2V	3	0	0	0	0
54	2W	3	0	0	0	0
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	193	0	0	0	0
54	2e	1	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2k	1	0	0	0	0
54	2o	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	36	0	29	1	0
55	2A	36	0	29	2	0
56	1A	52	0	72	0	0
56	2A	52	0	72	2	0
57	18	8	0	14	1	0
57	1A	8	0	14	0	0
57	1T	8	0	14	1	0
57	1a	8	0	12	5	0
57	2A	16	0	28	1	0
57	2B	8	0	14	0	0
58	1B	12	0	12	2	0
58	1F	12	0	12	2	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	2	0
60	2d	8	0	0	0	0
61	10	21	0	0	0	0
61	11	24	0	0	0	0
61	12	12	0	0	1	0
61	13	19	0	0	0	0
61	14	3	0	0	0	0
61	15	24	0	0	2	0
61	16	19	0	0	1	0
61	17	14	0	0	1	0
61	18	25	0	0	2	0
61	19	2	0	0	0	0
61	1A	3943	0	0	95	0
61	1B	106	0	0	6	0
61	1D	106	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1E	75	0	0	1	0
61	1F	62	0	0	1	0
61	1G	15	0	0	0	0
61	1H	13	0	0	0	0
61	1I	6	0	0	0	0
61	1N	50	0	0	0	0
61	1O	23	0	0	0	0
61	1P	56	0	0	3	0
61	1Q	38	0	0	1	0
61	1R	37	0	0	1	0
61	1S	11	0	0	1	0
61	1T	39	0	0	3	0
61	1U	43	0	0	4	0
61	1V	36	0	0	3	0
61	1W	29	0	0	0	0
61	1X	26	0	0	1	0
61	1Y	16	0	0	2	0
61	1Z	12	0	0	0	0
61	1a	465	0	0	16	0
61	1b	1	0	0	0	0
61	1d	8	0	0	0	0
61	1e	4	0	0	1	0
61	1f	1	0	0	0	0
61	1h	1	0	0	0	0
61	1i	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	4	0	0	0	0
61	1o	4	0	0	0	0
61	1t	1	0	0	0	0
61	1u	1	0	0	0	0
61	1y	3	0	0	1	0
61	20	6	0	0	0	0
61	21	12	0	0	1	0
61	23	1	0	0	1	0
61	25	6	0	0	0	0
61	26	5	0	0	1	0
61	27	5	0	0	0	0
61	28	8	0	0	0	0
61	2A	1664	0	0	82	0
61	2B	25	0	0	4	0
61	2D	38	0	0	0	0
61	2E	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2F	18	0	0	1	0
61	2G	4	0	0	0	0
61	2H	1	0	0	0	0
61	2I	1	0	0	0	0
61	2N	2	0	0	0	0
61	2O	11	0	0	1	0
61	2P	11	0	0	1	0
61	2Q	10	0	0	0	0
61	2R	16	0	0	2	0
61	2T	7	0	0	0	0
61	2U	8	0	0	1	0
61	2V	5	0	0	0	0
61	2W	17	0	0	0	0
61	2X	3	0	0	0	0
61	2Y	3	0	0	0	0
61	2Z	3	0	0	0	0
61	2a	245	0	0	20	0
61	2d	2	0	0	0	0
61	2e	1	0	0	0	0
61	2f	3	0	0	0	0
61	2l	3	0	0	0	0
61	2m	1	0	0	0	0
61	2o	2	0	0	0	0
61	2q	2	0	0	0	0
61	2r	1	0	0	0	0
61	2t	2	0	0	0	0
61	2y	2	0	0	0	0
All	All	296715	0	194718	3790	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 3790 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)
1:2A:2139:C:N4	1:2A:2152:G:H1	1.50	1.07
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.20	1.06
1:1A:2137:C:N4	1:1A:2154:G:H1	1.55	1.03
1:1A:1054:A:H61	1:1A:1105:U:H3	1.07	0.99
1:1A:1082:U:H3	1:1A:1086:A:H61	1.04	0.99

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	12	24
4	2E	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	12	24
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	24	43
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	43
6	1G	179/182 (98%)	165 (92%)	9 (5%)	5 (3%)	4	6
6	2G	179/182 (98%)	158 (88%)	18 (10%)	3 (2%)	7	13
7	1H	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
7	2H	171/180 (95%)	155 (91%)	15 (9%)	1 (1%)	21	38
8	1I	145/148 (98%)	128 (88%)	16 (11%)	1 (1%)	18	34
8	2I	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	18	34
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	34
11	2P	147/150 (98%)	136 (92%)	9 (6%)	2 (1%)	9	17
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	101 (94%)	6 (6%)	1 (1%)	14	27
15	1T	129/146 (88%)	122 (95%)	5 (4%)	2 (2%)	7	14
15	2T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	16	31
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	24
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	92 (99%)	0	1 (1%)	11	22
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	22
20	1Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	201/206 (98%)	189 (94%)	10 (5%)	2 (1%)	12	24
21	2Z	199/206 (97%)	179 (90%)	19 (10%)	1 (0%)	24	43
22	10	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
22	20	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	11	22
23	21	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	54 (81%)	7 (10%)	6 (9%)	0	0
26	24	67/71 (94%)	46 (69%)	17 (25%)	4 (6%)	1	1
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	195 (85%)	27 (12%)	7 (3%)	3	5
33	2b	229/256 (90%)	197 (86%)	23 (10%)	9 (4%)	2	3
34	1c	204/239 (85%)	193 (95%)	11 (5%)	0	100	100
34	2c	204/239 (85%)	176 (86%)	26 (13%)	2 (1%)	12	24
35	1d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
35	2d	206/209 (99%)	192 (93%)	14 (7%)	0	100	100
36	1e	146/162 (90%)	139 (95%)	4 (3%)	3 (2%)	5	9
36	2e	146/162 (90%)	135 (92%)	9 (6%)	2 (1%)	9	17
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	141 (92%)	11 (7%)	1 (1%)	18	34
38	2g	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	6	10
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
40	1i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16	31
40	2i	124/128 (97%)	105 (85%)	15 (12%)	4 (3%)	3	4
41	1j	95/105 (90%)	82 (86%)	8 (8%)	5 (5%)	1	1
41	2j	94/105 (90%)	76 (81%)	13 (14%)	5 (5%)	1	1
42	1k	112/129 (87%)	99 (88%)	13 (12%)	0	100	100
42	2k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	6	12
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
44	1m	114/126 (90%)	100 (88%)	10 (9%)	4 (4%)	3	4
44	2m	112/126 (89%)	100 (89%)	10 (9%)	2 (2%)	6	12
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	1o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	5	8
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	20
47	1p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	12	24
48	2q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	0	1 (2%)	8	16
49	2r	66/88 (75%)	58 (88%)	8 (12%)	0	100	100
50	1s	81/93 (87%)	75 (93%)	5 (6%)	1 (1%)	10	20
50	2s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
51	1t	94/106 (89%)	85 (90%)	9 (10%)	0	100	100
51	2t	96/106 (91%)	87 (91%)	6 (6%)	3 (3%)	3	5
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
53	1y	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
53	2y	94/113 (83%)	89 (95%)	5 (5%)	0	100	100
All	All	11629/12354 (94%)	10840 (93%)	689 (6%)	100 (1%)	14	27

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	71	GLY
6	1G	47	LYS
6	1G	50	ALA
21	1Z	53	ILE
26	14	55	ARG

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%)	199 (93%)	15 (7%)	14	29
3	2D	215/218 (99%)	197 (92%)	18 (8%)	10	22
4	1E	164/166 (99%)	156 (95%)	8 (5%)	22	45
4	2E	164/166 (99%)	156 (95%)	8 (5%)	22	45
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5	11
5	2F	159/166 (96%)	139 (87%)	20 (13%)	4	9
6	1G	144/156 (92%)	132 (92%)	12 (8%)	10	22
6	2G	142/156 (91%)	122 (86%)	20 (14%)	3	7
7	1H	144/148 (97%)	137 (95%)	7 (5%)	22	45
7	2H	143/148 (97%)	127 (89%)	16 (11%)	6	12
8	1I	111/124 (90%)	100 (90%)	11 (10%)	7	16
8	2I	108/124 (87%)	94 (87%)	14 (13%)	4	8
9	1N	119/119 (100%)	106 (89%)	13 (11%)	6	13
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	26
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22	44
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17	36
11	1P	115/116 (99%)	109 (95%)	6 (5%)	21	42
11	2P	115/116 (99%)	110 (96%)	5 (4%)	26	51
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11	23
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	34
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	20
13	2R	101/101 (100%)	94 (93%)	7 (7%)	14	30
14	1S	87/88 (99%)	79 (91%)	8 (9%)	8	19
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	11
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21	42
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16	34
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15	32
16	2U	93/94 (99%)	91 (98%)	2 (2%)	45	73
17	1V	81/82 (99%)	74 (91%)	7 (9%)	10	21
17	2V	80/82 (98%)	71 (89%)	9 (11%)	5	12
18	1W	90/92 (98%)	86 (96%)	4 (4%)	25	50
18	2W	90/92 (98%)	88 (98%)	2 (2%)	45	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	55
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	68
20	1Y	86/91 (94%)	75 (87%)	11 (13%)	4	9
20	2Y	86/91 (94%)	80 (93%)	6 (7%)	14	29
21	1Z	169/179 (94%)	157 (93%)	12 (7%)	13	29
21	2Z	165/179 (92%)	158 (96%)	7 (4%)	26	52
22	10	61/67 (91%)	61 (100%)	0	100	100
22	20	61/67 (91%)	58 (95%)	3 (5%)	22	45
23	11	79/83 (95%)	72 (91%)	7 (9%)	9	20
23	21	81/83 (98%)	72 (89%)	9 (11%)	6	12
24	12	65/67 (97%)	62 (95%)	3 (5%)	24	48
24	22	66/67 (98%)	56 (85%)	10 (15%)	3	5
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	24
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	24
26	14	58/63 (92%)	52 (90%)	6 (10%)	7	14
26	24	54/63 (86%)	48 (89%)	6 (11%)	6	12
27	15	51/52 (98%)	46 (90%)	5 (10%)	7	16
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	54
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	11
28	26	50/52 (96%)	47 (94%)	3 (6%)	17	36
29	17	41/42 (98%)	35 (85%)	6 (15%)	3	6
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	10
30	18	54/55 (98%)	53 (98%)	1 (2%)	50	76
30	28	54/55 (98%)	53 (98%)	1 (2%)	50	76
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	37
33	1b	191/220 (87%)	175 (92%)	16 (8%)	10	22
33	2b	187/220 (85%)	160 (86%)	27 (14%)	3	6
34	1c	144/188 (77%)	134 (93%)	10 (7%)	14	30
34	2c	140/188 (74%)	127 (91%)	13 (9%)	8	18
35	1d	171/181 (94%)	157 (92%)	14 (8%)	10	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	2d	172/181 (95%)	155 (90%)	17 (10%)	7	16
36	1e	114/123 (93%)	101 (89%)	13 (11%)	5	12
36	2e	114/123 (93%)	105 (92%)	9 (8%)	11	24
37	1f	85/90 (94%)	74 (87%)	11 (13%)	4	9
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	14
38	1g	120/127 (94%)	112 (93%)	8 (7%)	15	31
38	2g	119/127 (94%)	110 (92%)	9 (8%)	12	26
39	1h	116/119 (98%)	107 (92%)	9 (8%)	11	24
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	17
40	1i	91/99 (92%)	80 (88%)	11 (12%)	5	10
40	2i	88/99 (89%)	78 (89%)	10 (11%)	5	12
41	1j	68/92 (74%)	64 (94%)	4 (6%)	18	37
41	2j	68/92 (74%)	62 (91%)	6 (9%)	9	20
42	1k	83/99 (84%)	81 (98%)	2 (2%)	43	70
42	2k	83/99 (84%)	77 (93%)	6 (7%)	13	28
43	1l	96/108 (89%)	90 (94%)	6 (6%)	16	34
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	27
44	1m	90/101 (89%)	83 (92%)	7 (8%)	11	24
44	2m	87/101 (86%)	81 (93%)	6 (7%)	14	30
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	15
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3	6
46	1o	78/80 (98%)	72 (92%)	6 (8%)	12	25
46	2o	78/80 (98%)	72 (92%)	6 (8%)	12	25
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3	6
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	11
48	1q	94/97 (97%)	91 (97%)	3 (3%)	34	62
48	2q	94/97 (97%)	90 (96%)	4 (4%)	26	51
49	1r	59/77 (77%)	56 (95%)	3 (5%)	21	43
49	2r	59/77 (77%)	56 (95%)	3 (5%)	21	43
50	1s	68/80 (85%)	65 (96%)	3 (4%)	25	50
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	1t	71/82 (87%)	68 (96%)	3 (4%)	26	52
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18	39
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
53	1y	82/98 (84%)	79 (96%)	3 (4%)	30	57
53	2y	79/98 (81%)	68 (86%)	11 (14%)	3	7
All	All	9524/10260 (93%)	8766 (92%)	758 (8%)	11	24

5 of 758 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	2O	20	MET
29	27	48	LYS
12	2Q	75	THR
10	2O	8	LEU
20	2Y	3	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 136 such sidechains are listed below:

Mol	Chain	Res	Type
39	2h	81	HIS
41	2j	68	HIS
50	2s	83	HIS
36	1e	141	GLN
36	1e	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	399 (13%)	31 (1%)
1	2A	2858/2915 (98%)	463 (16%)	38 (1%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	119/121 (98%)	18 (15%)	0
32	1a	1497/1521 (98%)	241 (16%)	0
32	2a	1501/1521 (98%)	239 (15%)	0
All	All	8959/9114 (98%)	1372 (15%)	69 (0%)

5 of 1372 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	14	A
1	1A	15	G
1	1A	34	C

5 of 69 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1493	C
1	2A	2126	A
1	2A	2601	C
1	1A	2288	A
1	1A	2126	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	5MC	1a	1400	32	19,22,23	1.73	3 (15%)	26,32,35	1.14	2 (7%)
1	5MU	1A	1939	54,1	19,22,23	1.41	4 (21%)	27,32,35	2.13	6 (22%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.05	10 (30%)
1	OMG	2A	2251	54,1	23,26,27	1.21	2 (8%)	32,38,41	1.90	5 (15%)
32	PSU	2a	516	32,54	18,21,22	1.35	2 (11%)	21,30,33	2.10	5 (23%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	0.96	1 (4%)
1	PSU	2A	1911	1	18,21,22	1.39	3 (16%)	21,30,33	2.00	5 (23%)
32	2MG	2a	1207	32	23,26,27	1.26	4 (17%)	33,38,41	2.12	5 (15%)
1	5MC	1A	1942	54,1	19,22,23	1.62	3 (15%)	26,32,35	1.07	2 (7%)
32	MA6	1a	1518	32	23,26,27	0.39	0	33,38,41	1.88	9 (27%)
32	UR3	2a	1498	32,54	19,22,23	1.02	2 (10%)	26,32,35	1.62	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.78	0	25,31,34	0.87	1 (4%)

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	1.56	3 (15%)	26,32,35	1.16	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.02	4 (19%)
1	5MC	1A	1962	54,1	19,22,23	1.69	3 (15%)	26,32,35	1.09	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.70	3 (15%)	26,32,35	1.15	4 (15%)
1	5MU	2A	1939	54,1	19,22,23	1.39	5 (26%)	27,32,35	2.28	7 (25%)
1	PSU	2A	2605	1	18,21,22	1.38	4 (22%)	21,30,33	2.11	4 (19%)
1	2MU	2A	2552	54,1	19,22,24	1.33	4 (21%)	25,31,36	1.72	4 (16%)
32	2MG	1a	1207	32	23,26,27	1.25	2 (8%)	33,38,41	2.38	10 (30%)
32	5MC	2a	1407	32	19,22,23	1.66	3 (15%)	26,32,35	1.18	3 (11%)
32	PSU	1a	516	32,54	18,21,22	1.41	2 (11%)	21,30,33	1.95	4 (19%)
32	UR3	1a	1498	32	19,22,23	1.05	2 (10%)	26,32,35	1.85	4 (15%)
1	5MU	2A	1915	1	19,22,23	1.43	4 (21%)	27,32,35	2.22	8 (29%)
32	M2G	2a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.84	5 (15%)
1	OMC	1A	1920	1	19,22,23	0.83	0	25,31,34	0.99	1 (4%)
32	MA6	2a	1518	32	23,26,27	0.40	0	33,38,41	1.94	9 (27%)
1	PSU	1A	2605	1	18,21,22	1.47	3 (16%)	21,30,33	2.04	5 (23%)
1	PSU	2A	1917	1	18,21,22	1.35	3 (16%)	21,30,33	2.09	3 (14%)
1	5MC	2A	1942	54,1	19,22,23	1.75	3 (15%)	26,32,35	1.21	2 (7%)
32	5MC	2a	1404	32	19,22,23	1.91	3 (15%)	26,32,35	1.17	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.65	2 (10%)	26,32,35	1.13	2 (7%)
1	2MU	1A	2552	54,1	19,22,24	1.24	3 (15%)	25,31,36	1.97	6 (24%)
1	PSU	1A	1917	54,1	18,21,22	1.33	2 (11%)	21,30,33	1.97	3 (14%)
1	2MA	1A	2503	54,1	22,25,26	1.45	5 (22%)	32,37,40	2.27	7 (21%)
32	G7M	2a	527	32,54	23,26,27	2.35	5 (21%)	34,39,42	3.01	10 (29%)
1	5MU	1A	1915	54,1	19,22,23	1.48	5 (26%)	27,32,35	2.29	9 (33%)
43	0TD	2l	92	43	8,9,10	4.64	1 (12%)	6,11,13	7.26	2 (33%)
1	OMG	1A	2251	54,1	23,26,27	1.25	3 (13%)	32,38,41	2.06	6 (18%)
43	0TD	1l	92	43	8,9,10	4.59	2 (25%)	6,11,13	7.05	3 (50%)
32	5MC	2a	967	32	19,22,23	1.76	2 (10%)	26,32,35	1.03	2 (7%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.12	10 (30%)
1	2MA	2A	2503	54,1	22,25,26	1.49	4 (18%)	32,37,40	2.44	8 (25%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.94	1 (4%)
1	5MC	2A	1962	54,1	19,22,23	1.66	3 (15%)	26,32,35	1.20	2 (7%)
32	G7M	1a	527	32,54	23,26,27	2.38	5 (21%)	34,39,42	2.94	10 (29%)
32	5MC	2a	1400	32	19,22,23	1.59	3 (15%)	26,32,35	1.19	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	1a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.83	6 (18%)

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	1400	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	54,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
1	OMG	2A	2251	54,1	-	0/9/27/28	0/3/3/3
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
1	5MC	1A	1942	54,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	UR3	2a	1498	32,54	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	2/7/25/26	0/2/2/2
1	5MC	1A	1962	54,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	54,1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	54,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	54,1	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1917	54,1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	54,1	-	2/7/25/26	0/3/3/3
32	G7M	2a	527	32,54	-	2/7/25/26	0/3/3/3
1	5MU	1A	1915	54,1	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	OMG	1A	2251	54,1	-	1/9/27/28	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	2/11/29/30	0/3/3/3
1	2MA	2A	2503	54,1	-	0/7/25/26	0/3/3/3
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
1	5MC	2A	1962	54,1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,54	-	1/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.64	1.69	1.82
43	1l	92	0TD	CB-SB	-12.29	1.69	1.82
32	2a	527	G7M	C8-N7	7.57	1.46	1.33
32	1a	527	G7M	C8-N7	7.42	1.45	1.33
32	2a	1404	5MC	C5-C4	7.21	1.49	1.44

The worst 5 of 227 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-17.39	71.10	102.36
43	1l	92	0TD	CSB-SB-CB	-16.65	72.44	102.36
1	2A	2503	2MA	C5-C4-N3	-8.74	117.98	127.18
32	2a	527	G7M	CN7-N7-C8	-8.43	112.02	124.79
1	1A	2503	2MA	C5-C4-N3	-7.75	119.02	127.18

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
32	1a	1207	2MG	N1-C2-N2-CM2

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

There are no ring outliers.

19 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1400	5MC	2	0
1	1A	1939	5MU	1	0
32	1a	1519	MA6	2	0
1	2A	2251	OMG	2	0
32	1a	1402	4OC	1	0
32	2a	1207	2MG	1	0
32	1a	1518	MA6	3	0
1	2A	1920	OMC	1	0
1	2A	1939	5MU	3	0
1	2A	2552	2MU	1	0
32	1a	1498	UR3	1	0
1	2A	1915	5MU	1	0
1	1A	1920	OMC	1	0
32	2a	1518	MA6	2	0
32	2a	1404	5MC	1	0
32	2a	1519	MA6	2	0
1	2A	2503	2MA	1	0
32	2a	1402	4OC	3	0
32	2a	1400	5MC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2525 ligands modelled in this entry, 2510 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	MPD	18	103	-	7,7,7	0.32	0	9,10,10	0.52	0
57	MPD	2B	217	-	7,7,7	0.32	0	9,10,10	0.30	0
58	ARG	1B	230	-	10,11,11	0.76	1 (10%)	9,13,13	1.10	1 (11%)
57	MPD	1a	1882	32	7,7,7	0.41	0	9,10,10	0.64	0
58	ARG	1F	318	54	10,11,11	0.73	1 (10%)	9,13,13	0.94	1 (11%)
60	SF4	2d	501	35	0,12,12	-	-	-	-	-
55	HGR	1A	4022	-	39,39,39	2.48	11 (28%)	48,58,58	1.72	13 (27%)
57	MPD	2A	3733	-	7,7,7	0.30	0	9,10,10	0.36	0
57	MPD	1A	4024	-	7,7,7	0.38	0	9,10,10	0.37	0
56	ZIT	1A	4023	-	54,54,54	0.88	2 (3%)	82,83,83	1.35	11 (13%)
57	MPD	1T	204	-	7,7,7	0.30	0	9,10,10	0.34	0
55	HGR	2A	3730	-	39,39,39	2.42	10 (25%)	48,58,58	1.64	12 (25%)
60	SF4	1d	305	35	0,12,12	-	-	-	-	-
56	ZIT	2A	3731	-	54,54,54	0.89	2 (3%)	82,83,83	1.44	12 (14%)
57	MPD	2A	3732	-	7,7,7	0.33	0	9,10,10	0.22	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
57	MPD	18	103	-	-	3/5/5/5	-
57	MPD	2B	217	-	-	3/5/5/5	-
58	ARG	1B	230	-	-	2/11/11/11	-
57	MPD	1a	1882	32	-	3/5/5/5	-
58	ARG	1F	318	54	-	1/11/11/11	-
60	SF4	2d	501	35	-	-	0/6/5/5
55	HGR	1A	4022	-	-	6/20/79/79	0/4/4/4
57	MPD	2A	3733	-	-	4/5/5/5	-
57	MPD	1A	4024	-	-	1/5/5/5	-
56	ZIT	1A	4023	-	-	6/72/107/107	0/3/3/3
57	MPD	1T	204	-	-	3/5/5/5	-
55	HGR	2A	3730	-	-	9/20/79/79	0/4/4/4
60	SF4	1d	305	35	-	-	0/6/5/5
56	ZIT	2A	3731	-	-	8/72/107/107	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	2A	3732	-	-	0/5/5/5	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4022	HGR	C12-C14	9.19	1.55	1.33
55	2A	3730	HGR	C12-C14	8.94	1.54	1.33
55	2A	3730	HGR	C5-C4	-5.53	1.39	1.49
55	1A	4022	HGR	C5-C4	-5.46	1.39	1.49
55	2A	3730	HGR	C5-C6	-5.32	1.39	1.50

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1A	4022	HGR	C4-C5-C6	4.33	121.60	112.35
56	2A	3731	ZIT	O3B-C3B-C4B	4.20	109.94	103.86
55	2A	3730	HGR	C4-C5-C6	4.17	121.25	112.35
56	1A	4023	ZIT	O3B-C3B-C4B	3.95	109.58	103.86
56	2A	3731	ZIT	C6-C5-C4	-3.74	108.46	113.89

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	2A	3730	HGR	C2-C3-O3-C10
55	2A	3730	HGR	C14-C12-C6-C1
56	1A	4023	ZIT	C12-C11-N10-C9
56	1A	4023	ZIT	C22-C11-N10-C9
56	1A	4023	ZIT	C12-C11-N10-C21

There are no ring outliers.

10 monomers are involved in 19 short contacts:

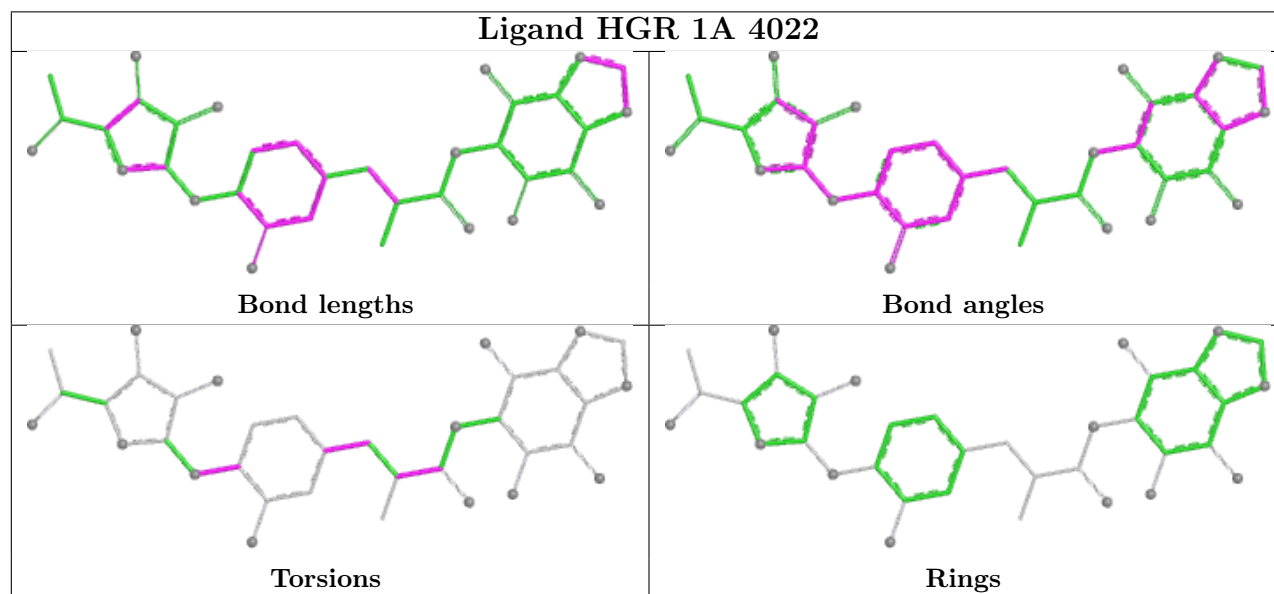
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	18	103	MPD	1	0
58	1B	230	ARG	2	0
57	1a	1882	MPD	5	0
58	1F	318	ARG	2	0
55	1A	4022	HGR	1	0
57	1T	204	MPD	1	0
55	2A	3730	HGR	2	0

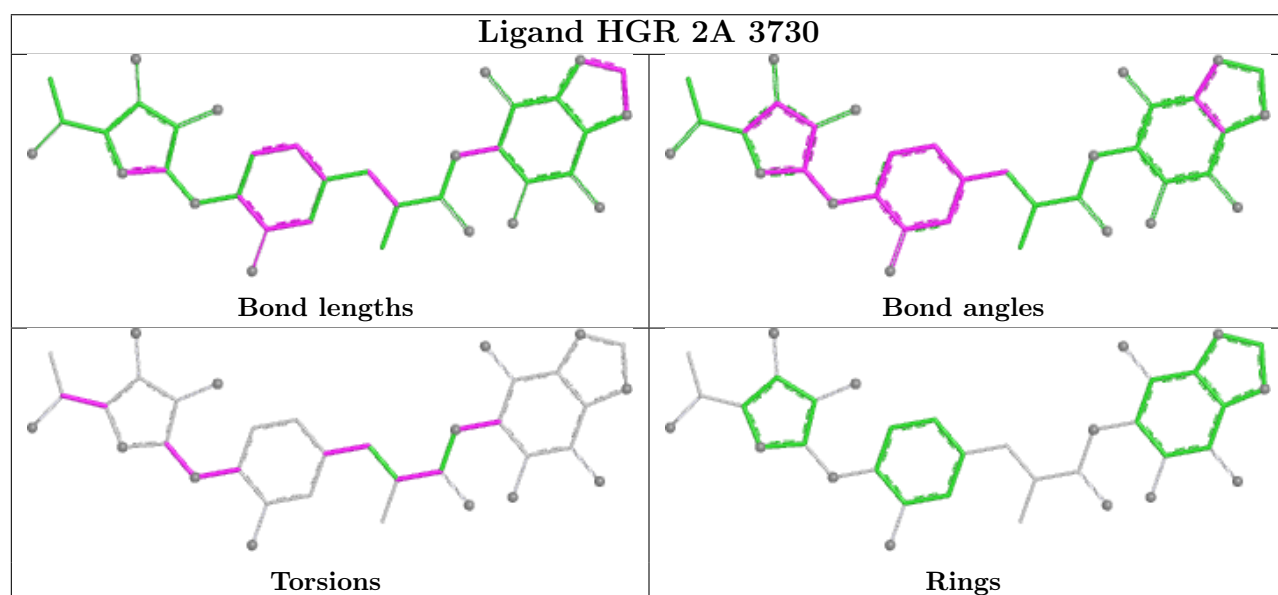
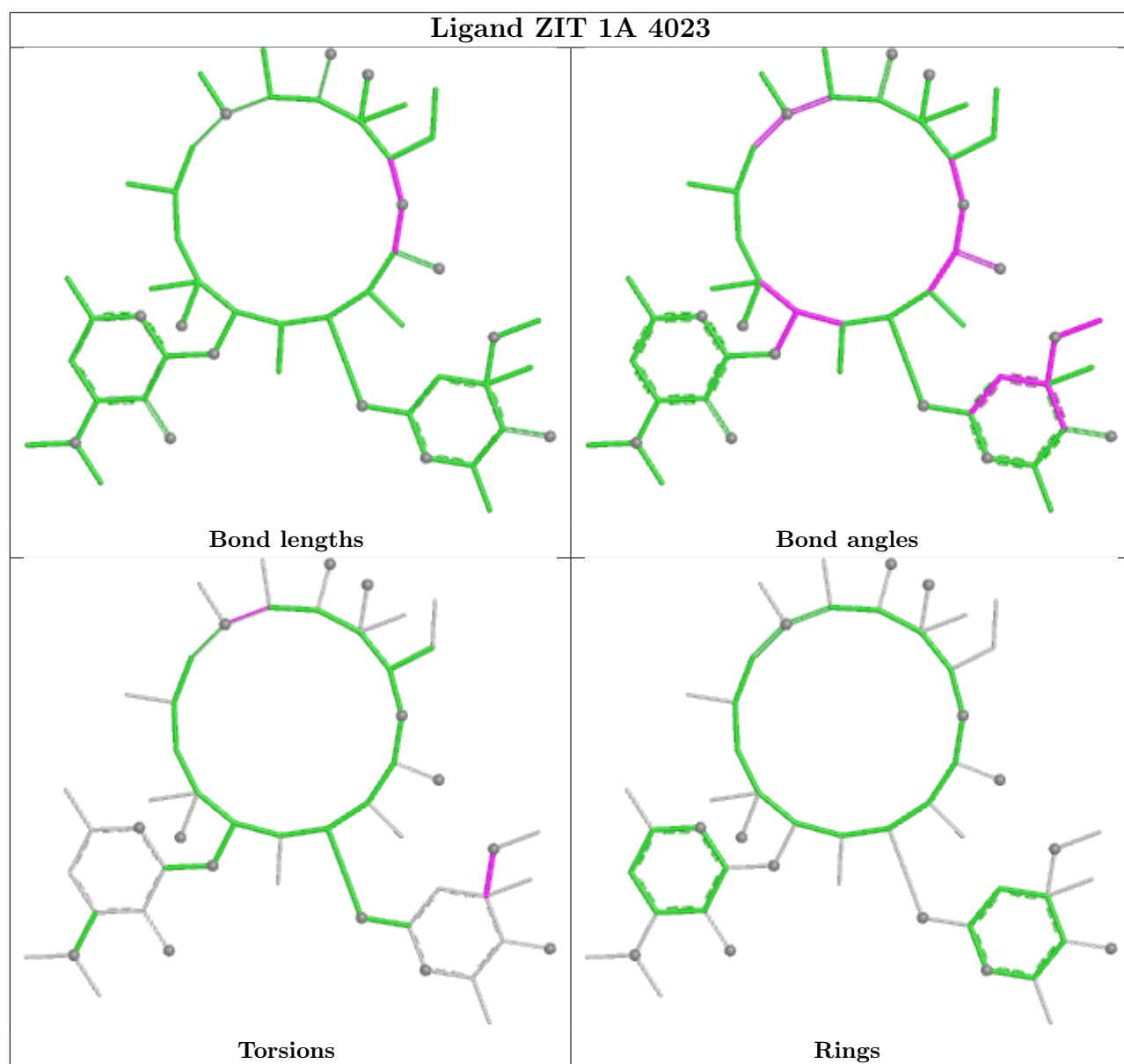
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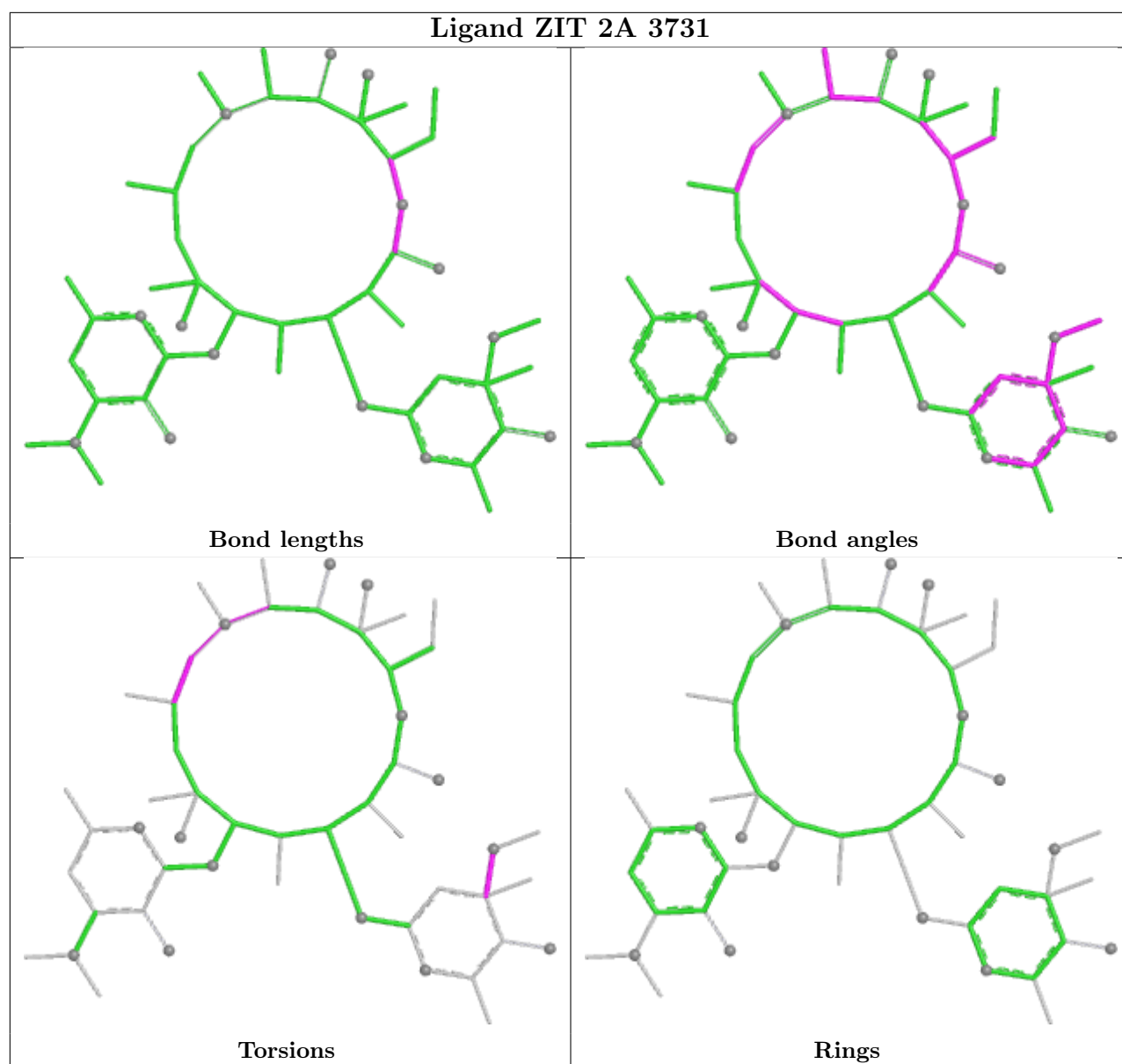
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1d	305	SF4	2	0
56	2A	3731	ZIT	2	0
57	2A	3732	MPD	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2861/2915 (98%)	-0.58	109 (3%) 44 39	26, 41, 95, 108	0
1	2A	2856/2915 (97%)	-0.21	127 (4%) 39 34	37, 59, 98, 107	0
2	1B	120/121 (99%)	-0.49	1 (0%) 82 80	36, 54, 69, 84	0
2	2B	120/121 (99%)	0.30	2 (1%) 69 65	61, 78, 86, 90	0
3	1D	275/276 (99%)	-0.08	1 (0%) 88 86	28, 43, 56, 75	0
3	2D	275/276 (99%)	0.17	1 (0%) 88 86	36, 54, 64, 79	0
4	1E	204/206 (99%)	-0.07	2 (0%) 79 76	26, 45, 65, 80	0
4	2E	204/206 (99%)	0.17	2 (0%) 79 76	37, 59, 73, 88	0
5	1F	203/210 (96%)	-0.10	1 (0%) 87 85	25, 46, 71, 86	0
5	2F	203/210 (96%)	0.42	2 (0%) 79 76	36, 67, 80, 87	0
6	1G	181/182 (99%)	0.47	6 (3%) 49 45	52, 67, 81, 86	0
6	2G	181/182 (99%)	1.33	31 (17%) 4 3	74, 82, 89, 93	0
7	1H	174/180 (96%)	0.15	1 (0%) 85 83	41, 56, 69, 74	0
7	2H	173/180 (96%)	1.08	15 (8%) 16 14	70, 81, 89, 92	0
8	1I	147/148 (99%)	0.71	3 (2%) 65 61	48, 73, 82, 87	0
8	2I	146/148 (98%)	1.12	19 (13%) 7 6	60, 75, 85, 90	0
9	1N	140/140 (100%)	-0.13	0 100 100	30, 43, 62, 77	0
9	2N	140/140 (100%)	0.40	1 (0%) 84 81	49, 64, 77, 79	0
10	1O	122/122 (100%)	-0.07	0 100 100	34, 45, 60, 66	0
10	2O	122/122 (100%)	0.39	2 (1%) 70 67	46, 57, 72, 76	0
11	1P	149/150 (99%)	0.03	0 100 100	26, 50, 68, 84	0
11	2P	149/150 (99%)	0.50	1 (0%) 84 81	43, 67, 81, 86	0
12	1Q	141/141 (100%)	-0.16	0 100 100	31, 44, 56, 72	0
12	2Q	141/141 (100%)	0.72	4 (2%) 55 50	47, 65, 74, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.25	0 100 100	31, 40, 51, 62	0
13	2R	118/118 (100%)	0.15	1 (0%) 82 80	41, 54, 64, 71	0
14	1S	110/112 (98%)	0.21	1 (0%) 81 78	44, 53, 65, 71	0
14	2S	110/112 (98%)	1.05	9 (8%) 17 15	65, 74, 79, 85	0
15	1T	131/146 (89%)	0.05	4 (3%) 51 47	38, 48, 70, 86	0
15	2T	131/146 (89%)	0.38	2 (1%) 72 68	51, 61, 79, 85	0
16	1U	116/118 (98%)	-0.33	0 100 100	27, 36, 49, 63	0
16	2U	116/118 (98%)	0.33	1 (0%) 81 78	42, 60, 72, 77	0
17	1V	101/101 (100%)	-0.22	0 100 100	28, 45, 61, 68	0
17	2V	101/101 (100%)	0.49	1 (0%) 79 76	42, 70, 78, 83	0
18	1W	112/113 (99%)	-0.21	1 (0%) 81 78	29, 37, 57, 81	0
18	2W	112/113 (99%)	0.14	1 (0%) 81 78	40, 51, 69, 87	0
19	1X	95/96 (98%)	0.08	3 (3%) 50 46	33, 41, 64, 76	0
19	2X	95/96 (98%)	0.42	3 (3%) 50 46	48, 62, 73, 81	0
20	1Y	107/110 (97%)	0.18	1 (0%) 81 78	40, 52, 65, 74	0
20	2Y	107/110 (97%)	0.80	4 (3%) 45 40	61, 70, 80, 85	0
21	1Z	203/206 (98%)	0.36	3 (1%) 72 68	41, 61, 75, 84	0
21	2Z	201/206 (97%)	1.00	12 (5%) 27 24	67, 78, 86, 89	0
22	10	77/85 (90%)	-0.04	1 (1%) 75 71	34, 42, 59, 66	0
22	20	77/85 (90%)	0.97	9 (11%) 9 7	50, 64, 72, 84	0
23	11	97/98 (98%)	0.09	1 (1%) 79 76	34, 48, 69, 74	0
23	21	97/98 (98%)	0.58	4 (4%) 41 37	43, 59, 75, 78	0
24	12	70/72 (97%)	0.25	2 (2%) 53 49	41, 53, 62, 79	0
24	22	70/72 (97%)	0.64	2 (2%) 53 49	60, 71, 78, 80	0
25	13	59/60 (98%)	-0.06	1 (1%) 69 65	28, 41, 66, 74	0
25	23	59/60 (98%)	0.34	0 100 100	53, 62, 74, 84	0
26	14	69/71 (97%)	0.90	11 (15%) 5 4	61, 79, 92, 93	0
26	24	69/71 (97%)	1.71	22 (31%) 1 1	82, 89, 94, 95	0
27	15	59/60 (98%)	-0.26	0 100 100	26, 39, 53, 63	0
27	25	59/60 (98%)	0.04	0 100 100	36, 52, 66, 75	0
28	16	53/54 (98%)	-0.11	0 100 100	38, 47, 59, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.51	3 (5%) 29 26	54, 63, 71, 76	0
29	17	48/49 (97%)	-0.18	2 (4%) 40 36	27, 34, 58, 67	0
29	27	48/49 (97%)	0.10	2 (4%) 40 36	38, 46, 66, 76	0
30	18	64/65 (98%)	-0.27	0 100 100	33, 39, 45, 55	0
30	28	64/65 (98%)	0.54	1 (1%) 70 67	49, 56, 63, 70	0
31	19	37/37 (100%)	0.02	0 100 100	36, 46, 60, 64	0
31	29	37/37 (100%)	0.89	1 (2%) 56 51	58, 66, 73, 76	0
32	1a	1488/1521 (97%)	0.04	26 (1%) 69 65	42, 71, 94, 109	0
32	2a	1492/1521 (98%)	0.30	35 (2%) 61 57	51, 78, 96, 107	0
33	1b	231/256 (90%)	1.07	30 (12%) 7 6	68, 80, 89, 95	0
33	2b	231/256 (90%)	1.53	60 (25%) 1 1	75, 85, 91, 95	0
34	1c	206/239 (86%)	0.83	13 (6%) 26 23	61, 74, 84, 90	0
34	2c	206/239 (86%)	1.37	42 (20%) 3 2	78, 84, 89, 91	0
35	1d	208/209 (99%)	0.97	20 (9%) 13 11	58, 72, 81, 89	0
35	2d	208/209 (99%)	0.85	7 (3%) 48 43	64, 74, 80, 83	0
36	1e	148/162 (91%)	0.45	0 100 100	57, 68, 76, 86	0
36	2e	148/162 (91%)	0.93	5 (3%) 48 43	63, 74, 82, 87	0
37	1f	100/101 (99%)	0.33	1 (1%) 79 76	59, 69, 78, 84	0
37	2f	100/101 (99%)	0.46	0 100 100	60, 71, 78, 86	0
38	1g	155/156 (99%)	0.62	6 (3%) 43 38	68, 75, 82, 86	0
38	2g	155/156 (99%)	1.14	20 (12%) 7 6	74, 82, 87, 91	0
39	1h	137/138 (99%)	0.52	4 (2%) 53 49	59, 70, 76, 81	0
39	2h	137/138 (99%)	0.77	3 (2%) 62 58	66, 75, 80, 83	0
40	1i	127/128 (99%)	1.26	18 (14%) 6 5	67, 79, 85, 87	0
40	2i	126/128 (98%)	1.97	58 (46%) 0 0	78, 86, 90, 93	0
41	1j	97/105 (92%)	1.53	29 (29%) 1 1	62, 79, 89, 91	0
41	2j	96/105 (91%)	1.80	35 (36%) 1 1	77, 86, 91, 94	0
42	1k	114/129 (88%)	0.54	3 (2%) 57 52	50, 68, 77, 85	0
42	2k	114/129 (88%)	0.82	5 (4%) 39 34	61, 75, 82, 86	0
43	1l	121/132 (91%)	0.53	4 (3%) 49 45	54, 62, 72, 75	0
43	2l	121/132 (91%)	0.71	4 (3%) 49 45	61, 69, 76, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.92	8 (6%) 23 20	62, 77, 82, 86	0
44	2m	114/126 (90%)	1.73	40 (35%) 1 1	77, 84, 89, 92	0
45	1n	60/61 (98%)	0.90	2 (3%) 49 45	65, 72, 79, 82	0
45	2n	60/61 (98%)	1.66	22 (36%) 1 1	77, 84, 89, 94	0
46	1o	88/89 (98%)	0.64	2 (2%) 61 57	53, 67, 78, 83	0
46	2o	88/89 (98%)	0.81	3 (3%) 48 43	62, 73, 81, 87	0
47	1p	82/88 (93%)	1.21	9 (10%) 10 8	62, 73, 82, 85	0
47	2p	82/88 (93%)	1.09	6 (7%) 21 19	64, 72, 80, 85	0
48	1q	99/105 (94%)	0.88	3 (3%) 52 48	59, 71, 78, 81	0
48	2q	99/105 (94%)	0.80	3 (3%) 52 48	59, 72, 79, 85	0
49	1r	68/88 (77%)	0.57	3 (4%) 39 34	61, 68, 80, 88	0
49	2r	68/88 (77%)	0.43	1 (1%) 72 68	65, 75, 83, 86	0
50	1s	83/93 (89%)	1.05	7 (8%) 17 15	70, 77, 83, 87	0
50	2s	83/93 (89%)	1.65	29 (34%) 1 1	79, 87, 91, 92	0
51	1t	96/106 (90%)	1.02	9 (9%) 14 12	64, 72, 80, 84	0
51	2t	98/106 (92%)	0.85	10 (10%) 12 10	60, 71, 81, 85	0
52	1u	23/27 (85%)	1.40	6 (26%) 1 1	71, 76, 78, 82	0
52	2u	23/27 (85%)	2.09	10 (43%) 0 0	79, 82, 85, 89	0
53	1y	97/113 (85%)	0.88	11 (11%) 10 8	59, 68, 77, 81	0
53	2y	96/113 (84%)	1.86	38 (39%) 1 0	73, 82, 89, 91	0
All	All	20766/21468 (96%)	0.26	1090 (5%) 33 29	25, 66, 89, 109	0

The worst 5 of 1090 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1087	G	12.1
1	1A	1089	G	8.9
1	1A	1090	U	8.2
1	1A	1091	G	7.5
45	2n	2	ALA	7.5

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MU	2A	1915	21/22	0.81	0.11	81,88,95,108	0
32	M2G	2a	966	25/26	0.86	0.16	67,77,87,95	0
32	2MG	2a	1207	24/25	0.86	0.13	83,89,95,100	0
1	5MU	1A	1915	21/22	0.88	0.11	76,81,85,87	0
1	PSU	2A	1911	20/21	0.89	0.09	64,75,83,88	0
1	PSU	2A	1917	20/21	0.90	0.08	72,80,90,94	0
1	PSU	1A	1917	20/21	0.91	0.10	69,74,81,85	0
43	0TD	1l	92	10/11	0.92	0.11	57,62,66,72	0
32	5MC	2a	967	21/22	0.92	0.12	72,78,84,88	0
32	2MG	1a	1207	24/25	0.92	0.10	65,75,77,81	0
43	0TD	2l	92	10/11	0.92	0.11	64,68,70,82	0
1	PSU	1A	1911	20/21	0.94	0.08	63,72,79,83	0
1	OMC	2A	1920	21/22	0.94	0.09	67,71,74,78	0
32	PSU	2a	516	20/21	0.94	0.08	70,78,80,80	0
32	G7M	2a	527	24/25	0.94	0.10	61,68,75,80	0
32	PSU	1a	516	20/21	0.95	0.08	58,66,71,73	0
32	4OC	2a	1402	22/23	0.95	0.09	60,69,74,76	0
32	5MC	2a	1404	21/22	0.95	0.09	60,68,71,75	0
32	5MC	1a	967	21/22	0.95	0.11	65,72,79,85	0
32	5MC	1a	1407	21/22	0.96	0.10	50,60,64,65	0
32	MA6	1a	1518	24/25	0.96	0.10	48,54,59,60	0
32	M2G	1a	966	25/26	0.96	0.10	60,66,70,74	0
1	OMC	1A	1920	21/22	0.96	0.10	46,62,65,65	0
32	G7M	1a	527	24/25	0.96	0.09	54,59,65,68	0
32	5MC	2a	1400	21/22	0.96	0.09	71,75,77,81	0
32	4OC	1a	1402	22/23	0.96	0.10	53,58,62,67	0
32	5MC	1a	1404	21/22	0.96	0.09	49,54,57,62	0
32	5MC	2a	1407	21/22	0.96	0.09	61,69,73,81	0
32	UR3	2a	1498	21/22	0.96	0.08	63,67,70,72	0
32	MA6	2a	1518	24/25	0.96	0.10	62,68,74,75	0
32	MA6	2a	1519	24/25	0.96	0.11	61,68,71,71	0
1	5MC	2A	1942	21/22	0.96	0.08	50,58,64,66	0
32	UR3	1a	1498	21/22	0.97	0.09	52,57,61,66	0
1	5MC	2A	1962	21/22	0.97	0.07	43,50,54,64	0
1	OMG	2A	2251	24/25	0.97	0.08	40,44,47,48	0
1	2MA	2A	2503	23/24	0.97	0.07	33,37,43,49	0
1	2MU	2A	2552	21/23	0.97	0.07	39,45,48,49	0
32	5MC	1a	1400	21/22	0.97	0.10	53,58,63,66	0
32	MA6	1a	1519	24/25	0.97	0.09	46,55,60,61	0
1	PSU	1A	2605	20/21	0.97	0.09	29,34,40,40	0
1	5MU	2A	1939	21/22	0.97	0.08	35,42,47,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PSU	2A	2605	20/21	0.98	0.07	34,42,46,48	0
1	5MU	1A	1939	21/22	0.98	0.07	29,33,37,38	0
1	5MC	1A	1942	21/22	0.98	0.06	35,44,49,58	0
1	5MC	1A	1962	21/22	0.98	0.07	35,40,43,45	0
1	OMG	1A	2251	24/25	0.98	0.07	26,32,35,35	0
1	2MA	1A	2503	23/24	0.98	0.06	21,29,32,34	0
1	2MU	1A	2552	21/23	0.98	0.07	28,36,39,45	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	3985	1/1	0.54	0.18	41,41,41,41	0
54	MG	2a	3182	1/1	0.59	0.32	84,84,84,84	0
54	MG	2A	3327	1/1	0.61	0.34	78,78,78,78	0
54	MG	1a	1778	1/1	0.61	0.19	79,79,79,79	0
54	MG	2A	3534	1/1	0.63	0.32	74,74,74,74	0
54	MG	2A	3468	1/1	0.66	0.33	67,67,67,67	0
54	MG	1B	226	1/1	0.68	0.15	81,81,81,81	0
54	MG	2A	3476	1/1	0.68	0.27	65,65,65,65	0
54	MG	1a	1878	1/1	0.69	0.20	88,88,88,88	0
54	MG	1a	1744	1/1	0.69	0.25	86,86,86,86	0
54	MG	1A	3292	1/1	0.69	0.16	84,84,84,84	0
54	MG	2G	201	1/1	0.70	0.22	81,81,81,81	0
54	MG	2A	3501	1/1	0.71	0.22	70,70,70,70	0
54	MG	2A	3463	1/1	0.71	0.39	61,61,61,61	0
54	MG	2A	3265	1/1	0.71	0.27	85,85,85,85	0
54	MG	2A	3193	1/1	0.71	0.30	78,78,78,78	0
54	MG	1a	1805	1/1	0.72	0.16	81,81,81,81	0
54	MG	1A	3989	1/1	0.72	0.21	80,80,80,80	0
54	MG	1a	1786	1/1	0.73	0.25	74,74,74,74	0
54	MG	1A	3533	1/1	0.73	0.16	59,59,59,59	0
54	MG	2A	3713	1/1	0.73	0.17	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3186	1/1	0.73	0.19	64,64,64,64	0
54	MG	2O	202	1/1	0.73	0.15	82,82,82,82	0
54	MG	2a	3020	1/1	0.73	0.17	90,90,90,90	0
54	MG	2A	3499	1/1	0.73	0.24	81,81,81,81	0
54	MG	1A	3464	1/1	0.74	0.12	59,59,59,59	0
54	MG	1A	3832	1/1	0.74	0.27	47,47,47,47	0
54	MG	1a	1811	1/1	0.75	0.19	85,85,85,85	0
54	MG	1a	1722	1/1	0.75	0.24	77,77,77,77	0
54	MG	1a	1781	1/1	0.75	0.14	67,67,67,67	0
54	MG	2A	3723	1/1	0.75	0.38	77,77,77,77	0
54	MG	1A	3621	1/1	0.76	0.20	69,69,69,69	0
54	MG	2A	3666	1/1	0.76	0.20	82,82,82,82	0
54	MG	2A	3675	1/1	0.76	0.32	71,71,71,71	0
54	MG	2A	3345	1/1	0.76	0.29	81,81,81,81	0
54	MG	1a	1773	1/1	0.76	0.17	72,72,72,72	0
54	MG	1A	3664	1/1	0.76	0.17	70,70,70,70	0
54	MG	2A	3111	1/1	0.76	0.16	78,78,78,78	0
54	MG	1A	3198	1/1	0.76	0.12	67,67,67,67	0
54	MG	2a	3024	1/1	0.76	0.28	85,85,85,85	0
54	MG	1A	3960	1/1	0.76	0.15	84,84,84,84	0
54	MG	2A	3638	1/1	0.77	0.17	77,77,77,77	0
54	MG	15	106	1/1	0.77	0.18	49,49,49,49	0
54	MG	1a	1670	1/1	0.77	0.26	81,81,81,81	0
54	MG	2A	3230	1/1	0.77	0.25	83,83,83,83	0
54	MG	1a	1685	1/1	0.77	0.34	75,75,75,75	0
54	MG	1A	3649	1/1	0.77	0.23	62,62,62,62	0
54	MG	2A	3519	1/1	0.77	0.19	64,64,64,64	0
54	MG	2A	3080	1/1	0.77	0.22	84,84,84,84	0
54	MG	2A	3554	1/1	0.77	0.20	71,71,71,71	0
54	MG	2a	3046	1/1	0.77	0.26	81,81,81,81	0
54	MG	2A	3614	1/1	0.77	0.20	62,62,62,62	0
54	MG	2j	201	1/1	0.77	0.24	74,74,74,74	0
58	ARG	1F	318	12/12	0.77	0.16	57,65,72,73	0
54	MG	1A	3862	1/1	0.78	0.14	70,70,70,70	0
54	MG	1A	3700	1/1	0.78	0.14	74,74,74,74	0
54	MG	1A	3516	1/1	0.78	0.14	56,56,56,56	0
54	MG	1a	1796	1/1	0.78	0.21	80,80,80,80	0
54	MG	2A	3263	1/1	0.78	0.14	79,79,79,79	0
54	MG	1a	1728	1/1	0.78	0.24	67,67,67,67	0
54	MG	2A	3549	1/1	0.78	0.20	61,61,61,61	0
54	MG	1a	1808	1/1	0.78	0.22	86,86,86,86	0
54	MG	2a	3055	1/1	0.78	0.28	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3060	1/1	0.78	0.31	82,82,82,82	0
54	MG	2a	3113	1/1	0.78	0.29	77,77,77,77	0
54	MG	2a	3129	1/1	0.78	0.37	82,82,82,82	0
54	MG	2a	3144	1/1	0.78	0.31	81,81,81,81	0
54	MG	1a	1641	1/1	0.78	0.25	74,74,74,74	0
54	MG	2a	3188	1/1	0.78	0.18	73,73,73,73	0
54	MG	2A	3411	1/1	0.78	0.15	70,70,70,70	0
54	MG	1a	1651	1/1	0.78	0.12	65,65,65,65	0
54	MG	2B	204	1/1	0.79	0.20	81,81,81,81	0
54	MG	2A	3488	1/1	0.79	0.17	61,61,61,61	0
54	MG	2A	3489	1/1	0.79	0.17	77,77,77,77	0
54	MG	1a	1853	1/1	0.79	0.15	75,75,75,75	0
54	MG	1A	3462	1/1	0.79	0.20	80,80,80,80	0
54	MG	2A	3290	1/1	0.79	0.26	87,87,87,87	0
54	MG	2A	3291	1/1	0.79	0.14	64,64,64,64	0
54	MG	2A	3326	1/1	0.79	0.24	67,67,67,67	0
54	MG	2a	3067	1/1	0.79	0.22	76,76,76,76	0
54	MG	1d	301	1/1	0.79	0.26	83,83,83,83	0
54	MG	2A	3054	1/1	0.79	0.32	76,76,76,76	0
54	MG	1a	1757	1/1	0.79	0.20	82,82,82,82	0
54	MG	2A	3440	1/1	0.79	0.22	88,88,88,88	0
54	MG	1a	1701	1/1	0.79	0.33	82,82,82,82	0
54	MG	2a	3193	1/1	0.79	0.18	84,84,84,84	0
54	MG	1A	3495	1/1	0.79	0.13	40,40,40,40	0
54	MG	2o	101	1/1	0.79	0.13	70,70,70,70	0
54	MG	1A	3660	1/1	0.79	0.17	72,72,72,72	0
54	MG	1T	202	1/1	0.80	0.19	70,70,70,70	0
54	MG	2A	3205	1/1	0.80	0.32	72,72,72,72	0
54	MG	14	101	1/1	0.80	0.10	65,65,65,65	0
54	MG	2G	202	1/1	0.80	0.21	81,81,81,81	0
54	MG	2A	3253	1/1	0.80	0.16	69,69,69,69	0
54	MG	1A	3477	1/1	0.80	0.23	67,67,67,67	0
54	MG	1A	3502	1/1	0.80	0.12	63,63,63,63	0
54	MG	1a	1873	1/1	0.80	0.20	75,75,75,75	0
54	MG	1a	1876	1/1	0.80	0.12	63,63,63,63	0
54	MG	2A	3541	1/1	0.80	0.14	73,73,73,73	0
54	MG	1A	3597	1/1	0.80	0.14	56,56,56,56	0
54	MG	2a	3111	1/1	0.80	0.35	73,73,73,73	0
54	MG	1A	3835	1/1	0.80	0.14	68,68,68,68	0
54	MG	2A	3053	1/1	0.80	0.40	80,80,80,80	0
54	MG	2A	3629	1/1	0.80	0.13	44,44,44,44	0
54	MG	2A	3633	1/1	0.80	0.34	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3842	1/1	0.80	0.11	63,63,63,63	0
54	MG	2A	3433	1/1	0.80	0.17	52,52,52,52	0
54	MG	2A	3669	1/1	0.80	0.22	59,59,59,59	0
54	MG	1a	1698	1/1	0.80	0.20	67,67,67,67	0
54	MG	1D	311	1/1	0.80	0.36	54,54,54,54	0
54	MG	2A	3023	1/1	0.81	0.21	64,64,64,64	0
54	MG	2A	3457	1/1	0.81	0.23	70,70,70,70	0
54	MG	2A	3036	1/1	0.81	0.26	76,76,76,76	0
54	MG	1A	3851	1/1	0.81	0.13	63,63,63,63	0
54	MG	2A	3469	1/1	0.81	0.18	63,63,63,63	0
54	MG	2A	3273	1/1	0.81	0.45	80,80,80,80	0
54	MG	1a	1813	1/1	0.81	0.15	81,81,81,81	0
54	MG	1A	3580	1/1	0.81	0.21	64,64,64,64	0
54	MG	1A	3088	1/1	0.81	0.18	64,64,64,64	0
54	MG	1A	3657	1/1	0.81	0.27	69,69,69,69	0
54	MG	1a	1761	1/1	0.81	0.24	70,70,70,70	0
54	MG	2a	3187	1/1	0.81	0.20	45,45,45,45	0
54	MG	2A	3399	1/1	0.81	0.15	72,72,72,72	0
54	MG	2A	3216	1/1	0.81	0.27	73,73,73,73	0
54	MG	1a	1714	1/1	0.81	0.33	73,73,73,73	0
54	MG	2T	202	1/1	0.81	0.23	77,77,77,77	0
54	MG	2a	3011	1/1	0.81	0.23	74,74,74,74	0
54	MG	2A	3679	1/1	0.82	0.16	75,75,75,75	0
54	MG	1A	3918	1/1	0.82	0.14	53,53,53,53	0
54	MG	2A	3717	1/1	0.82	0.17	64,64,64,64	0
54	MG	1a	1753	1/1	0.82	0.28	64,64,64,64	0
54	MG	2A	3728	1/1	0.82	0.21	69,69,69,69	0
54	MG	1A	3217	1/1	0.82	0.33	84,84,84,84	0
54	MG	1A	3647	1/1	0.82	0.19	75,75,75,75	0
54	MG	2A	3264	1/1	0.82	0.26	71,71,71,71	0
54	MG	1a	1652	1/1	0.82	0.29	73,73,73,73	0
54	MG	1A	3542	1/1	0.82	0.17	60,60,60,60	0
54	MG	2a	3010	1/1	0.82	0.30	75,75,75,75	0
54	MG	1B	220	1/1	0.82	0.17	57,57,57,57	0
54	MG	2A	3502	1/1	0.82	0.17	70,70,70,70	0
54	MG	1A	3272	1/1	0.82	0.33	79,79,79,79	0
54	MG	2A	3317	1/1	0.82	0.55	77,77,77,77	0
54	MG	2A	3324	1/1	0.82	0.35	69,69,69,69	0
54	MG	1A	3591	1/1	0.82	0.13	44,44,44,44	0
54	MG	1a	1707	1/1	0.82	0.26	71,71,71,71	0
54	MG	2a	3072	1/1	0.82	0.18	70,70,70,70	0
54	MG	2a	3081	1/1	0.82	0.20	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3089	1/1	0.82	0.33	81,81,81,81	0
54	MG	2A	3564	1/1	0.82	0.20	74,74,74,74	0
54	MG	2A	3587	1/1	0.82	0.17	48,48,48,48	0
54	MG	2A	3591	1/1	0.82	0.19	60,60,60,60	0
54	MG	2A	3608	1/1	0.82	0.23	68,68,68,68	0
54	MG	2A	3335	1/1	0.82	0.28	70,70,70,70	0
54	MG	1O	201	1/1	0.82	0.23	67,67,67,67	0
54	MG	2A	3128	1/1	0.82	0.29	76,76,76,76	0
54	MG	2A	3189	1/1	0.82	0.32	58,58,58,58	0
54	MG	1A	3483	1/1	0.82	0.14	60,60,60,60	0
54	MG	1A	3886	1/1	0.82	0.12	70,70,70,70	0
54	MG	2A	3208	1/1	0.82	0.17	69,69,69,69	0
54	MG	2A	3699	1/1	0.83	0.20	70,70,70,70	0
54	MG	1A	3894	1/1	0.83	0.12	59,59,59,59	0
54	MG	1A	3453	1/1	0.83	0.22	74,74,74,74	0
54	MG	1A	3942	1/1	0.83	0.19	61,61,61,61	0
54	MG	1A	3189	1/1	0.83	0.12	66,66,66,66	0
54	MG	2B	202	1/1	0.83	0.17	78,78,78,78	0
54	MG	2A	3214	1/1	0.83	0.28	74,74,74,74	0
54	MG	1A	3982	1/1	0.83	0.17	66,66,66,66	0
54	MG	1A	3244	1/1	0.83	0.12	70,70,70,70	0
54	MG	2O	201	1/1	0.83	0.21	63,63,63,63	0
54	MG	2A	3493	1/1	0.83	0.20	56,56,56,56	0
54	MG	2A	3250	1/1	0.83	0.25	70,70,70,70	0
54	MG	1A	3191	1/1	0.83	0.21	82,82,82,82	0
54	MG	1a	1704	1/1	0.83	0.25	76,76,76,76	0
54	MG	1A	3789	1/1	0.83	0.14	36,36,36,36	0
54	MG	2A	3532	1/1	0.83	0.15	73,73,73,73	0
54	MG	2a	3038	1/1	0.83	0.12	82,82,82,82	0
54	MG	1a	1710	1/1	0.83	0.12	72,72,72,72	0
54	MG	2A	3540	1/1	0.83	0.17	41,41,41,41	0
54	MG	1A	3126	1/1	0.83	0.32	66,66,66,66	0
54	MG	2a	3061	1/1	0.83	0.32	75,75,75,75	0
54	MG	2a	3062	1/1	0.83	0.26	76,76,76,76	0
54	MG	1A	3421	1/1	0.83	0.17	61,61,61,61	0
54	MG	1d	302	1/1	0.83	0.23	77,77,77,77	0
54	MG	1D	316	1/1	0.83	0.13	68,68,68,68	0
54	MG	2a	3087	1/1	0.83	0.14	78,78,78,78	0
54	MG	2A	3035	1/1	0.83	0.19	64,64,64,64	0
54	MG	2a	3106	1/1	0.83	0.42	67,67,67,67	0
54	MG	1A	3635	1/1	0.83	0.12	29,29,29,29	0
54	MG	1A	3447	1/1	0.83	0.16	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3119	1/1	0.83	0.13	67,67,67,67	0
54	MG	2A	3609	1/1	0.83	0.22	62,62,62,62	0
54	MG	1l	104	1/1	0.83	0.13	70,70,70,70	0
54	MG	1A	3449	1/1	0.83	0.18	57,57,57,57	0
54	MG	2A	3094	1/1	0.83	0.26	66,66,66,66	0
54	MG	1A	3652	1/1	0.83	0.36	47,47,47,47	0
54	MG	2A	3421	1/1	0.83	0.21	74,74,74,74	0
54	MG	2A	3123	1/1	0.83	0.25	79,79,79,79	0
54	MG	1a	1640	1/1	0.83	0.21	69,69,69,69	0
57	MPD	2B	217	8/8	0.83	0.26	61,68,76,77	0
54	MG	2A	3444	1/1	0.83	0.15	73,73,73,73	0
54	MG	1A	3816	1/1	0.84	0.11	80,80,80,80	0
54	MG	1l	202	1/1	0.84	0.14	81,81,81,81	0
54	MG	2a	3022	1/1	0.84	0.27	74,74,74,74	0
54	MG	2A	3232	1/1	0.84	0.26	64,64,64,64	0
54	MG	2a	3028	1/1	0.84	0.14	77,77,77,77	0
54	MG	1A	3344	1/1	0.84	0.11	59,59,59,59	0
54	MG	2A	3616	1/1	0.84	0.12	65,65,65,65	0
54	MG	1a	1783	1/1	0.84	0.14	74,74,74,74	0
54	MG	2a	3057	1/1	0.84	0.27	72,72,72,72	0
54	MG	1A	3170	1/1	0.84	0.17	66,66,66,66	0
54	MG	1a	1604	1/1	0.84	0.17	69,69,69,69	0
54	MG	2A	3641	1/1	0.84	0.13	74,74,74,74	0
54	MG	2a	3063	1/1	0.84	0.28	84,84,84,84	0
54	MG	1A	3926	1/1	0.84	0.12	32,32,32,32	0
54	MG	1B	229	1/1	0.84	0.14	80,80,80,80	0
54	MG	2A	3280	1/1	0.84	0.27	75,75,75,75	0
54	MG	2a	3084	1/1	0.84	0.47	68,68,68,68	0
54	MG	1A	3687	1/1	0.84	0.17	64,64,64,64	0
54	MG	2A	3682	1/1	0.84	0.17	65,65,65,65	0
54	MG	1A	3548	1/1	0.84	0.14	51,51,51,51	0
54	MG	2A	3118	1/1	0.84	0.25	76,76,76,76	0
54	MG	1G	202	1/1	0.84	0.16	63,63,63,63	0
54	MG	2A	3513	1/1	0.84	0.13	55,55,55,55	0
54	MG	1a	1863	1/1	0.84	0.20	72,72,72,72	0
54	MG	1a	1872	1/1	0.84	0.19	84,84,84,84	0
54	MG	2A	3190	1/1	0.84	0.20	61,61,61,61	0
54	MG	1a	1674	1/1	0.84	0.27	69,69,69,69	0
54	MG	2A	3350	1/1	0.84	0.16	59,59,59,59	0
54	MG	2A	3358	1/1	0.84	0.15	60,60,60,60	0
54	MG	1A	3963	1/1	0.84	0.18	70,70,70,70	0
54	MG	1A	3294	1/1	0.84	0.17	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	2a	3005	1/1	0.84	0.15	66,66,66,66	0
54	MG	1a	1775	1/1	0.84	0.15	76,76,76,76	0
54	MG	1A	3327	1/1	0.85	0.26	61,61,61,61	0
54	MG	1A	3983	1/1	0.85	0.10	71,71,71,71	0
54	MG	1a	1681	1/1	0.85	0.19	88,88,88,88	0
54	MG	1A	3792	1/1	0.85	0.14	45,45,45,45	0
54	MG	2A	3336	1/1	0.85	0.15	41,41,41,41	0
54	MG	2A	3703	1/1	0.85	0.13	68,68,68,68	0
54	MG	2A	3704	1/1	0.85	0.12	79,79,79,79	0
54	MG	1A	3027	1/1	0.85	0.15	71,71,71,71	0
54	MG	1B	210	1/1	0.85	0.31	70,70,70,70	0
54	MG	1A	3450	1/1	0.85	0.20	63,63,63,63	0
54	MG	2A	3362	1/1	0.85	0.21	77,77,77,77	0
54	MG	1B	224	1/1	0.85	0.15	65,65,65,65	0
54	MG	1A	3354	1/1	0.85	0.14	73,73,73,73	0
54	MG	1A	3360	1/1	0.85	0.18	55,55,55,55	0
54	MG	2A	3042	1/1	0.85	0.28	81,81,81,81	0
54	MG	1A	3848	1/1	0.85	0.16	60,60,60,60	0
54	MG	1A	3310	1/1	0.85	0.19	73,73,73,73	0
54	MG	1A	3574	1/1	0.85	0.10	49,49,49,49	0
54	MG	2a	3002	1/1	0.85	0.27	70,70,70,70	0
54	MG	2a	3003	1/1	0.85	0.21	71,71,71,71	0
54	MG	1a	1746	1/1	0.85	0.18	81,81,81,81	0
54	MG	1a	1748	1/1	0.85	0.21	79,79,79,79	0
54	MG	2A	3114	1/1	0.85	0.25	65,65,65,65	0
54	MG	1H	201	1/1	0.85	0.14	64,64,64,64	0
54	MG	1A	3882	1/1	0.85	0.14	55,55,55,55	0
54	MG	1R	208	1/1	0.85	0.21	53,53,53,53	0
54	MG	2A	3162	1/1	0.85	0.35	72,72,72,72	0
54	MG	1A	3468	1/1	0.85	0.14	66,66,66,66	0
54	MG	10	106	1/1	0.85	0.14	66,66,66,66	0
54	MG	10	107	1/1	0.85	0.17	69,69,69,69	0
54	MG	2A	3203	1/1	0.85	0.20	68,68,68,68	0
54	MG	1A	3680	1/1	0.85	0.40	39,39,39,39	0
54	MG	2A	3520	1/1	0.85	0.10	67,67,67,67	0
54	MG	2A	3523	1/1	0.85	0.12	63,63,63,63	0
54	MG	1A	3424	1/1	0.85	0.16	78,78,78,78	0
54	MG	1A	3695	1/1	0.85	0.09	77,77,77,77	0
54	MG	2a	3069	1/1	0.85	0.20	73,73,73,73	0
54	MG	1a	1793	1/1	0.85	0.14	68,68,68,68	0
54	MG	2a	3080	1/1	0.85	0.09	73,73,73,73	0
54	MG	1A	3932	1/1	0.85	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1802	1/1	0.85	0.13	79,79,79,79	0
54	MG	2A	3249	1/1	0.85	0.19	64,64,64,64	0
54	MG	2a	3088	1/1	0.85	0.20	70,70,70,70	0
54	MG	1a	1624	1/1	0.85	0.17	66,66,66,66	0
54	MG	2A	3583	1/1	0.85	0.14	47,47,47,47	0
54	MG	1A	3436	1/1	0.85	0.11	66,66,66,66	0
54	MG	2A	3590	1/1	0.85	0.16	66,66,66,66	0
54	MG	1A	3945	1/1	0.85	0.12	69,69,69,69	0
54	MG	1A	3707	1/1	0.85	0.19	71,71,71,71	0
54	MG	2a	3142	1/1	0.85	0.25	67,67,67,67	0
54	MG	1a	1820	1/1	0.85	0.12	76,76,76,76	0
54	MG	2a	3180	1/1	0.85	0.14	76,76,76,76	0
54	MG	1a	1839	1/1	0.85	0.15	77,77,77,77	0
54	MG	2a	3183	1/1	0.85	0.21	69,69,69,69	0
54	MG	2A	3275	1/1	0.85	0.27	73,73,73,73	0
54	MG	1a	1842	1/1	0.85	0.14	62,62,62,62	0
54	MG	1a	1844	1/1	0.85	0.16	75,75,75,75	0
54	MG	1A	3780	1/1	0.85	0.11	38,38,38,38	0
54	MG	1a	1664	1/1	0.85	0.23	77,77,77,77	0
57	MPD	1a	1882	8/8	0.85	0.14	55,67,72,79	0
54	MG	2A	3655	1/1	0.85	0.23	78,78,78,78	0
54	MG	2A	3323	1/1	0.85	0.25	63,63,63,63	0
54	MG	1a	1881	1/1	0.86	0.23	66,66,66,66	0
54	MG	2A	3640	1/1	0.86	0.27	62,62,62,62	0
54	MG	1A	3861	1/1	0.86	0.15	48,48,48,48	0
54	MG	2A	3643	1/1	0.86	0.10	69,69,69,69	0
54	MG	2A	3296	1/1	0.86	0.28	61,61,61,61	0
54	MG	1A	3196	1/1	0.86	0.14	57,57,57,57	0
54	MG	1h	202	1/1	0.86	0.20	74,74,74,74	0
54	MG	1A	3865	1/1	0.86	0.10	63,63,63,63	0
54	MG	1t	201	1/1	0.86	0.13	69,69,69,69	0
54	MG	1A	4001	1/1	0.86	0.24	60,60,60,60	0
54	MG	2A	3683	1/1	0.86	0.16	62,62,62,62	0
54	MG	2A	3687	1/1	0.86	0.14	55,55,55,55	0
54	MG	2A	3693	1/1	0.86	0.10	46,46,46,46	0
54	MG	2A	3328	1/1	0.86	0.43	67,67,67,67	0
54	MG	2A	3329	1/1	0.86	0.18	66,66,66,66	0
54	MG	2A	3033	1/1	0.86	0.11	68,68,68,68	0
54	MG	1a	1637	1/1	0.86	0.24	60,60,60,60	0
54	MG	1A	3874	1/1	0.86	0.17	68,68,68,68	0
54	MG	2A	3348	1/1	0.86	0.19	63,63,63,63	0
54	MG	1A	3793	1/1	0.86	0.14	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	1765	1/1	0.86	0.23	70,70,70,70	0
54	MG	1A	3798	1/1	0.86	0.23	65,65,65,65	0
54	MG	2B	208	1/1	0.86	0.20	73,73,73,73	0
54	MG	2B	211	1/1	0.86	0.22	66,66,66,66	0
54	MG	2A	3368	1/1	0.86	0.17	59,59,59,59	0
54	MG	2A	3068	1/1	0.86	0.28	64,64,64,64	0
54	MG	1A	3893	1/1	0.86	0.18	48,48,48,48	0
54	MG	2A	3088	1/1	0.86	0.20	76,76,76,76	0
54	MG	2A	3428	1/1	0.86	0.09	40,40,40,40	0
54	MG	2W	203	1/1	0.86	0.18	77,77,77,77	0
54	MG	27	103	1/1	0.86	0.17	68,68,68,68	0
54	MG	2A	3432	1/1	0.86	0.17	56,56,56,56	0
54	MG	1a	1657	1/1	0.86	0.11	73,73,73,73	0
54	MG	2A	3438	1/1	0.86	0.25	65,65,65,65	0
54	MG	2a	3006	1/1	0.86	0.39	78,78,78,78	0
54	MG	1A	3328	1/1	0.86	0.38	69,69,69,69	0
54	MG	2A	3441	1/1	0.86	0.24	80,80,80,80	0
54	MG	2a	3012	1/1	0.86	0.25	78,78,78,78	0
54	MG	2A	3113	1/1	0.86	0.19	59,59,59,59	0
54	MG	2A	3453	1/1	0.86	0.21	73,73,73,73	0
54	MG	1A	3912	1/1	0.86	0.12	33,33,33,33	0
54	MG	1a	1672	1/1	0.86	0.39	71,71,71,71	0
54	MG	2a	3032	1/1	0.86	0.22	77,77,77,77	0
54	MG	2a	3037	1/1	0.86	0.20	68,68,68,68	0
54	MG	2A	3464	1/1	0.86	0.14	61,61,61,61	0
54	MG	2a	3039	1/1	0.86	0.12	86,86,86,86	0
54	MG	1A	3830	1/1	0.86	0.16	76,76,76,76	0
54	MG	1a	1678	1/1	0.86	0.16	55,55,55,55	0
54	MG	2A	3148	1/1	0.86	0.20	69,69,69,69	0
54	MG	2A	3485	1/1	0.86	0.13	71,71,71,71	0
54	MG	1a	1798	1/1	0.86	0.11	73,73,73,73	0
54	MG	2A	3163	1/1	0.86	0.25	84,84,84,84	0
54	MG	2A	3184	1/1	0.86	0.14	70,70,70,70	0
54	MG	1A	3601	1/1	0.86	0.13	49,49,49,49	0
54	MG	1a	1684	1/1	0.86	0.23	66,66,66,66	0
54	MG	1A	3479	1/1	0.86	0.12	42,42,42,42	0
54	MG	1a	1686	1/1	0.86	0.19	75,75,75,75	0
54	MG	2A	3516	1/1	0.86	0.11	46,46,46,46	0
54	MG	1A	3838	1/1	0.86	0.15	69,69,69,69	0
54	MG	1P	204	1/1	0.86	0.24	47,47,47,47	0
54	MG	2A	3210	1/1	0.86	0.18	66,66,66,66	0
54	MG	2A	3213	1/1	0.86	0.15	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	2a	3101	1/1	0.86	0.21	71,71,71,71	0
54	MG	1a	1824	1/1	0.86	0.21	69,69,69,69	0
54	MG	1A	3840	1/1	0.86	0.11	68,68,68,68	0
54	MG	2a	3112	1/1	0.86	0.27	75,75,75,75	0
54	MG	2A	3229	1/1	0.86	0.15	68,68,68,68	0
54	MG	1a	1706	1/1	0.86	0.18	80,80,80,80	0
54	MG	1A	3764	1/1	0.86	0.30	67,67,67,67	0
54	MG	1a	1847	1/1	0.86	0.16	68,68,68,68	0
54	MG	2A	3568	1/1	0.86	0.17	66,66,66,66	0
54	MG	2a	3171	1/1	0.86	0.17	71,71,71,71	0
54	MG	1A	3576	1/1	0.86	0.11	56,56,56,56	0
54	MG	1A	3967	1/1	0.86	0.15	77,77,77,77	0
54	MG	1a	1869	1/1	0.86	0.20	82,82,82,82	0
54	MG	1a	1715	1/1	0.86	0.31	75,75,75,75	0
54	MG	1a	1718	1/1	0.86	0.12	69,69,69,69	0
54	MG	2A	3271	1/1	0.86	0.17	70,70,70,70	0
54	MG	1A	3438	1/1	0.86	0.11	46,46,46,46	0
54	MG	1a	1726	1/1	0.86	0.16	68,68,68,68	0
54	MG	1a	1880	1/1	0.86	0.26	69,69,69,69	0
54	MG	2A	3284	1/1	0.86	0.19	68,68,68,68	0
54	MG	2A	3634	1/1	0.86	0.15	37,37,37,37	0
54	MG	19	102	1/1	0.87	0.14	64,64,64,64	0
54	MG	2B	214	1/1	0.87	0.12	72,72,72,72	0
54	MG	2D	311	1/1	0.87	0.09	36,36,36,36	0
54	MG	1A	3476	1/1	0.87	0.13	51,51,51,51	0
54	MG	2A	3272	1/1	0.87	0.12	65,65,65,65	0
54	MG	2I	201	1/1	0.87	0.13	77,77,77,77	0
54	MG	2A	3047	1/1	0.87	0.20	66,66,66,66	0
54	MG	2A	3510	1/1	0.87	0.09	68,68,68,68	0
54	MG	1A	3446	1/1	0.87	0.19	52,52,52,52	0
54	MG	1a	1636	1/1	0.87	0.34	72,72,72,72	0
54	MG	1A	3098	1/1	0.87	0.12	67,67,67,67	0
54	MG	1A	3389	1/1	0.87	0.16	55,55,55,55	0
54	MG	1A	3490	1/1	0.87	0.10	31,31,31,31	0
54	MG	2A	3529	1/1	0.87	0.19	60,60,60,60	0
54	MG	2A	3089	1/1	0.87	0.32	72,72,72,72	0
54	MG	2A	3311	1/1	0.87	0.22	60,60,60,60	0
54	MG	2A	3316	1/1	0.87	0.38	71,71,71,71	0
54	MG	1a	1717	1/1	0.87	0.12	72,72,72,72	0
54	MG	1a	1646	1/1	0.87	0.25	70,70,70,70	0
54	MG	2A	3553	1/1	0.87	0.14	71,71,71,71	0
54	MG	1a	1826	1/1	0.87	0.26	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3026	1/1	0.87	0.22	79,79,79,79	0
54	MG	1a	1837	1/1	0.87	0.27	68,68,68,68	0
54	MG	1a	1720	1/1	0.87	0.13	68,68,68,68	0
54	MG	1A	3396	1/1	0.87	0.12	54,54,54,54	0
54	MG	2A	3584	1/1	0.87	0.12	44,44,44,44	0
54	MG	1a	1725	1/1	0.87	0.23	70,70,70,70	0
54	MG	2A	3333	1/1	0.87	0.17	60,60,60,60	0
54	MG	2A	3133	1/1	0.87	0.23	67,67,67,67	0
54	MG	1A	3335	1/1	0.87	0.18	62,62,62,62	0
54	MG	1A	3949	1/1	0.87	0.12	51,51,51,51	0
54	MG	1a	1662	1/1	0.87	0.11	74,74,74,74	0
54	MG	1A	3958	1/1	0.87	0.11	62,62,62,62	0
54	MG	2A	3618	1/1	0.87	0.11	60,60,60,60	0
54	MG	2a	3066	1/1	0.87	0.27	69,69,69,69	0
54	MG	2A	3351	1/1	0.87	0.13	46,46,46,46	0
54	MG	2A	3631	1/1	0.87	0.17	82,82,82,82	0
54	MG	1A	3337	1/1	0.87	0.35	68,68,68,68	0
54	MG	1A	3880	1/1	0.87	0.19	42,42,42,42	0
54	MG	2A	3191	1/1	0.87	0.13	54,54,54,54	0
54	MG	1A	3173	1/1	0.87	0.15	55,55,55,55	0
54	MG	1a	1677	1/1	0.87	0.15	65,65,65,65	0
54	MG	1a	1879	1/1	0.87	0.32	75,75,75,75	0
54	MG	2A	3207	1/1	0.87	0.29	70,70,70,70	0
54	MG	2a	3095	1/1	0.87	0.44	74,74,74,74	0
54	MG	2a	3098	1/1	0.87	0.21	72,72,72,72	0
54	MG	1A	3222	1/1	0.87	0.14	65,65,65,65	0
54	MG	1A	3888	1/1	0.87	0.09	32,32,32,32	0
54	MG	2a	3108	1/1	0.87	0.30	64,64,64,64	0
54	MG	2A	3671	1/1	0.87	0.13	75,75,75,75	0
54	MG	2A	3212	1/1	0.87	0.31	64,64,64,64	0
54	MG	1A	3891	1/1	0.87	0.17	57,57,57,57	0
54	MG	1a	1777	1/1	0.87	0.14	64,64,64,64	0
54	MG	2a	3126	1/1	0.87	0.14	74,74,74,74	0
54	MG	1d	304	1/1	0.87	0.09	86,86,86,86	0
54	MG	1e	204	1/1	0.87	0.13	77,77,77,77	0
54	MG	1A	3892	1/1	0.87	0.11	56,56,56,56	0
54	MG	2a	3156	1/1	0.87	0.17	80,80,80,80	0
54	MG	2a	3157	1/1	0.87	0.14	70,70,70,70	0
54	MG	2a	3159	1/1	0.87	0.15	76,76,76,76	0
54	MG	2A	3695	1/1	0.87	0.14	69,69,69,69	0
54	MG	2a	3172	1/1	0.87	0.30	76,76,76,76	0
54	MG	2A	3462	1/1	0.87	0.22	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	3997	1/1	0.87	0.15	76,76,76,76	0
54	MG	2A	3241	1/1	0.87	0.21	60,60,60,60	0
54	MG	2a	3186	1/1	0.87	0.43	72,72,72,72	0
54	MG	2A	3466	1/1	0.87	0.14	85,85,85,85	0
54	MG	1a	1689	1/1	0.87	0.36	68,68,68,68	0
54	MG	2A	3021	1/1	0.87	0.33	56,56,56,56	0
54	MG	2A	3251	1/1	0.87	0.26	67,67,67,67	0
54	MG	2B	201	1/1	0.87	0.14	74,74,74,74	0
54	MG	1a	1696	1/1	0.87	0.19	73,73,73,73	0
54	MG	1a	1790	1/1	0.87	0.22	74,74,74,74	0
54	MG	1A	3731	1/1	0.87	0.13	52,52,52,52	0
54	MG	2A	3137	1/1	0.88	0.22	69,69,69,69	0
54	MG	1a	1690	1/1	0.88	0.48	76,76,76,76	0
54	MG	1a	1819	1/1	0.88	0.16	73,73,73,73	0
54	MG	1A	3673	1/1	0.88	0.09	35,35,35,35	0
54	MG	2A	3725	1/1	0.88	0.14	69,69,69,69	0
54	MG	2A	3170	1/1	0.88	0.12	47,47,47,47	0
54	MG	2A	3178	1/1	0.88	0.21	70,70,70,70	0
54	MG	2A	3182	1/1	0.88	0.15	61,61,61,61	0
54	MG	2B	203	1/1	0.88	0.27	74,74,74,74	0
54	MG	1N	204	1/1	0.88	0.24	59,59,59,59	0
54	MG	2A	3186	1/1	0.88	0.19	67,67,67,67	0
54	MG	1A	3594	1/1	0.88	0.20	59,59,59,59	0
54	MG	2B	213	1/1	0.88	0.21	72,72,72,72	0
54	MG	1a	1827	1/1	0.88	0.17	64,64,64,64	0
54	MG	1A	3947	1/1	0.88	0.08	45,45,45,45	0
54	MG	2A	3192	1/1	0.88	0.27	71,71,71,71	0
54	MG	1a	1705	1/1	0.88	0.50	78,78,78,78	0
54	MG	1a	1840	1/1	0.88	0.19	81,81,81,81	0
54	MG	2A	3467	1/1	0.88	0.15	49,49,49,49	0
54	MG	1A	3595	1/1	0.88	0.30	47,47,47,47	0
54	MG	2P	202	1/1	0.88	0.25	77,77,77,77	0
54	MG	2Q	202	1/1	0.88	0.34	63,63,63,63	0
54	MG	1A	3022	1/1	0.88	0.10	52,52,52,52	0
54	MG	2A	3472	1/1	0.88	0.16	68,68,68,68	0
54	MG	2I	101	1/1	0.88	0.28	73,73,73,73	0
54	MG	1a	1845	1/1	0.88	0.26	76,76,76,76	0
54	MG	1A	3546	1/1	0.88	0.10	55,55,55,55	0
54	MG	1a	1711	1/1	0.88	0.30	66,66,66,66	0
54	MG	1A	3547	1/1	0.88	0.15	40,40,40,40	0
54	MG	1A	3964	1/1	0.88	0.13	66,66,66,66	0
54	MG	2A	3494	1/1	0.88	0.24	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	2A	3215	1/1	0.88	0.16	59,59,59,59	0
54	MG	2A	3500	1/1	0.88	0.23	71,71,71,71	0
54	MG	1a	1716	1/1	0.88	0.26	68,68,68,68	0
54	MG	2A	3224	1/1	0.88	0.11	63,63,63,63	0
54	MG	1A	3716	1/1	0.88	0.13	60,60,60,60	0
54	MG	1A	3630	1/1	0.88	0.29	66,66,66,66	0
54	MG	1A	3041	1/1	0.88	0.19	58,58,58,58	0
54	MG	1A	3768	1/1	0.88	0.16	65,65,65,65	0
54	MG	1a	1623	1/1	0.88	0.17	63,63,63,63	0
54	MG	1A	3778	1/1	0.88	0.15	76,76,76,76	0
54	MG	1a	1633	1/1	0.88	0.14	66,66,66,66	0
54	MG	1a	1732	1/1	0.88	0.15	75,75,75,75	0
54	MG	2a	3048	1/1	0.88	0.25	75,75,75,75	0
54	MG	1a	1736	1/1	0.88	0.18	79,79,79,79	0
54	MG	1A	3992	1/1	0.88	0.27	60,60,60,60	0
54	MG	1A	3994	1/1	0.88	0.16	47,47,47,47	0
54	MG	2A	3544	1/1	0.88	0.15	62,62,62,62	0
54	MG	2A	3548	1/1	0.88	0.19	70,70,70,70	0
54	MG	1i	3101	1/1	0.88	0.16	66,66,66,66	0
54	MG	1A	3282	1/1	0.88	0.14	56,56,56,56	0
54	MG	1A	3999	1/1	0.88	0.12	64,64,64,64	0
54	MG	2A	3558	1/1	0.88	0.11	51,51,51,51	0
54	MG	1a	1755	1/1	0.88	0.17	63,63,63,63	0
54	MG	2a	3075	1/1	0.88	0.40	76,76,76,76	0
54	MG	2A	3565	1/1	0.88	0.11	65,65,65,65	0
54	MG	1a	1644	1/1	0.88	0.24	64,64,64,64	0
54	MG	1A	4000	1/1	0.88	0.17	70,70,70,70	0
54	MG	1A	3367	1/1	0.88	0.15	57,57,57,57	0
54	MG	1A	4006	1/1	0.88	0.31	63,63,63,63	0
54	MG	1A	4008	1/1	0.88	0.25	64,64,64,64	0
54	MG	2a	3090	1/1	0.88	0.32	64,64,64,64	0
54	MG	2a	3092	1/1	0.88	0.12	70,70,70,70	0
54	MG	2a	3093	1/1	0.88	0.18	67,67,67,67	0
54	MG	2a	3094	1/1	0.88	0.38	75,75,75,75	0
54	MG	2A	3302	1/1	0.88	0.32	59,59,59,59	0
54	MG	1B	203	1/1	0.88	0.18	61,61,61,61	0
54	MG	1B	206	1/1	0.88	0.21	61,61,61,61	0
54	MG	2a	3102	1/1	0.88	0.37	73,73,73,73	0
54	MG	1a	1665	1/1	0.88	0.10	72,72,72,72	0
54	MG	2A	3321	1/1	0.88	0.12	63,63,63,63	0
54	MG	2a	3109	1/1	0.88	0.42	70,70,70,70	0
54	MG	2A	3062	1/1	0.88	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3578	1/1	0.88	0.13	61,61,61,61	0
54	MG	2A	3079	1/1	0.88	0.17	61,61,61,61	0
54	MG	2a	3117	1/1	0.88	0.12	78,78,78,78	0
54	MG	1A	3655	1/1	0.88	0.25	45,45,45,45	0
54	MG	2a	3125	1/1	0.88	0.17	89,89,89,89	0
54	MG	1A	3656	1/1	0.88	0.11	69,69,69,69	0
54	MG	2A	3635	1/1	0.88	0.19	55,55,55,55	0
54	MG	2a	3138	1/1	0.88	0.16	80,80,80,80	0
54	MG	1A	3318	1/1	0.88	0.38	72,72,72,72	0
54	MG	1B	228	1/1	0.88	0.08	63,63,63,63	0
54	MG	2a	3153	1/1	0.88	0.21	82,82,82,82	0
54	MG	1A	3658	1/1	0.88	0.15	67,67,67,67	0
54	MG	1a	1801	1/1	0.88	0.11	69,69,69,69	0
54	MG	1A	3831	1/1	0.88	0.12	24,24,24,24	0
54	MG	2a	3164	1/1	0.88	0.12	71,71,71,71	0
54	MG	1a	1804	1/1	0.88	0.18	75,75,75,75	0
54	MG	2A	3668	1/1	0.88	0.14	73,73,73,73	0
54	MG	1A	3588	1/1	0.88	0.17	76,76,76,76	0
54	MG	2A	3126	1/1	0.88	0.15	73,73,73,73	0
54	MG	1E	302	1/1	0.88	0.17	38,38,38,38	0
54	MG	2A	3676	1/1	0.88	0.19	66,66,66,66	0
54	MG	2A	3359	1/1	0.88	0.16	54,54,54,54	0
54	MG	2A	3131	1/1	0.88	0.33	65,65,65,65	0
54	MG	2a	3189	1/1	0.88	0.28	69,69,69,69	0
54	MG	2a	3192	1/1	0.88	0.21	62,62,62,62	0
54	MG	1A	3455	1/1	0.88	0.20	67,67,67,67	0
54	MG	2A	3394	1/1	0.88	0.13	48,48,48,48	0
54	MG	2A	3396	1/1	0.88	0.15	52,52,52,52	0
54	MG	2A	3135	1/1	0.88	0.12	57,57,57,57	0
54	MG	2A	3400	1/1	0.88	0.13	54,54,54,54	0
54	MG	2A	3404	1/1	0.88	0.16	56,56,56,56	0
54	MG	1A	3334	1/1	0.89	0.21	65,65,65,65	0
54	MG	1a	1767	1/1	0.89	0.18	61,61,61,61	0
54	MG	2A	3164	1/1	0.89	0.13	70,70,70,70	0
54	MG	2A	3546	1/1	0.89	0.23	65,65,65,65	0
54	MG	1A	3796	1/1	0.89	0.13	60,60,60,60	0
54	MG	1a	1774	1/1	0.89	0.13	66,66,66,66	0
54	MG	2A	3180	1/1	0.89	0.21	76,76,76,76	0
54	MG	1a	1688	1/1	0.89	0.18	56,56,56,56	0
54	MG	1A	3205	1/1	0.89	0.19	56,56,56,56	0
54	MG	1A	3156	1/1	0.89	0.24	66,66,66,66	0
54	MG	2a	3014	1/1	0.89	0.26	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	1692	1/1	0.89	0.22	74,74,74,74	0
54	MG	1e	201	1/1	0.89	0.16	72,72,72,72	0
54	MG	2A	3573	1/1	0.89	0.10	67,67,67,67	0
54	MG	1a	1694	1/1	0.89	0.15	72,72,72,72	0
54	MG	1f	201	1/1	0.89	0.29	75,75,75,75	0
54	MG	1A	3608	1/1	0.89	0.16	67,67,67,67	0
54	MG	1B	201	1/1	0.89	0.17	63,63,63,63	0
54	MG	2A	3375	1/1	0.89	0.16	60,60,60,60	0
54	MG	2A	3595	1/1	0.89	0.15	72,72,72,72	0
54	MG	2a	3040	1/1	0.89	0.19	64,64,64,64	0
54	MG	2a	3041	1/1	0.89	0.15	78,78,78,78	0
54	MG	2A	3388	1/1	0.89	0.26	63,63,63,63	0
54	MG	1A	3610	1/1	0.89	0.17	48,48,48,48	0
54	MG	1n	101	1/1	0.89	0.11	63,63,63,63	0
54	MG	1A	3471	1/1	0.89	0.13	57,57,57,57	0
54	MG	1y	202	1/1	0.89	0.13	74,74,74,74	0
54	MG	2A	3621	1/1	0.89	0.14	54,54,54,54	0
54	MG	2A	3622	1/1	0.89	0.10	62,62,62,62	0
54	MG	2A	3623	1/1	0.89	0.13	46,46,46,46	0
54	MG	2A	3401	1/1	0.89	0.16	54,54,54,54	0
54	MG	1y	203	1/1	0.89	0.14	83,83,83,83	0
54	MG	2A	3001	1/1	0.89	0.13	57,57,57,57	0
54	MG	1A	3549	1/1	0.89	0.13	57,57,57,57	0
54	MG	2A	3424	1/1	0.89	0.19	63,63,63,63	0
54	MG	2a	3079	1/1	0.89	0.24	70,70,70,70	0
54	MG	1B	211	1/1	0.89	0.11	55,55,55,55	0
54	MG	2A	3429	1/1	0.89	0.09	43,43,43,43	0
54	MG	1B	216	1/1	0.89	0.20	67,67,67,67	0
54	MG	2A	3219	1/1	0.89	0.11	61,61,61,61	0
54	MG	2A	3436	1/1	0.89	0.13	49,49,49,49	0
54	MG	2A	3661	1/1	0.89	0.14	41,41,41,41	0
54	MG	2A	3437	1/1	0.89	0.14	60,60,60,60	0
54	MG	2A	3221	1/1	0.89	0.24	73,73,73,73	0
54	MG	2A	3034	1/1	0.89	0.27	66,66,66,66	0
54	MG	1A	3702	1/1	0.89	0.17	77,77,77,77	0
54	MG	1a	1639	1/1	0.89	0.19	71,71,71,71	0
54	MG	1a	1713	1/1	0.89	0.27	52,52,52,52	0
54	MG	2a	3100	1/1	0.89	0.30	78,78,78,78	0
54	MG	1A	3573	1/1	0.89	0.19	67,67,67,67	0
54	MG	1B	225	1/1	0.89	0.11	49,49,49,49	0
54	MG	1a	1818	1/1	0.89	0.17	69,69,69,69	0
54	MG	1A	3841	1/1	0.89	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3063	1/1	0.89	0.15	60,60,60,60	0
54	MG	2a	3110	1/1	0.89	0.26	67,67,67,67	0
54	MG	1A	3639	1/1	0.89	0.13	67,67,67,67	0
54	MG	1A	3717	1/1	0.89	0.10	64,64,64,64	0
54	MG	1A	3720	1/1	0.89	0.12	58,58,58,58	0
54	MG	2a	3116	1/1	0.89	0.14	54,54,54,54	0
54	MG	2A	3270	1/1	0.89	0.26	74,74,74,74	0
54	MG	2A	3707	1/1	0.89	0.21	68,68,68,68	0
54	MG	1a	1655	1/1	0.89	0.21	63,63,63,63	0
54	MG	2A	3716	1/1	0.89	0.11	79,79,79,79	0
54	MG	1a	1831	1/1	0.89	0.09	92,92,92,92	0
54	MG	1A	3498	1/1	0.89	0.12	42,42,42,42	0
54	MG	2A	3102	1/1	0.89	0.34	67,67,67,67	0
54	MG	2A	3727	1/1	0.89	0.19	62,62,62,62	0
54	MG	2a	3145	1/1	0.89	0.34	70,70,70,70	0
54	MG	2A	3490	1/1	0.89	0.15	65,65,65,65	0
54	MG	2A	3491	1/1	0.89	0.21	65,65,65,65	0
54	MG	1a	1658	1/1	0.89	0.26	51,51,51,51	0
54	MG	1A	3746	1/1	0.89	0.11	52,52,52,52	0
54	MG	2a	3160	1/1	0.89	0.13	75,75,75,75	0
54	MG	2A	3496	1/1	0.89	0.14	60,60,60,60	0
54	MG	2A	3288	1/1	0.89	0.26	78,78,78,78	0
54	MG	1F	316	1/1	0.89	0.10	62,62,62,62	0
54	MG	1A	3762	1/1	0.89	0.29	41,41,41,41	0
54	MG	1A	3501	1/1	0.89	0.10	30,30,30,30	0
54	MG	1A	3474	1/1	0.89	0.11	51,51,51,51	0
54	MG	2E	305	1/1	0.89	0.11	41,41,41,41	0
54	MG	2F	302	1/1	0.89	0.13	55,55,55,55	0
54	MG	2F	303	1/1	0.89	0.15	62,62,62,62	0
54	MG	1A	3439	1/1	0.89	0.11	34,34,34,34	0
54	MG	2A	3313	1/1	0.89	0.25	74,74,74,74	0
54	MG	1A	3521	1/1	0.89	0.12	75,75,75,75	0
54	MG	1A	3531	1/1	0.89	0.14	65,65,65,65	0
54	MG	1a	1871	1/1	0.89	0.08	84,84,84,84	0
57	MPD	1T	204	8/8	0.89	0.19	68,72,74,77	0
54	MG	1A	3361	1/1	0.89	0.13	58,58,58,58	0
57	MPD	2A	3732	8/8	0.89	0.23	50,56,61,64	0
54	MG	1Z	301	1/1	0.89	0.13	71,71,71,71	0
54	MG	2A	3325	1/1	0.89	0.24	65,65,65,65	0
54	MG	1a	1743	1/1	0.90	0.11	62,62,62,62	0
54	MG	1A	3382	1/1	0.90	0.19	66,66,66,66	0
54	MG	2A	3459	1/1	0.90	0.21	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	2A	3461	1/1	0.90	0.24	74,74,74,74	0
54	MG	1A	4003	1/1	0.90	0.25	42,42,42,42	0
54	MG	1A	3387	1/1	0.90	0.21	69,69,69,69	0
54	MG	1a	1643	1/1	0.90	0.26	63,63,63,63	0
54	MG	1A	3696	1/1	0.90	0.11	54,54,54,54	0
54	MG	2D	301	1/1	0.90	0.35	53,53,53,53	0
54	MG	2D	310	1/1	0.90	0.14	52,52,52,52	0
54	MG	1f	202	1/1	0.90	0.12	56,56,56,56	0
54	MG	2A	3218	1/1	0.90	0.23	71,71,71,71	0
54	MG	1A	4015	1/1	0.90	0.09	46,46,46,46	0
54	MG	1A	3211	1/1	0.90	0.20	61,61,61,61	0
54	MG	1k	201	1/1	0.90	0.20	57,57,57,57	0
54	MG	1B	202	1/1	0.90	0.20	63,63,63,63	0
54	MG	1A	3147	1/1	0.90	0.15	58,58,58,58	0
54	MG	2I	202	1/1	0.90	0.14	70,70,70,70	0
54	MG	1B	205	1/1	0.90	0.08	50,50,50,50	0
54	MG	1A	3611	1/1	0.90	0.10	64,64,64,64	0
54	MG	2A	3248	1/1	0.90	0.17	62,62,62,62	0
54	MG	1A	3613	1/1	0.90	0.11	52,52,52,52	0
54	MG	1A	3614	1/1	0.90	0.10	50,50,50,50	0
54	MG	2W	202	1/1	0.90	0.20	57,57,57,57	0
54	MG	1A	3620	1/1	0.90	0.35	33,33,33,33	0
54	MG	1A	3723	1/1	0.90	0.17	42,42,42,42	0
54	MG	2A	3259	1/1	0.90	0.17	64,64,64,64	0
54	MG	1a	1782	1/1	0.90	0.13	68,68,68,68	0
54	MG	1A	3724	1/1	0.90	0.14	34,34,34,34	0
54	MG	1A	3470	1/1	0.90	0.10	55,55,55,55	0
54	MG	2A	3267	1/1	0.90	0.26	64,64,64,64	0
54	MG	1A	3125	1/1	0.90	0.17	46,46,46,46	0
54	MG	2A	3037	1/1	0.90	0.11	49,49,49,49	0
54	MG	2A	3038	1/1	0.90	0.26	69,69,69,69	0
54	MG	1a	1792	1/1	0.90	0.18	70,70,70,70	0
54	MG	2A	3528	1/1	0.90	0.17	68,68,68,68	0
54	MG	2A	3044	1/1	0.90	0.19	59,59,59,59	0
54	MG	2a	3023	1/1	0.90	0.15	58,58,58,58	0
54	MG	2A	3531	1/1	0.90	0.12	71,71,71,71	0
54	MG	2a	3025	1/1	0.90	0.12	71,71,71,71	0
54	MG	2A	3276	1/1	0.90	0.17	70,70,70,70	0
54	MG	2A	3278	1/1	0.90	0.12	63,63,63,63	0
54	MG	1A	3633	1/1	0.90	0.15	73,73,73,73	0
54	MG	2a	3034	1/1	0.90	0.27	64,64,64,64	0
54	MG	1A	3225	1/1	0.90	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3286	1/1	0.90	0.30	66,66,66,66	0
54	MG	1a	1797	1/1	0.90	0.13	78,78,78,78	0
54	MG	2A	3060	1/1	0.90	0.26	71,71,71,71	0
54	MG	1A	3434	1/1	0.90	0.13	65,65,65,65	0
54	MG	2a	3042	1/1	0.90	0.37	75,75,75,75	0
54	MG	2A	3550	1/1	0.90	0.25	75,75,75,75	0
54	MG	1D	315	1/1	0.90	0.30	51,51,51,51	0
54	MG	2A	3067	1/1	0.90	0.16	63,63,63,63	0
54	MG	2A	3557	1/1	0.90	0.08	40,40,40,40	0
54	MG	2A	3308	1/1	0.90	0.39	68,68,68,68	0
54	MG	1A	3646	1/1	0.90	0.12	32,32,32,32	0
54	MG	1D	318	1/1	0.90	0.16	66,66,66,66	0
54	MG	1A	3166	1/1	0.90	0.17	56,56,56,56	0
54	MG	1a	1806	1/1	0.90	0.10	73,73,73,73	0
54	MG	2A	3580	1/1	0.90	0.11	65,65,65,65	0
54	MG	2A	3581	1/1	0.90	0.20	66,66,66,66	0
54	MG	1E	304	1/1	0.90	0.09	28,28,28,28	0
54	MG	2a	3073	1/1	0.90	0.19	71,71,71,71	0
54	MG	2A	3322	1/1	0.90	0.31	68,68,68,68	0
54	MG	2A	3092	1/1	0.90	0.27	66,66,66,66	0
54	MG	1A	3788	1/1	0.90	0.11	48,48,48,48	0
54	MG	2A	3095	1/1	0.90	0.27	68,68,68,68	0
54	MG	2A	3096	1/1	0.90	0.09	63,63,63,63	0
54	MG	1A	3557	1/1	0.90	0.08	37,37,37,37	0
54	MG	1A	3790	1/1	0.90	0.19	50,50,50,50	0
54	MG	1A	3195	1/1	0.90	0.13	68,68,68,68	0
54	MG	1A	3342	1/1	0.90	0.12	62,62,62,62	0
54	MG	1P	203	1/1	0.90	0.23	77,77,77,77	0
54	MG	1A	3957	1/1	0.90	0.15	50,50,50,50	0
54	MG	1R	204	1/1	0.90	0.15	43,43,43,43	0
54	MG	1A	3795	1/1	0.90	0.14	54,54,54,54	0
54	MG	2A	3627	1/1	0.90	0.20	61,61,61,61	0
54	MG	1a	1834	1/1	0.90	0.20	74,74,74,74	0
54	MG	2A	3630	1/1	0.90	0.19	63,63,63,63	0
54	MG	1a	1709	1/1	0.90	0.41	73,73,73,73	0
54	MG	2A	3356	1/1	0.90	0.19	67,67,67,67	0
54	MG	2A	3357	1/1	0.90	0.16	59,59,59,59	0
54	MG	1a	1838	1/1	0.90	0.09	67,67,67,67	0
54	MG	1A	3489	1/1	0.90	0.12	53,53,53,53	0
54	MG	1W	201	1/1	0.90	0.22	50,50,50,50	0
54	MG	2A	3152	1/1	0.90	0.28	64,64,64,64	0
54	MG	2A	3371	1/1	0.90	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3646	1/1	0.90	0.08	58,58,58,58	0
54	MG	2A	3649	1/1	0.90	0.20	67,67,67,67	0
54	MG	2A	3654	1/1	0.90	0.11	54,54,54,54	0
54	MG	2a	3123	1/1	0.90	0.16	70,70,70,70	0
54	MG	2A	3154	1/1	0.90	0.20	63,63,63,63	0
54	MG	2A	3658	1/1	0.90	0.14	60,60,60,60	0
54	MG	2A	3160	1/1	0.90	0.16	50,50,50,50	0
54	MG	2a	3131	1/1	0.90	0.19	64,64,64,64	0
54	MG	1A	3797	1/1	0.90	0.09	38,38,38,38	0
54	MG	1A	3010	1/1	0.90	0.21	56,56,56,56	0
54	MG	2A	3398	1/1	0.90	0.08	42,42,42,42	0
54	MG	1A	3800	1/1	0.90	0.12	59,59,59,59	0
54	MG	1A	3197	1/1	0.90	0.35	69,69,69,69	0
54	MG	2a	3155	1/1	0.90	0.18	70,70,70,70	0
54	MG	1a	1852	1/1	0.90	0.13	75,75,75,75	0
54	MG	1A	3817	1/1	0.90	0.19	33,33,33,33	0
54	MG	2A	3680	1/1	0.90	0.13	65,65,65,65	0
54	MG	2A	3681	1/1	0.90	0.12	56,56,56,56	0
54	MG	2A	3181	1/1	0.90	0.16	69,69,69,69	0
54	MG	1a	1854	1/1	0.90	0.16	76,76,76,76	0
54	MG	1A	3172	1/1	0.90	0.14	62,62,62,62	0
54	MG	2A	3425	1/1	0.90	0.21	64,64,64,64	0
54	MG	2A	3694	1/1	0.90	0.13	58,58,58,58	0
54	MG	1A	3986	1/1	0.90	0.10	52,52,52,52	0
54	MG	1A	3661	1/1	0.90	0.14	48,48,48,48	0
54	MG	2A	3700	1/1	0.90	0.11	64,64,64,64	0
54	MG	1A	3298	1/1	0.90	0.17	56,56,56,56	0
54	MG	1A	3672	1/1	0.90	0.09	44,44,44,44	0
54	MG	1A	3129	1/1	0.90	0.25	63,63,63,63	0
54	MG	1a	1729	1/1	0.90	0.23	70,70,70,70	0
54	MG	2A	3201	1/1	0.90	0.11	58,58,58,58	0
54	MG	2A	3439	1/1	0.90	0.16	50,50,50,50	0
54	MG	1A	3679	1/1	0.90	0.19	64,64,64,64	0
54	MG	1A	3509	1/1	0.90	0.14	44,44,44,44	0
54	MG	2A	3726	1/1	0.90	0.29	71,71,71,71	0
54	MG	1a	1741	1/1	0.90	0.15	75,75,75,75	0
54	MG	2A	3446	1/1	0.90	0.09	40,40,40,40	0
54	MG	1a	1612	1/1	0.91	0.27	67,67,67,67	0
54	MG	1a	1742	1/1	0.91	0.14	68,68,68,68	0
54	MG	2A	3194	1/1	0.91	0.34	68,68,68,68	0
54	MG	2A	3195	1/1	0.91	0.34	68,68,68,68	0
54	MG	2A	3196	1/1	0.91	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3159	1/1	0.91	0.08	49,49,49,49	0
54	MG	1A	3615	1/1	0.91	0.09	50,50,50,50	0
54	MG	1a	1631	1/1	0.91	0.28	55,55,55,55	0
54	MG	1A	3403	1/1	0.91	0.09	24,24,24,24	0
54	MG	2A	3449	1/1	0.91	0.11	41,41,41,41	0
54	MG	1a	1750	1/1	0.91	0.14	68,68,68,68	0
54	MG	2B	206	1/1	0.91	0.17	73,73,73,73	0
54	MG	1A	3412	1/1	0.91	0.07	44,44,44,44	0
54	MG	2A	3211	1/1	0.91	0.19	59,59,59,59	0
54	MG	1A	3708	1/1	0.91	0.08	45,45,45,45	0
54	MG	1A	3711	1/1	0.91	0.14	54,54,54,54	0
54	MG	1A	3165	1/1	0.91	0.32	66,66,66,66	0
54	MG	1A	3853	1/1	0.91	0.08	57,57,57,57	0
54	MG	1a	1766	1/1	0.91	0.12	68,68,68,68	0
54	MG	1A	3856	1/1	0.91	0.14	58,58,58,58	0
54	MG	1o	101	1/1	0.91	0.32	77,77,77,77	0
54	MG	1A	3554	1/1	0.91	0.08	58,58,58,58	0
54	MG	1A	4016	1/1	0.91	0.12	61,61,61,61	0
54	MG	1A	3047	1/1	0.91	0.28	68,68,68,68	0
54	MG	2A	3483	1/1	0.91	0.10	52,52,52,52	0
54	MG	1A	3262	1/1	0.91	0.17	53,53,53,53	0
54	MG	2A	3231	1/1	0.91	0.24	62,62,62,62	0
54	MG	2A	3007	1/1	0.91	0.11	45,45,45,45	0
54	MG	2A	3236	1/1	0.91	0.11	66,66,66,66	0
54	MG	1A	3057	1/1	0.91	0.14	49,49,49,49	0
54	MG	2A	3243	1/1	0.91	0.33	56,56,56,56	0
54	MG	1A	3729	1/1	0.91	0.11	50,50,50,50	0
54	MG	2A	3495	1/1	0.91	0.13	64,64,64,64	0
54	MG	2A	3030	1/1	0.91	0.14	69,69,69,69	0
54	MG	1A	3280	1/1	0.91	0.16	69,69,69,69	0
54	MG	28	102	1/1	0.91	0.21	64,64,64,64	0
54	MG	1A	3066	1/1	0.91	0.10	56,56,56,56	0
54	MG	1A	3748	1/1	0.91	0.10	38,38,38,38	0
54	MG	1B	214	1/1	0.91	0.09	58,58,58,58	0
54	MG	2A	3509	1/1	0.91	0.13	69,69,69,69	0
54	MG	2a	3007	1/1	0.91	0.11	64,64,64,64	0
54	MG	1a	1791	1/1	0.91	0.07	76,76,76,76	0
54	MG	2A	3512	1/1	0.91	0.14	64,64,64,64	0
54	MG	1A	3757	1/1	0.91	0.13	67,67,67,67	0
54	MG	1A	3440	1/1	0.91	0.14	43,43,43,43	0
54	MG	1A	3654	1/1	0.91	0.27	39,39,39,39	0
54	MG	1A	3585	1/1	0.91	0.21	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3048	1/1	0.91	0.20	58,58,58,58	0
54	MG	2A	3052	1/1	0.91	0.16	54,54,54,54	0
54	MG	1A	3895	1/1	0.91	0.16	63,63,63,63	0
54	MG	2A	3530	1/1	0.91	0.20	66,66,66,66	0
54	MG	2a	3027	1/1	0.91	0.34	72,72,72,72	0
54	MG	1a	1799	1/1	0.91	0.22	81,81,81,81	0
54	MG	2A	3057	1/1	0.91	0.18	52,52,52,52	0
54	MG	2A	3277	1/1	0.91	0.22	61,61,61,61	0
54	MG	1A	3771	1/1	0.91	0.10	57,57,57,57	0
54	MG	1A	3586	1/1	0.91	0.10	43,43,43,43	0
54	MG	2A	3542	1/1	0.91	0.11	66,66,66,66	0
54	MG	2A	3281	1/1	0.91	0.28	74,74,74,74	0
54	MG	1A	3920	1/1	0.91	0.12	55,55,55,55	0
54	MG	1A	3291	1/1	0.91	0.11	72,72,72,72	0
54	MG	2a	3043	1/1	0.91	0.23	66,66,66,66	0
54	MG	2A	3287	1/1	0.91	0.21	65,65,65,65	0
54	MG	2a	3047	1/1	0.91	0.32	68,68,68,68	0
54	MG	1A	3589	1/1	0.91	0.09	61,61,61,61	0
54	MG	2a	3051	1/1	0.91	0.31	73,73,73,73	0
54	MG	2a	3052	1/1	0.91	0.37	67,67,67,67	0
54	MG	2a	3054	1/1	0.91	0.25	72,72,72,72	0
54	MG	2A	3076	1/1	0.91	0.19	55,55,55,55	0
54	MG	1a	1807	1/1	0.91	0.17	61,61,61,61	0
54	MG	1A	3201	1/1	0.91	0.35	48,48,48,48	0
54	MG	2A	3297	1/1	0.91	0.28	61,61,61,61	0
54	MG	2A	3561	1/1	0.91	0.09	58,58,58,58	0
54	MG	2A	3562	1/1	0.91	0.16	58,58,58,58	0
54	MG	2a	3065	1/1	0.91	0.18	70,70,70,70	0
54	MG	2A	3300	1/1	0.91	0.30	69,69,69,69	0
54	MG	2A	3083	1/1	0.91	0.15	62,62,62,62	0
54	MG	2A	3305	1/1	0.91	0.19	66,66,66,66	0
54	MG	2A	3086	1/1	0.91	0.11	52,52,52,52	0
54	MG	2A	3579	1/1	0.91	0.17	67,67,67,67	0
54	MG	1a	1809	1/1	0.91	0.14	74,74,74,74	0
54	MG	2a	3076	1/1	0.91	0.32	57,57,57,57	0
54	MG	1a	1810	1/1	0.91	0.11	65,65,65,65	0
54	MG	1A	3943	1/1	0.91	0.08	51,51,51,51	0
54	MG	2A	3093	1/1	0.91	0.15	70,70,70,70	0
54	MG	2A	3318	1/1	0.91	0.15	63,63,63,63	0
54	MG	2a	3086	1/1	0.91	0.35	64,64,64,64	0
54	MG	1A	3004	1/1	0.91	0.15	53,53,53,53	0
54	MG	1F	315	1/1	0.91	0.24	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3152	1/1	0.91	0.16	69,69,69,69	0
54	MG	2A	3599	1/1	0.91	0.20	62,62,62,62	0
54	MG	2A	3101	1/1	0.91	0.20	57,57,57,57	0
54	MG	1A	3451	1/1	0.91	0.19	64,64,64,64	0
54	MG	2A	3103	1/1	0.91	0.31	66,66,66,66	0
54	MG	1A	3308	1/1	0.91	0.10	47,47,47,47	0
54	MG	1H	202	1/1	0.91	0.08	56,56,56,56	0
54	MG	1N	203	1/1	0.91	0.09	55,55,55,55	0
54	MG	1A	3676	1/1	0.91	0.16	68,68,68,68	0
54	MG	1A	3677	1/1	0.91	0.11	30,30,30,30	0
54	MG	1A	3961	1/1	0.91	0.10	48,48,48,48	0
54	MG	2A	3342	1/1	0.91	0.10	44,44,44,44	0
54	MG	1A	3008	1/1	0.91	0.12	48,48,48,48	0
54	MG	1A	3458	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3965	1/1	0.91	0.11	62,62,62,62	0
54	MG	1A	3681	1/1	0.91	0.16	64,64,64,64	0
54	MG	1A	3978	1/1	0.91	0.13	61,61,61,61	0
54	MG	2A	3141	1/1	0.91	0.15	58,58,58,58	0
54	MG	1A	3219	1/1	0.91	0.11	46,46,46,46	0
54	MG	2A	3151	1/1	0.91	0.34	58,58,58,58	0
54	MG	1a	1846	1/1	0.91	0.10	69,69,69,69	0
54	MG	2a	3124	1/1	0.91	0.10	76,76,76,76	0
54	MG	2A	3644	1/1	0.91	0.16	71,71,71,71	0
54	MG	1A	3821	1/1	0.91	0.09	48,48,48,48	0
54	MG	2A	3158	1/1	0.91	0.11	70,70,70,70	0
54	MG	2A	3372	1/1	0.91	0.09	51,51,51,51	0
54	MG	1a	1848	1/1	0.91	0.11	74,74,74,74	0
54	MG	2A	3377	1/1	0.91	0.09	47,47,47,47	0
54	MG	2A	3387	1/1	0.91	0.14	66,66,66,66	0
54	MG	2A	3662	1/1	0.91	0.14	44,44,44,44	0
54	MG	2a	3152	1/1	0.91	0.19	72,72,72,72	0
54	MG	1A	3692	1/1	0.91	0.09	71,71,71,71	0
54	MG	1A	3694	1/1	0.91	0.07	79,79,79,79	0
54	MG	2A	3395	1/1	0.91	0.22	78,78,78,78	0
54	MG	1A	3987	1/1	0.91	0.08	74,74,74,74	0
54	MG	2A	3674	1/1	0.91	0.18	52,52,52,52	0
54	MG	2A	3397	1/1	0.91	0.11	45,45,45,45	0
54	MG	2A	3165	1/1	0.91	0.18	67,67,67,67	0
54	MG	2a	3169	1/1	0.91	0.08	68,68,68,68	0
54	MG	2a	3170	1/1	0.91	0.19	63,63,63,63	0
54	MG	1A	3988	1/1	0.91	0.11	49,49,49,49	0
54	MG	2A	3172	1/1	0.91	0.14	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3177	1/1	0.91	0.20	76,76,76,76	0
54	MG	1a	1867	1/1	0.91	0.09	59,59,59,59	0
54	MG	19	101	1/1	0.91	0.14	57,57,57,57	0
54	MG	2A	3406	1/1	0.91	0.20	66,66,66,66	0
54	MG	2a	3184	1/1	0.91	0.33	66,66,66,66	0
54	MG	1a	1870	1/1	0.91	0.16	69,69,69,69	0
54	MG	2A	3689	1/1	0.91	0.20	57,57,57,57	0
54	MG	2A	3690	1/1	0.91	0.08	66,66,66,66	0
54	MG	2A	3414	1/1	0.91	0.10	67,67,67,67	0
54	MG	2a	3190	1/1	0.91	0.27	77,77,77,77	0
54	MG	1A	3395	1/1	0.91	0.13	52,52,52,52	0
54	MG	2A	3423	1/1	0.91	0.26	80,80,80,80	0
54	MG	1A	3991	1/1	0.91	0.08	25,25,25,25	0
54	MG	1a	1608	1/1	0.91	0.09	66,66,66,66	0
54	MG	1a	1609	1/1	0.91	0.12	69,69,69,69	0
54	MG	1a	1739	1/1	0.91	0.12	74,74,74,74	0
54	MG	2A	3706	1/1	0.91	0.10	68,68,68,68	0
54	MG	2A	3430	1/1	0.91	0.12	62,62,62,62	0
54	MG	1a	1740	1/1	0.91	0.12	66,66,66,66	0
54	MG	2A	3256	1/1	0.92	0.23	60,60,60,60	0
54	MG	1A	3825	1/1	0.92	0.15	69,69,69,69	0
54	MG	1a	1785	1/1	0.92	0.22	62,62,62,62	0
54	MG	2D	302	1/1	0.92	0.13	57,57,57,57	0
54	MG	1A	3567	1/1	0.92	0.17	61,61,61,61	0
54	MG	1A	3995	1/1	0.92	0.11	61,61,61,61	0
54	MG	2D	312	1/1	0.92	0.19	63,63,63,63	0
54	MG	1A	3034	1/1	0.92	0.09	57,57,57,57	0
54	MG	1A	3452	1/1	0.92	0.07	59,59,59,59	0
54	MG	2A	3498	1/1	0.92	0.10	58,58,58,58	0
54	MG	2A	3058	1/1	0.92	0.11	59,59,59,59	0
54	MG	1A	3365	1/1	0.92	0.14	63,63,63,63	0
54	MG	1A	3836	1/1	0.92	0.11	58,58,58,58	0
54	MG	1A	3071	1/1	0.92	0.36	40,40,40,40	0
54	MG	2A	3504	1/1	0.92	0.35	63,63,63,63	0
54	MG	2A	3505	1/1	0.92	0.14	74,74,74,74	0
54	MG	1A	3371	1/1	0.92	0.07	48,48,48,48	0
54	MG	2Q	201	1/1	0.92	0.17	60,60,60,60	0
54	MG	1A	3583	1/1	0.92	0.07	22,22,22,22	0
54	MG	2A	3072	1/1	0.92	0.20	59,59,59,59	0
54	MG	1A	4010	1/1	0.92	0.14	63,63,63,63	0
54	MG	1A	4011	1/1	0.92	0.16	62,62,62,62	0
54	MG	20	103	1/1	0.92	0.11	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	3517	1/1	0.92	0.16	69,69,69,69	0
54	MG	25	101	1/1	0.92	0.45	48,48,48,48	0
54	MG	1a	1803	1/1	0.92	0.20	67,67,67,67	0
54	MG	2A	3081	1/1	0.92	0.24	70,70,70,70	0
54	MG	28	103	1/1	0.92	0.20	60,60,60,60	0
54	MG	1a	1656	1/1	0.92	0.11	74,74,74,74	0
54	MG	1A	3376	1/1	0.92	0.09	51,51,51,51	0
54	MG	2A	3087	1/1	0.92	0.07	42,42,42,42	0
54	MG	1A	3463	1/1	0.92	0.08	57,57,57,57	0
54	MG	2A	3295	1/1	0.92	0.30	67,67,67,67	0
54	MG	2a	3008	1/1	0.92	0.25	60,60,60,60	0
54	MG	1a	1659	1/1	0.92	0.26	71,71,71,71	0
54	MG	1a	1661	1/1	0.92	0.18	66,66,66,66	0
54	MG	2A	3536	1/1	0.92	0.14	65,65,65,65	0
54	MG	2A	3537	1/1	0.92	0.08	68,68,68,68	0
54	MG	2a	3017	1/1	0.92	0.09	67,67,67,67	0
54	MG	1A	4017	1/1	0.92	0.17	53,53,53,53	0
54	MG	1A	3377	1/1	0.92	0.08	38,38,38,38	0
54	MG	2A	3303	1/1	0.92	0.24	58,58,58,58	0
54	MG	1A	3380	1/1	0.92	0.10	29,29,29,29	0
54	MG	2A	3545	1/1	0.92	0.13	65,65,65,65	0
54	MG	1A	3228	1/1	0.92	0.17	45,45,45,45	0
54	MG	2A	3098	1/1	0.92	0.11	52,52,52,52	0
54	MG	1a	1814	1/1	0.92	0.07	62,62,62,62	0
54	MG	2a	3030	1/1	0.92	0.15	68,68,68,68	0
54	MG	2A	3315	1/1	0.92	0.28	73,73,73,73	0
54	MG	1A	3858	1/1	0.92	0.12	45,45,45,45	0
54	MG	2a	3035	1/1	0.92	0.39	76,76,76,76	0
54	MG	1A	3386	1/1	0.92	0.09	37,37,37,37	0
54	MG	1B	207	1/1	0.92	0.30	63,63,63,63	0
54	MG	2A	3319	1/1	0.92	0.36	66,66,66,66	0
54	MG	1B	209	1/1	0.92	0.12	56,56,56,56	0
54	MG	1A	3073	1/1	0.92	0.12	50,50,50,50	0
54	MG	1A	3316	1/1	0.92	0.39	53,53,53,53	0
54	MG	1A	3598	1/1	0.92	0.09	48,48,48,48	0
54	MG	2a	3044	1/1	0.92	0.19	74,74,74,74	0
54	MG	2a	3045	1/1	0.92	0.16	74,74,74,74	0
54	MG	2A	3566	1/1	0.92	0.09	74,74,74,74	0
54	MG	1B	215	1/1	0.92	0.14	51,51,51,51	0
54	MG	2A	3571	1/1	0.92	0.25	64,64,64,64	0
54	MG	1a	1835	1/1	0.92	0.12	72,72,72,72	0
54	MG	2A	3129	1/1	0.92	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3391	1/1	0.92	0.10	44,44,44,44	0
54	MG	1A	3603	1/1	0.92	0.08	61,61,61,61	0
54	MG	1A	3393	1/1	0.92	0.10	59,59,59,59	0
54	MG	2a	3059	1/1	0.92	0.11	72,72,72,72	0
54	MG	1a	1691	1/1	0.92	0.08	58,58,58,58	0
54	MG	1A	3251	1/1	0.92	0.13	51,51,51,51	0
54	MG	2A	3337	1/1	0.92	0.21	67,67,67,67	0
54	MG	2A	3147	1/1	0.92	0.12	55,55,55,55	0
54	MG	2A	3593	1/1	0.92	0.26	56,56,56,56	0
54	MG	1A	3890	1/1	0.92	0.08	33,33,33,33	0
54	MG	2A	3596	1/1	0.92	0.09	52,52,52,52	0
54	MG	1A	3321	1/1	0.92	0.11	54,54,54,54	0
54	MG	1A	3402	1/1	0.92	0.08	29,29,29,29	0
54	MG	1A	3325	1/1	0.92	0.09	51,51,51,51	0
54	MG	1A	3406	1/1	0.92	0.08	47,47,47,47	0
54	MG	1a	1851	1/1	0.92	0.09	55,55,55,55	0
54	MG	1A	3257	1/1	0.92	0.13	44,44,44,44	0
54	MG	1A	3897	1/1	0.92	0.23	47,47,47,47	0
54	MG	1A	3898	1/1	0.92	0.12	63,63,63,63	0
54	MG	2a	3082	1/1	0.92	0.11	65,65,65,65	0
54	MG	2a	3083	1/1	0.92	0.26	70,70,70,70	0
54	MG	1A	3416	1/1	0.92	0.06	22,22,22,22	0
54	MG	1A	3751	1/1	0.92	0.08	47,47,47,47	0
54	MG	1A	3629	1/1	0.92	0.17	58,58,58,58	0
54	MG	2A	3173	1/1	0.92	0.09	71,71,71,71	0
54	MG	1A	3758	1/1	0.92	0.14	60,60,60,60	0
54	MG	2A	3179	1/1	0.92	0.25	70,70,70,70	0
54	MG	2a	3091	1/1	0.92	0.09	69,69,69,69	0
54	MG	1A	3503	1/1	0.92	0.08	31,31,31,31	0
54	MG	1A	3077	1/1	0.92	0.24	56,56,56,56	0
54	MG	1N	202	1/1	0.92	0.19	51,51,51,51	0
54	MG	1a	1874	1/1	0.92	0.15	83,83,83,83	0
54	MG	2a	3096	1/1	0.92	0.25	76,76,76,76	0
54	MG	1A	3131	1/1	0.92	0.13	40,40,40,40	0
54	MG	2A	3188	1/1	0.92	0.22	73,73,73,73	0
54	MG	1A	3517	1/1	0.92	0.12	43,43,43,43	0
54	MG	1A	3776	1/1	0.92	0.14	57,57,57,57	0
54	MG	2a	3104	1/1	0.92	0.28	60,60,60,60	0
54	MG	1A	3641	1/1	0.92	0.09	28,28,28,28	0
54	MG	1A	3432	1/1	0.92	0.13	32,32,32,32	0
54	MG	2A	3405	1/1	0.92	0.12	73,73,73,73	0
54	MG	1A	3783	1/1	0.92	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3277	1/1	0.92	0.26	59,59,59,59	0
54	MG	1A	3139	1/1	0.92	0.08	50,50,50,50	0
54	MG	1U	202	1/1	0.92	0.41	45,45,45,45	0
54	MG	2a	3114	1/1	0.92	0.31	62,62,62,62	0
54	MG	2A	3667	1/1	0.92	0.10	53,53,53,53	0
54	MG	2A	3197	1/1	0.92	0.11	51,51,51,51	0
54	MG	1V	205	1/1	0.92	0.13	67,67,67,67	0
54	MG	1A	3650	1/1	0.92	0.14	54,54,54,54	0
54	MG	1Y	201	1/1	0.92	0.17	56,56,56,56	0
54	MG	1A	3538	1/1	0.92	0.09	65,65,65,65	0
54	MG	1A	3340	1/1	0.92	0.14	49,49,49,49	0
54	MG	1A	3084	1/1	0.92	0.14	59,59,59,59	0
54	MG	1l	102	1/1	0.92	0.19	59,59,59,59	0
54	MG	2A	3435	1/1	0.92	0.24	50,50,50,50	0
54	MG	2a	3140	1/1	0.92	0.21	71,71,71,71	0
54	MG	1A	3968	1/1	0.92	0.16	57,57,57,57	0
54	MG	2a	3143	1/1	0.92	0.12	70,70,70,70	0
54	MG	1n	102	1/1	0.92	0.15	68,68,68,68	0
54	MG	1A	3975	1/1	0.92	0.11	56,56,56,56	0
54	MG	2a	3150	1/1	0.92	0.19	78,78,78,78	0
54	MG	1A	3289	1/1	0.92	0.19	64,64,64,64	0
54	MG	18	102	1/1	0.92	0.15	46,46,46,46	0
54	MG	1A	3981	1/1	0.92	0.09	80,80,80,80	0
54	MG	1A	3345	1/1	0.92	0.09	29,29,29,29	0
54	MG	2A	3220	1/1	0.92	0.13	57,57,57,57	0
54	MG	2A	3698	1/1	0.92	0.13	67,67,67,67	0
54	MG	2A	3448	1/1	0.92	0.10	57,57,57,57	0
54	MG	2a	3162	1/1	0.92	0.09	62,62,62,62	0
54	MG	1A	3002	1/1	0.92	0.09	48,48,48,48	0
54	MG	2a	3165	1/1	0.92	0.15	68,68,68,68	0
54	MG	2A	3452	1/1	0.92	0.08	39,39,39,39	0
54	MG	2A	3015	1/1	0.92	0.29	76,76,76,76	0
54	MG	1A	3659	1/1	0.92	0.11	40,40,40,40	0
54	MG	2A	3022	1/1	0.92	0.16	67,67,67,67	0
54	MG	2a	3173	1/1	0.92	0.15	69,69,69,69	0
54	MG	2A	3711	1/1	0.92	0.14	66,66,66,66	0
54	MG	1A	3803	1/1	0.92	0.13	59,59,59,59	0
54	MG	2a	3181	1/1	0.92	0.16	77,77,77,77	0
54	MG	1A	3357	1/1	0.92	0.08	44,44,44,44	0
54	MG	2A	3233	1/1	0.92	0.16	66,66,66,66	0
54	MG	2A	3718	1/1	0.92	0.10	65,65,65,65	0
54	MG	2A	3234	1/1	0.92	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1617	1/1	0.92	0.16	67,67,67,67	0
54	MG	2A	3238	1/1	0.92	0.07	60,60,60,60	0
54	MG	1a	1618	1/1	0.92	0.14	63,63,63,63	0
54	MG	1a	1621	1/1	0.92	0.21	59,59,59,59	0
54	MG	2A	3729	1/1	0.92	0.10	62,62,62,62	0
54	MG	1A	3097	1/1	0.92	0.18	57,57,57,57	0
54	MG	1A	3820	1/1	0.92	0.12	65,65,65,65	0
54	MG	2A	3481	1/1	0.92	0.14	60,60,60,60	0
55	HGR	2A	3730	36/36	0.92	0.13	35,49,57,66	0
57	MPD	1A	4024	8/8	0.92	0.20	50,57,60,63	0
54	MG	1a	1780	1/1	0.92	0.13	60,60,60,60	0
54	MG	2B	205	1/1	0.92	0.22	73,73,73,73	0
54	MG	1a	1628	1/1	0.92	0.10	74,74,74,74	0
57	MPD	2A	3733	8/8	0.92	0.17	54,63,65,65	0
54	MG	2A	3487	1/1	0.92	0.11	60,60,60,60	0
54	MG	1A	3563	1/1	0.92	0.09	63,63,63,63	0
54	MG	1A	3605	1/1	0.93	0.17	61,61,61,61	0
54	MG	2B	212	1/1	0.93	0.22	69,69,69,69	0
54	MG	1A	3526	1/1	0.93	0.11	31,31,31,31	0
54	MG	2A	3474	1/1	0.93	0.09	42,42,42,42	0
54	MG	2B	215	1/1	0.93	0.08	80,80,80,80	0
54	MG	2A	3032	1/1	0.93	0.24	60,60,60,60	0
54	MG	2A	3477	1/1	0.93	0.12	50,50,50,50	0
54	MG	1A	3528	1/1	0.93	0.07	42,42,42,42	0
54	MG	2A	3482	1/1	0.93	0.12	63,63,63,63	0
54	MG	1a	1616	1/1	0.93	0.19	79,79,79,79	0
54	MG	2E	304	1/1	0.93	0.27	51,51,51,51	0
54	MG	1A	3107	1/1	0.93	0.18	41,41,41,41	0
54	MG	2E	307	1/1	0.93	0.21	68,68,68,68	0
54	MG	2A	3486	1/1	0.93	0.17	56,56,56,56	0
54	MG	1A	3067	1/1	0.93	0.14	58,58,58,58	0
54	MG	2A	3245	1/1	0.93	0.17	64,64,64,64	0
54	MG	1a	1776	1/1	0.93	0.16	65,65,65,65	0
54	MG	1a	1620	1/1	0.93	0.07	68,68,68,68	0
54	MG	1A	3837	1/1	0.93	0.10	59,59,59,59	0
54	MG	2A	3043	1/1	0.93	0.17	54,54,54,54	0
54	MG	1a	1779	1/1	0.93	0.20	71,71,71,71	0
54	MG	2P	201	1/1	0.93	0.22	64,64,64,64	0
54	MG	1A	3534	1/1	0.93	0.07	24,24,24,24	0
54	MG	1A	3224	1/1	0.93	0.22	41,41,41,41	0
54	MG	1A	3068	1/1	0.93	0.12	46,46,46,46	0
54	MG	2R	201	1/1	0.93	0.28	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	2R	202	1/1	0.93	0.14	53,53,53,53	0
54	MG	1a	1629	1/1	0.93	0.24	65,65,65,65	0
54	MG	2T	204	1/1	0.93	0.08	48,48,48,48	0
54	MG	1A	3710	1/1	0.93	0.11	46,46,46,46	0
54	MG	1A	3347	1/1	0.93	0.21	55,55,55,55	0
54	MG	20	101	1/1	0.93	0.10	55,55,55,55	0
54	MG	1a	1787	1/1	0.93	0.14	71,71,71,71	0
54	MG	1a	1789	1/1	0.93	0.20	55,55,55,55	0
54	MG	1A	4013	1/1	0.93	0.24	42,42,42,42	0
54	MG	1A	3713	1/1	0.93	0.15	58,58,58,58	0
54	MG	2A	3064	1/1	0.93	0.08	45,45,45,45	0
54	MG	2A	3511	1/1	0.93	0.24	68,68,68,68	0
54	MG	2A	3065	1/1	0.93	0.08	56,56,56,56	0
54	MG	1A	3627	1/1	0.93	0.16	49,49,49,49	0
54	MG	1A	3628	1/1	0.93	0.15	39,39,39,39	0
54	MG	1a	1795	1/1	0.93	0.07	74,74,74,74	0
54	MG	2A	3073	1/1	0.93	0.24	67,67,67,67	0
54	MG	2A	3074	1/1	0.93	0.20	54,54,54,54	0
54	MG	1A	4019	1/1	0.93	0.21	84,84,84,84	0
54	MG	2A	3077	1/1	0.93	0.11	59,59,59,59	0
54	MG	1A	4020	1/1	0.93	0.12	65,65,65,65	0
54	MG	1A	3719	1/1	0.93	0.09	70,70,70,70	0
54	MG	2a	3016	1/1	0.93	0.11	60,60,60,60	0
54	MG	1A	3405	1/1	0.93	0.08	41,41,41,41	0
54	MG	2a	3019	1/1	0.93	0.22	60,60,60,60	0
54	MG	2A	3292	1/1	0.93	0.12	64,64,64,64	0
54	MG	2A	3293	1/1	0.93	0.39	79,79,79,79	0
54	MG	1A	3070	1/1	0.93	0.29	45,45,45,45	0
54	MG	1A	3407	1/1	0.93	0.07	40,40,40,40	0
54	MG	1A	3726	1/1	0.93	0.08	66,66,66,66	0
54	MG	2A	3299	1/1	0.93	0.08	50,50,50,50	0
54	MG	1A	3727	1/1	0.93	0.23	43,43,43,43	0
54	MG	1A	3550	1/1	0.93	0.08	62,62,62,62	0
54	MG	1A	3638	1/1	0.93	0.11	35,35,35,35	0
54	MG	2A	3304	1/1	0.93	0.25	61,61,61,61	0
54	MG	2a	3033	1/1	0.93	0.17	71,71,71,71	0
54	MG	2A	3547	1/1	0.93	0.18	57,57,57,57	0
54	MG	1A	3738	1/1	0.93	0.12	70,70,70,70	0
54	MG	1A	3234	1/1	0.93	0.11	55,55,55,55	0
54	MG	2A	3310	1/1	0.93	0.35	65,65,65,65	0
54	MG	2A	3552	1/1	0.93	0.22	65,65,65,65	0
54	MG	1A	3747	1/1	0.93	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3300	1/1	0.93	0.13	59,59,59,59	0
54	MG	2A	3555	1/1	0.93	0.10	63,63,63,63	0
54	MG	2A	3556	1/1	0.93	0.20	66,66,66,66	0
54	MG	2A	3314	1/1	0.93	0.27	61,61,61,61	0
54	MG	1B	218	1/1	0.93	0.07	47,47,47,47	0
54	MG	1A	3645	1/1	0.93	0.08	43,43,43,43	0
54	MG	1B	221	1/1	0.93	0.11	61,61,61,61	0
54	MG	1a	1815	1/1	0.93	0.12	69,69,69,69	0
54	MG	2a	3049	1/1	0.93	0.26	59,59,59,59	0
54	MG	2a	3050	1/1	0.93	0.19	76,76,76,76	0
54	MG	2A	3104	1/1	0.93	0.15	66,66,66,66	0
54	MG	2A	3107	1/1	0.93	0.11	57,57,57,57	0
54	MG	2a	3053	1/1	0.93	0.23	61,61,61,61	0
54	MG	2A	3108	1/1	0.93	0.14	67,67,67,67	0
54	MG	1A	3754	1/1	0.93	0.16	48,48,48,48	0
54	MG	1A	3092	1/1	0.93	0.09	50,50,50,50	0
54	MG	1A	3199	1/1	0.93	0.27	67,67,67,67	0
54	MG	2A	3115	1/1	0.93	0.21	72,72,72,72	0
54	MG	2A	3117	1/1	0.93	0.20	58,58,58,58	0
54	MG	1A	3761	1/1	0.93	0.09	29,29,29,29	0
54	MG	1A	3902	1/1	0.93	0.11	58,58,58,58	0
54	MG	2a	3064	1/1	0.93	0.35	75,75,75,75	0
54	MG	2A	3586	1/1	0.93	0.10	46,46,46,46	0
54	MG	1A	3570	1/1	0.93	0.17	58,58,58,58	0
54	MG	1a	1829	1/1	0.93	0.07	72,72,72,72	0
54	MG	1A	3427	1/1	0.93	0.18	52,52,52,52	0
54	MG	2A	3130	1/1	0.93	0.19	66,66,66,66	0
54	MG	2A	3341	1/1	0.93	0.15	59,59,59,59	0
54	MG	1a	1833	1/1	0.93	0.24	73,73,73,73	0
54	MG	1A	3256	1/1	0.93	0.21	51,51,51,51	0
54	MG	2a	3078	1/1	0.93	0.08	63,63,63,63	0
54	MG	1A	3653	1/1	0.93	0.18	66,66,66,66	0
54	MG	2A	3349	1/1	0.93	0.13	54,54,54,54	0
54	MG	1D	320	1/1	0.93	0.08	52,52,52,52	0
54	MG	1A	3773	1/1	0.93	0.13	45,45,45,45	0
54	MG	2A	3352	1/1	0.93	0.09	45,45,45,45	0
54	MG	2A	3353	1/1	0.93	0.07	49,49,49,49	0
54	MG	1A	3368	1/1	0.93	0.12	62,62,62,62	0
54	MG	1a	1693	1/1	0.93	0.10	74,74,74,74	0
54	MG	1E	306	1/1	0.93	0.13	54,54,54,54	0
54	MG	2A	3628	1/1	0.93	0.16	63,63,63,63	0
54	MG	1E	308	1/1	0.93	0.08	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	1F	313	1/1	0.93	0.09	49,49,49,49	0
54	MG	2A	3367	1/1	0.93	0.09	56,56,56,56	0
54	MG	2A	3155	1/1	0.93	0.27	60,60,60,60	0
54	MG	2A	3156	1/1	0.93	0.13	57,57,57,57	0
54	MG	1a	1699	1/1	0.93	0.25	66,66,66,66	0
54	MG	1a	1700	1/1	0.93	0.36	67,67,67,67	0
54	MG	2A	3639	1/1	0.93	0.09	54,54,54,54	0
54	MG	1A	3777	1/1	0.93	0.07	40,40,40,40	0
54	MG	2A	3382	1/1	0.93	0.07	36,36,36,36	0
54	MG	2A	3385	1/1	0.93	0.08	36,36,36,36	0
54	MG	1a	1849	1/1	0.93	0.23	63,63,63,63	0
54	MG	2A	3645	1/1	0.93	0.21	61,61,61,61	0
54	MG	1A	3944	1/1	0.93	0.10	60,60,60,60	0
54	MG	1A	3132	1/1	0.93	0.14	53,53,53,53	0
54	MG	2A	3652	1/1	0.93	0.12	64,64,64,64	0
54	MG	1A	3579	1/1	0.93	0.12	62,62,62,62	0
54	MG	1A	3492	1/1	0.93	0.06	26,26,26,26	0
54	MG	2A	3657	1/1	0.93	0.11	61,61,61,61	0
54	MG	1A	3950	1/1	0.93	0.14	70,70,70,70	0
54	MG	1A	3261	1/1	0.93	0.32	71,71,71,71	0
54	MG	1A	3014	1/1	0.93	0.19	62,62,62,62	0
54	MG	1A	3265	1/1	0.93	0.07	76,76,76,76	0
54	MG	2a	3121	1/1	0.93	0.12	62,62,62,62	0
54	MG	1A	3791	1/1	0.93	0.09	50,50,50,50	0
54	MG	1A	3208	1/1	0.93	0.30	67,67,67,67	0
54	MG	1A	3663	1/1	0.93	0.07	54,54,54,54	0
54	MG	1R	207	1/1	0.93	0.14	57,57,57,57	0
54	MG	2a	3127	1/1	0.93	0.19	58,58,58,58	0
54	MG	2a	3128	1/1	0.93	0.10	67,67,67,67	0
54	MG	2A	3673	1/1	0.93	0.09	52,52,52,52	0
54	MG	2A	3409	1/1	0.93	0.14	69,69,69,69	0
54	MG	2a	3136	1/1	0.93	0.11	72,72,72,72	0
54	MG	1A	3329	1/1	0.93	0.10	44,44,44,44	0
54	MG	1a	1877	1/1	0.93	0.10	58,58,58,58	0
54	MG	2a	3141	1/1	0.93	0.10	60,60,60,60	0
54	MG	2A	3416	1/1	0.93	0.25	63,63,63,63	0
54	MG	2A	3419	1/1	0.93	0.07	44,44,44,44	0
54	MG	1A	3665	1/1	0.93	0.07	39,39,39,39	0
54	MG	2A	3422	1/1	0.93	0.10	52,52,52,52	0
54	MG	1a	1721	1/1	0.93	0.33	82,82,82,82	0
54	MG	2a	3151	1/1	0.93	0.12	80,80,80,80	0
54	MG	2A	3686	1/1	0.93	0.12	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3505	1/1	0.93	0.07	44,44,44,44	0
54	MG	1a	1723	1/1	0.93	0.10	51,51,51,51	0
54	MG	1b	301	1/1	0.93	0.11	78,78,78,78	0
54	MG	2A	3691	1/1	0.93	0.17	45,45,45,45	0
54	MG	1V	204	1/1	0.93	0.12	57,57,57,57	0
54	MG	1A	3035	1/1	0.93	0.10	45,45,45,45	0
54	MG	2a	3161	1/1	0.93	0.09	65,65,65,65	0
54	MG	1A	3511	1/1	0.93	0.15	59,59,59,59	0
54	MG	2A	3199	1/1	0.93	0.15	62,62,62,62	0
54	MG	2A	3434	1/1	0.93	0.07	44,44,44,44	0
54	MG	2a	3166	1/1	0.93	0.16	72,72,72,72	0
54	MG	1A	3106	1/1	0.93	0.11	42,42,42,42	0
54	MG	2A	3701	1/1	0.93	0.08	55,55,55,55	0
54	MG	1a	1730	1/1	0.93	0.14	63,63,63,63	0
54	MG	1A	3804	1/1	0.93	0.14	60,60,60,60	0
54	MG	2A	3206	1/1	0.93	0.28	64,64,64,64	0
54	MG	2a	3174	1/1	0.93	0.20	64,64,64,64	0
54	MG	1A	3806	1/1	0.93	0.07	55,55,55,55	0
54	MG	2A	3710	1/1	0.93	0.07	46,46,46,46	0
54	MG	1A	3814	1/1	0.93	0.09	63,63,63,63	0
54	MG	1A	3281	1/1	0.93	0.12	64,64,64,64	0
54	MG	1A	3599	1/1	0.93	0.15	66,66,66,66	0
54	MG	13	102	1/1	0.93	0.25	61,61,61,61	0
54	MG	2a	3185	1/1	0.93	0.23	71,71,71,71	0
54	MG	2A	3447	1/1	0.93	0.14	63,63,63,63	0
54	MG	1A	3520	1/1	0.93	0.09	27,27,27,27	0
54	MG	2A	3724	1/1	0.93	0.21	63,63,63,63	0
54	MG	1A	3392	1/1	0.93	0.11	75,75,75,75	0
54	MG	1a	1745	1/1	0.93	0.12	78,78,78,78	0
54	MG	15	107	1/1	0.93	0.08	57,57,57,57	0
54	MG	17	105	1/1	0.93	0.21	64,64,64,64	0
54	MG	2e	201	1/1	0.93	0.35	72,72,72,72	0
54	MG	1A	3990	1/1	0.93	0.07	55,55,55,55	0
54	MG	1A	3689	1/1	0.93	0.07	69,69,69,69	0
54	MG	1A	3827	1/1	0.93	0.15	42,42,42,42	0
54	MG	1A	3993	1/1	0.93	0.12	40,40,40,40	0
54	MG	2A	3226	1/1	0.93	0.18	42,42,42,42	0
54	MG	2A	3018	1/1	0.93	0.34	54,54,54,54	0
54	MG	1a	1758	1/1	0.93	0.20	49,49,49,49	0
54	MG	2B	207	1/1	0.93	0.18	72,72,72,72	0
54	MG	1a	1605	1/1	0.93	0.23	72,72,72,72	0
58	ARG	1B	230	12/12	0.93	0.10	34,54,66,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2B	209	1/1	0.93	0.10	69,69,69,69	0
54	MG	2A	3150	1/1	0.94	0.20	72,72,72,72	0
54	MG	1a	1630	1/1	0.94	0.10	62,62,62,62	0
54	MG	1A	3535	1/1	0.94	0.12	53,53,53,53	0
54	MG	2A	3153	1/1	0.94	0.11	46,46,46,46	0
54	MG	1a	1632	1/1	0.94	0.23	59,59,59,59	0
54	MG	1A	3017	1/1	0.94	0.23	36,36,36,36	0
54	MG	1a	1635	1/1	0.94	0.12	57,57,57,57	0
54	MG	1a	1816	1/1	0.94	0.13	68,68,68,68	0
54	MG	1A	3541	1/1	0.94	0.33	39,39,39,39	0
54	MG	2A	3161	1/1	0.94	0.10	66,66,66,66	0
54	MG	1A	3108	1/1	0.94	0.07	43,43,43,43	0
54	MG	1a	1638	1/1	0.94	0.17	51,51,51,51	0
54	MG	1a	1822	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3349	1/1	0.94	0.08	29,29,29,29	0
54	MG	2A	3169	1/1	0.94	0.17	61,61,61,61	0
54	MG	1A	3441	1/1	0.94	0.11	27,27,27,27	0
54	MG	1A	3200	1/1	0.94	0.28	44,44,44,44	0
54	MG	1A	3998	1/1	0.94	0.06	57,57,57,57	0
54	MG	2A	3176	1/1	0.94	0.12	60,60,60,60	0
54	MG	2B	216	1/1	0.94	0.09	59,59,59,59	0
54	MG	1A	3268	1/1	0.94	0.30	40,40,40,40	0
54	MG	1a	1832	1/1	0.94	0.11	70,70,70,70	0
54	MG	2D	304	1/1	0.94	0.17	57,57,57,57	0
54	MG	2D	307	1/1	0.94	0.28	44,44,44,44	0
54	MG	1a	1645	1/1	0.94	0.22	62,62,62,62	0
54	MG	1A	3805	1/1	0.94	0.20	64,64,64,64	0
54	MG	1A	3110	1/1	0.94	0.12	61,61,61,61	0
54	MG	1A	4002	1/1	0.94	0.08	62,62,62,62	0
54	MG	1A	3809	1/1	0.94	0.09	63,63,63,63	0
54	MG	2A	3187	1/1	0.94	0.11	64,64,64,64	0
54	MG	1A	4005	1/1	0.94	0.13	69,69,69,69	0
54	MG	1A	3811	1/1	0.94	0.23	41,41,41,41	0
54	MG	1A	3812	1/1	0.94	0.12	67,67,67,67	0
54	MG	1A	4009	1/1	0.94	0.14	61,61,61,61	0
54	MG	2A	3465	1/1	0.94	0.15	45,45,45,45	0
54	MG	1A	3552	1/1	0.94	0.18	68,68,68,68	0
54	MG	1A	3202	1/1	0.94	0.09	50,50,50,50	0
54	MG	1a	1663	1/1	0.94	0.15	68,68,68,68	0
54	MG	1A	3204	1/1	0.94	0.10	54,54,54,54	0
54	MG	1A	4014	1/1	0.94	0.08	52,52,52,52	0
54	MG	2A	3473	1/1	0.94	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	1a	1850	1/1	0.94	0.11	75,75,75,75	0
54	MG	2Q	203	1/1	0.94	0.18	64,64,64,64	0
54	MG	2A	3198	1/1	0.94	0.16	65,65,65,65	0
54	MG	1a	1668	1/1	0.94	0.33	60,60,60,60	0
54	MG	2A	3479	1/1	0.94	0.09	55,55,55,55	0
54	MG	2A	3480	1/1	0.94	0.10	62,62,62,62	0
54	MG	2U	201	1/1	0.94	0.05	65,65,65,65	0
54	MG	1a	1669	1/1	0.94	0.19	62,62,62,62	0
54	MG	2A	3202	1/1	0.94	0.22	48,48,48,48	0
54	MG	2Y	201	1/1	0.94	0.16	71,71,71,71	0
54	MG	1A	3560	1/1	0.94	0.13	52,52,52,52	0
54	MG	1a	1671	1/1	0.94	0.14	66,66,66,66	0
54	MG	1a	1858	1/1	0.94	0.10	72,72,72,72	0
54	MG	1A	3666	1/1	0.94	0.18	61,61,61,61	0
54	MG	25	103	1/1	0.94	0.10	61,61,61,61	0
54	MG	1a	1673	1/1	0.94	0.19	62,62,62,62	0
54	MG	1A	3822	1/1	0.94	0.05	40,40,40,40	0
54	MG	1A	4018	1/1	0.94	0.10	52,52,52,52	0
54	MG	2a	3001	1/1	0.94	0.09	47,47,47,47	0
54	MG	1A	3116	1/1	0.94	0.09	46,46,46,46	0
54	MG	2A	3492	1/1	0.94	0.10	49,49,49,49	0
54	MG	2a	3004	1/1	0.94	0.09	58,58,58,58	0
54	MG	1a	1679	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	3087	1/1	0.94	0.43	41,41,41,41	0
54	MG	1a	1682	1/1	0.94	0.08	66,66,66,66	0
54	MG	1A	3674	1/1	0.94	0.12	68,68,68,68	0
54	MG	2a	3009	1/1	0.94	0.07	76,76,76,76	0
54	MG	2A	3217	1/1	0.94	0.13	58,58,58,58	0
54	MG	1A	3675	1/1	0.94	0.06	19,19,19,19	0
54	MG	1A	3210	1/1	0.94	0.22	52,52,52,52	0
54	MG	1a	1687	1/1	0.94	0.15	60,60,60,60	0
54	MG	2a	3015	1/1	0.94	0.16	62,62,62,62	0
54	MG	1A	3571	1/1	0.94	0.08	42,42,42,42	0
54	MG	2A	3503	1/1	0.94	0.08	56,56,56,56	0
54	MG	1A	3572	1/1	0.94	0.10	54,54,54,54	0
54	MG	2A	3225	1/1	0.94	0.09	53,53,53,53	0
54	MG	1A	3168	1/1	0.94	0.12	49,49,49,49	0
54	MG	1A	3460	1/1	0.94	0.11	50,50,50,50	0
54	MG	1A	3216	1/1	0.94	0.39	45,45,45,45	0
54	MG	1d	303	1/1	0.94	0.21	71,71,71,71	0
54	MG	1A	3577	1/1	0.94	0.08	60,60,60,60	0
54	MG	1A	3691	1/1	0.94	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1695	1/1	0.94	0.07	68,68,68,68	0
54	MG	1A	3843	1/1	0.94	0.07	48,48,48,48	0
54	MG	1A	3169	1/1	0.94	0.09	32,32,32,32	0
54	MG	1h	201	1/1	0.94	0.20	62,62,62,62	0
54	MG	2A	3526	1/1	0.94	0.08	44,44,44,44	0
54	MG	2A	3242	1/1	0.94	0.17	64,64,64,64	0
54	MG	1A	3218	1/1	0.94	0.40	42,42,42,42	0
54	MG	2A	3244	1/1	0.94	0.08	62,62,62,62	0
54	MG	1A	3060	1/1	0.94	0.08	54,54,54,54	0
54	MG	1A	3128	1/1	0.94	0.15	53,53,53,53	0
54	MG	1a	1702	1/1	0.94	0.37	66,66,66,66	0
54	MG	2A	3535	1/1	0.94	0.07	63,63,63,63	0
54	MG	1m	201	1/1	0.94	0.07	74,74,74,74	0
54	MG	1A	3309	1/1	0.94	0.22	63,63,63,63	0
54	MG	2A	3252	1/1	0.94	0.18	61,61,61,61	0
54	MG	1A	3701	1/1	0.94	0.15	66,66,66,66	0
54	MG	1A	3223	1/1	0.94	0.08	57,57,57,57	0
54	MG	1A	3475	1/1	0.94	0.08	29,29,29,29	0
54	MG	1a	1708	1/1	0.94	0.24	62,62,62,62	0
54	MG	1A	3868	1/1	0.94	0.11	49,49,49,49	0
54	MG	1D	307	1/1	0.94	0.19	48,48,48,48	0
54	MG	2A	3004	1/1	0.94	0.10	67,67,67,67	0
54	MG	2A	3268	1/1	0.94	0.18	55,55,55,55	0
54	MG	1A	3062	1/1	0.94	0.18	42,42,42,42	0
54	MG	2A	3009	1/1	0.94	0.15	58,58,58,58	0
54	MG	2a	3056	1/1	0.94	0.16	71,71,71,71	0
54	MG	1a	1712	1/1	0.94	0.38	73,73,73,73	0
54	MG	1D	313	1/1	0.94	0.18	40,40,40,40	0
54	MG	1A	3875	1/1	0.94	0.08	47,47,47,47	0
54	MG	1A	3877	1/1	0.94	0.11	60,60,60,60	0
54	MG	1D	317	1/1	0.94	0.11	68,68,68,68	0
54	MG	2A	3024	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3027	1/1	0.94	0.17	57,57,57,57	0
54	MG	1A	3878	1/1	0.94	0.08	33,33,33,33	0
54	MG	2A	3282	1/1	0.94	0.34	70,70,70,70	0
54	MG	2A	3031	1/1	0.94	0.13	52,52,52,52	0
54	MG	2a	3068	1/1	0.94	0.07	81,81,81,81	0
54	MG	1A	3590	1/1	0.94	0.08	26,26,26,26	0
54	MG	2a	3071	1/1	0.94	0.10	67,67,67,67	0
54	MG	1a	1719	1/1	0.94	0.26	70,70,70,70	0
54	MG	2A	3569	1/1	0.94	0.17	70,70,70,70	0
54	MG	2A	3570	1/1	0.94	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3181	1/1	0.94	0.14	53,53,53,53	0
54	MG	2a	3077	1/1	0.94	0.17	72,72,72,72	0
54	MG	2A	3572	1/1	0.94	0.09	63,63,63,63	0
54	MG	1A	3319	1/1	0.94	0.12	44,44,44,44	0
54	MG	1A	3481	1/1	0.94	0.09	53,53,53,53	0
54	MG	1A	3596	1/1	0.94	0.30	60,60,60,60	0
54	MG	1F	312	1/1	0.94	0.37	51,51,51,51	0
54	MG	2A	3040	1/1	0.94	0.15	52,52,52,52	0
54	MG	1A	3227	1/1	0.94	0.13	46,46,46,46	0
54	MG	1a	1727	1/1	0.94	0.19	72,72,72,72	0
54	MG	2A	3298	1/1	0.94	0.38	66,66,66,66	0
54	MG	1A	3487	1/1	0.94	0.08	57,57,57,57	0
54	MG	1A	3721	1/1	0.94	0.11	47,47,47,47	0
54	MG	2A	3301	1/1	0.94	0.31	57,57,57,57	0
54	MG	2A	3594	1/1	0.94	0.12	56,56,56,56	0
54	MG	1A	3398	1/1	0.94	0.18	61,61,61,61	0
54	MG	2A	3049	1/1	0.94	0.26	66,66,66,66	0
54	MG	2A	3597	1/1	0.94	0.07	49,49,49,49	0
54	MG	1G	204	1/1	0.94	0.08	56,56,56,56	0
54	MG	2A	3603	1/1	0.94	0.08	62,62,62,62	0
54	MG	2A	3607	1/1	0.94	0.05	70,70,70,70	0
54	MG	2a	3099	1/1	0.94	0.26	64,64,64,64	0
54	MG	1A	3399	1/1	0.94	0.12	58,58,58,58	0
54	MG	1A	3896	1/1	0.94	0.16	40,40,40,40	0
54	MG	2A	3612	1/1	0.94	0.09	69,69,69,69	0
54	MG	2A	3309	1/1	0.94	0.42	53,53,53,53	0
54	MG	2A	3055	1/1	0.94	0.24	65,65,65,65	0
54	MG	2a	3107	1/1	0.94	0.31	53,53,53,53	0
54	MG	2A	3617	1/1	0.94	0.07	65,65,65,65	0
54	MG	1A	3725	1/1	0.94	0.17	51,51,51,51	0
54	MG	2A	3620	1/1	0.94	0.08	44,44,44,44	0
54	MG	1A	3322	1/1	0.94	0.18	62,62,62,62	0
54	MG	1A	3493	1/1	0.94	0.07	31,31,31,31	0
54	MG	1A	3910	1/1	0.94	0.13	38,38,38,38	0
54	MG	2A	3625	1/1	0.94	0.08	56,56,56,56	0
54	MG	1P	201	1/1	0.94	0.27	39,39,39,39	0
54	MG	1A	3038	1/1	0.94	0.24	58,58,58,58	0
54	MG	1A	3496	1/1	0.94	0.11	39,39,39,39	0
54	MG	2a	3120	1/1	0.94	0.11	65,65,65,65	0
54	MG	1R	203	1/1	0.94	0.21	53,53,53,53	0
54	MG	1A	3737	1/1	0.94	0.12	48,48,48,48	0
54	MG	1R	205	1/1	0.94	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3232	1/1	0.94	0.13	40,40,40,40	0
54	MG	1A	3743	1/1	0.94	0.12	67,67,67,67	0
54	MG	2A	3636	1/1	0.94	0.11	56,56,56,56	0
54	MG	2A	3075	1/1	0.94	0.16	55,55,55,55	0
54	MG	1A	3937	1/1	0.94	0.11	68,68,68,68	0
54	MG	2a	3130	1/1	0.94	0.10	79,79,79,79	0
54	MG	1T	203	1/1	0.94	0.06	70,70,70,70	0
54	MG	1A	3612	1/1	0.94	0.08	56,56,56,56	0
54	MG	2A	3642	1/1	0.94	0.09	74,74,74,74	0
54	MG	1A	3499	1/1	0.94	0.08	29,29,29,29	0
54	MG	1A	3051	1/1	0.94	0.29	56,56,56,56	0
54	MG	2A	3082	1/1	0.94	0.10	46,46,46,46	0
54	MG	1A	3101	1/1	0.94	0.23	42,42,42,42	0
54	MG	1A	3411	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3339	1/1	0.94	0.08	50,50,50,50	0
54	MG	2a	3148	1/1	0.94	0.13	78,78,78,78	0
54	MG	1A	3948	1/1	0.94	0.07	30,30,30,30	0
54	MG	1A	3756	1/1	0.94	0.19	67,67,67,67	0
54	MG	1A	3504	1/1	0.94	0.06	31,31,31,31	0
54	MG	2A	3091	1/1	0.94	0.14	60,60,60,60	0
54	MG	10	108	1/1	0.94	0.08	60,60,60,60	0
54	MG	1A	3954	1/1	0.94	0.07	29,29,29,29	0
54	MG	1A	3956	1/1	0.94	0.10	59,59,59,59	0
54	MG	1A	3623	1/1	0.94	0.15	33,33,33,33	0
54	MG	1A	3330	1/1	0.94	0.08	52,52,52,52	0
54	MG	2A	3355	1/1	0.94	0.07	42,42,42,42	0
54	MG	1A	3959	1/1	0.94	0.07	71,71,71,71	0
54	MG	1A	3331	1/1	0.94	0.10	54,54,54,54	0
54	MG	1A	3763	1/1	0.94	0.11	46,46,46,46	0
54	MG	17	106	1/1	0.94	0.08	50,50,50,50	0
54	MG	2a	3168	1/1	0.94	0.14	66,66,66,66	0
54	MG	2A	3360	1/1	0.94	0.10	45,45,45,45	0
54	MG	1a	1788	1/1	0.94	0.12	74,74,74,74	0
54	MG	1A	3417	1/1	0.94	0.07	26,26,26,26	0
54	MG	1A	3420	1/1	0.94	0.07	32,32,32,32	0
54	MG	2A	3109	1/1	0.94	0.11	59,59,59,59	0
54	MG	2A	3110	1/1	0.94	0.08	69,69,69,69	0
54	MG	1A	3143	1/1	0.94	0.05	30,30,30,30	0
54	MG	1a	1602	1/1	0.94	0.10	79,79,79,79	0
54	MG	1A	3519	1/1	0.94	0.06	46,46,46,46	0
54	MG	2A	3383	1/1	0.94	0.07	48,48,48,48	0
54	MG	1A	3253	1/1	0.94	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3116	1/1	0.94	0.09	57,57,57,57	0
54	MG	1A	3970	1/1	0.94	0.08	53,53,53,53	0
54	MG	1A	3425	1/1	0.94	0.08	31,31,31,31	0
54	MG	2A	3697	1/1	0.94	0.09	66,66,66,66	0
54	MG	1A	3078	1/1	0.94	0.35	42,42,42,42	0
54	MG	1a	1615	1/1	0.94	0.09	63,63,63,63	0
54	MG	1a	1800	1/1	0.94	0.10	70,70,70,70	0
54	MG	1A	3980	1/1	0.94	0.15	56,56,56,56	0
54	MG	1A	3643	1/1	0.94	0.08	47,47,47,47	0
54	MG	1A	3527	1/1	0.94	0.11	27,27,27,27	0
54	MG	2A	3705	1/1	0.94	0.09	79,79,79,79	0
54	MG	1A	3787	1/1	0.94	0.10	60,60,60,60	0
54	MG	2t	201	1/1	0.94	0.19	53,53,53,53	0
54	MG	1A	3150	1/1	0.94	0.08	56,56,56,56	0
54	MG	1A	3433	1/1	0.94	0.13	27,27,27,27	0
54	MG	1A	3648	1/1	0.94	0.07	39,39,39,39	0
54	MG	2A	3143	1/1	0.94	0.19	49,49,49,49	0
54	MG	2A	3144	1/1	0.94	0.13	65,65,65,65	0
54	MG	2A	3146	1/1	0.94	0.14	43,43,43,43	0
54	MG	1A	3258	1/1	0.94	0.09	48,48,48,48	0
54	MG	2A	3417	1/1	0.94	0.13	57,57,57,57	0
54	MG	1A	3260	1/1	0.94	0.24	65,65,65,65	0
54	MG	1Q	203	1/1	0.95	0.08	50,50,50,50	0
54	MG	2A	3454	1/1	0.95	0.08	55,55,55,55	0
54	MG	1A	3556	1/1	0.95	0.06	39,39,39,39	0
54	MG	2A	3458	1/1	0.95	0.11	51,51,51,51	0
54	MG	1A	3775	1/1	0.95	0.07	57,57,57,57	0
54	MG	1A	3465	1/1	0.95	0.10	52,52,52,52	0
54	MG	1R	206	1/1	0.95	0.11	34,34,34,34	0
54	MG	1A	3235	1/1	0.95	0.12	36,36,36,36	0
54	MG	1A	3952	1/1	0.95	0.07	41,41,41,41	0
54	MG	1A	3469	1/1	0.95	0.07	63,63,63,63	0
54	MG	1A	3955	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3779	1/1	0.95	0.11	55,55,55,55	0
54	MG	1A	3565	1/1	0.95	0.21	37,37,37,37	0
54	MG	1A	3237	1/1	0.95	0.23	41,41,41,41	0
54	MG	2A	3005	1/1	0.95	0.09	60,60,60,60	0
54	MG	2D	305	1/1	0.95	0.41	50,50,50,50	0
54	MG	2D	306	1/1	0.95	0.10	61,61,61,61	0
54	MG	2A	3222	1/1	0.95	0.10	57,57,57,57	0
54	MG	2A	3223	1/1	0.95	0.10	69,69,69,69	0
54	MG	1V	206	1/1	0.95	0.09	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	3568	1/1	0.95	0.11	59,59,59,59	0
54	MG	2A	3478	1/1	0.95	0.08	64,64,64,64	0
54	MG	2A	3011	1/1	0.95	0.15	69,69,69,69	0
54	MG	2A	3227	1/1	0.95	0.15	62,62,62,62	0
54	MG	1a	1731	1/1	0.95	0.09	57,57,57,57	0
54	MG	1A	3569	1/1	0.95	0.09	54,54,54,54	0
54	MG	1A	3149	1/1	0.95	0.32	35,35,35,35	0
54	MG	2A	3484	1/1	0.95	0.16	65,65,65,65	0
54	MG	1a	1738	1/1	0.95	0.08	46,46,46,46	0
54	MG	10	102	1/1	0.95	0.15	49,49,49,49	0
54	MG	10	103	1/1	0.95	0.10	62,62,62,62	0
54	MG	2A	3235	1/1	0.95	0.13	59,59,59,59	0
54	MG	1A	3962	1/1	0.95	0.09	65,65,65,65	0
54	MG	1A	3394	1/1	0.95	0.07	39,39,39,39	0
54	MG	2A	3239	1/1	0.95	0.31	48,48,48,48	0
54	MG	1A	3320	1/1	0.95	0.07	34,34,34,34	0
54	MG	11	101	1/1	0.95	0.13	51,51,51,51	0
54	MG	1A	3245	1/1	0.95	0.28	64,64,64,64	0
54	MG	1A	3397	1/1	0.95	0.08	50,50,50,50	0
54	MG	2T	201	1/1	0.95	0.11	53,53,53,53	0
54	MG	11	105	1/1	0.95	0.08	44,44,44,44	0
54	MG	2T	203	1/1	0.95	0.14	71,71,71,71	0
54	MG	2A	3247	1/1	0.95	0.07	66,66,66,66	0
54	MG	1A	3246	1/1	0.95	0.33	59,59,59,59	0
54	MG	1a	1751	1/1	0.95	0.09	62,62,62,62	0
54	MG	1a	1752	1/1	0.95	0.12	65,65,65,65	0
54	MG	2A	3039	1/1	0.95	0.12	54,54,54,54	0
54	MG	1A	3969	1/1	0.95	0.11	52,52,52,52	0
54	MG	20	102	1/1	0.95	0.40	61,61,61,61	0
54	MG	2A	3041	1/1	0.95	0.06	26,26,26,26	0
54	MG	15	105	1/1	0.95	0.24	32,32,32,32	0
54	MG	23	101	1/1	0.95	0.16	61,61,61,61	0
54	MG	2A	3507	1/1	0.95	0.08	69,69,69,69	0
54	MG	25	102	1/1	0.95	0.11	61,61,61,61	0
54	MG	2A	3508	1/1	0.95	0.09	33,33,33,33	0
54	MG	27	101	1/1	0.95	0.21	49,49,49,49	0
54	MG	27	102	1/1	0.95	0.15	45,45,45,45	0
54	MG	1A	3249	1/1	0.95	0.22	54,54,54,54	0
54	MG	2A	3262	1/1	0.95	0.09	68,68,68,68	0
54	MG	1A	3971	1/1	0.95	0.15	53,53,53,53	0
54	MG	2A	3045	1/1	0.95	0.21	65,65,65,65	0
54	MG	1A	3973	1/1	0.95	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1762	1/1	0.95	0.21	56,56,56,56	0
54	MG	1a	1764	1/1	0.95	0.15	67,67,67,67	0
54	MG	1A	3974	1/1	0.95	0.09	65,65,65,65	0
54	MG	1A	3011	1/1	0.95	0.08	52,52,52,52	0
54	MG	2A	3521	1/1	0.95	0.07	47,47,47,47	0
54	MG	1A	3667	1/1	0.95	0.14	55,55,55,55	0
54	MG	1a	1770	1/1	0.95	0.14	61,61,61,61	0
54	MG	2A	3527	1/1	0.95	0.08	63,63,63,63	0
54	MG	2A	3056	1/1	0.95	0.08	37,37,37,37	0
54	MG	1a	1771	1/1	0.95	0.16	67,67,67,67	0
54	MG	1a	1772	1/1	0.95	0.18	59,59,59,59	0
54	MG	1A	3799	1/1	0.95	0.12	65,65,65,65	0
54	MG	2A	3061	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3670	1/1	0.95	0.38	52,52,52,52	0
54	MG	1A	3802	1/1	0.95	0.12	60,60,60,60	0
54	MG	1A	3113	1/1	0.95	0.08	44,44,44,44	0
54	MG	2a	3021	1/1	0.95	0.07	63,63,63,63	0
54	MG	1a	1606	1/1	0.95	0.07	62,62,62,62	0
54	MG	2A	3538	1/1	0.95	0.16	56,56,56,56	0
54	MG	1a	1607	1/1	0.95	0.11	55,55,55,55	0
54	MG	1A	3153	1/1	0.95	0.18	57,57,57,57	0
54	MG	2A	3289	1/1	0.95	0.15	50,50,50,50	0
54	MG	2A	3543	1/1	0.95	0.08	44,44,44,44	0
54	MG	1A	3581	1/1	0.95	0.07	53,53,53,53	0
54	MG	2a	3029	1/1	0.95	0.15	66,66,66,66	0
54	MG	1a	1610	1/1	0.95	0.07	62,62,62,62	0
54	MG	1A	3582	1/1	0.95	0.21	49,49,49,49	0
54	MG	1a	1613	1/1	0.95	0.16	35,35,35,35	0
54	MG	2A	3294	1/1	0.95	0.23	65,65,65,65	0
54	MG	1A	3807	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3808	1/1	0.95	0.15	51,51,51,51	0
54	MG	2A	3551	1/1	0.95	0.16	60,60,60,60	0
54	MG	2A	3078	1/1	0.95	0.11	64,64,64,64	0
54	MG	1A	3114	1/1	0.95	0.18	47,47,47,47	0
54	MG	1A	3025	1/1	0.95	0.21	45,45,45,45	0
54	MG	1A	3259	1/1	0.95	0.21	55,55,55,55	0
54	MG	1A	3160	1/1	0.95	0.20	37,37,37,37	0
54	MG	1A	3815	1/1	0.95	0.22	52,52,52,52	0
54	MG	1A	3413	1/1	0.95	0.06	54,54,54,54	0
54	MG	1A	3683	1/1	0.95	0.06	55,55,55,55	0
54	MG	1A	3819	1/1	0.95	0.08	33,33,33,33	0
54	MG	2A	3563	1/1	0.95	0.19	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	3686	1/1	0.95	0.10	46,46,46,46	0
54	MG	2A	3090	1/1	0.95	0.13	51,51,51,51	0
54	MG	1A	3054	1/1	0.95	0.21	39,39,39,39	0
54	MG	1A	3093	1/1	0.95	0.19	46,46,46,46	0
54	MG	2A	3312	1/1	0.95	0.28	65,65,65,65	0
54	MG	1A	3592	1/1	0.95	0.05	31,31,31,31	0
54	MG	1A	3593	1/1	0.95	0.10	37,37,37,37	0
54	MG	1A	3829	1/1	0.95	0.24	44,44,44,44	0
54	MG	1A	3419	1/1	0.95	0.07	34,34,34,34	0
54	MG	2A	3574	1/1	0.95	0.07	43,43,43,43	0
54	MG	2A	3575	1/1	0.95	0.09	59,59,59,59	0
54	MG	1A	3056	1/1	0.95	0.09	47,47,47,47	0
54	MG	1A	3036	1/1	0.95	0.06	39,39,39,39	0
54	MG	1A	3834	1/1	0.95	0.06	27,27,27,27	0
54	MG	1A	3697	1/1	0.95	0.11	42,42,42,42	0
54	MG	1A	3422	1/1	0.95	0.10	50,50,50,50	0
54	MG	2A	3585	1/1	0.95	0.07	68,68,68,68	0
54	MG	1A	3212	1/1	0.95	0.14	42,42,42,42	0
54	MG	1A	3273	1/1	0.95	0.12	41,41,41,41	0
54	MG	1A	3099	1/1	0.95	0.08	41,41,41,41	0
54	MG	2a	3070	1/1	0.95	0.15	72,72,72,72	0
54	MG	1a	1648	1/1	0.95	0.20	46,46,46,46	0
54	MG	1A	3512	1/1	0.95	0.16	37,37,37,37	0
54	MG	1A	3604	1/1	0.95	0.09	58,58,58,58	0
54	MG	1a	1654	1/1	0.95	0.17	62,62,62,62	0
54	MG	2A	3330	1/1	0.95	0.10	44,44,44,44	0
54	MG	2A	3332	1/1	0.95	0.11	65,65,65,65	0
54	MG	2A	3598	1/1	0.95	0.08	55,55,55,55	0
54	MG	1A	3430	1/1	0.95	0.06	38,38,38,38	0
54	MG	2A	3600	1/1	0.95	0.08	57,57,57,57	0
54	MG	2A	3601	1/1	0.95	0.15	50,50,50,50	0
54	MG	1a	1817	1/1	0.95	0.10	61,61,61,61	0
54	MG	1A	3353	1/1	0.95	0.13	38,38,38,38	0
54	MG	1A	3714	1/1	0.95	0.21	56,56,56,56	0
54	MG	2A	3120	1/1	0.95	0.12	50,50,50,50	0
54	MG	2A	3340	1/1	0.95	0.09	22,22,22,22	0
54	MG	1A	3012	1/1	0.95	0.18	43,43,43,43	0
54	MG	2A	3124	1/1	0.95	0.21	48,48,48,48	0
54	MG	2A	3343	1/1	0.95	0.06	44,44,44,44	0
54	MG	1A	3356	1/1	0.95	0.09	48,48,48,48	0
54	MG	2A	3619	1/1	0.95	0.10	49,49,49,49	0
54	MG	2A	3347	1/1	0.95	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1B	204	1/1	0.95	0.07	54,54,54,54	0
54	MG	1A	3133	1/1	0.95	0.22	51,51,51,51	0
54	MG	1A	3358	1/1	0.95	0.07	31,31,31,31	0
54	MG	1A	3179	1/1	0.95	0.25	56,56,56,56	0
54	MG	1a	1830	1/1	0.95	0.06	72,72,72,72	0
54	MG	1B	208	1/1	0.95	0.06	46,46,46,46	0
54	MG	2A	3354	1/1	0.95	0.08	37,37,37,37	0
54	MG	2A	3136	1/1	0.95	0.07	47,47,47,47	0
54	MG	2a	3103	1/1	0.95	0.30	53,53,53,53	0
54	MG	1A	3864	1/1	0.95	0.08	53,53,53,53	0
54	MG	2a	3105	1/1	0.95	0.40	67,67,67,67	0
54	MG	2A	3632	1/1	0.95	0.14	58,58,58,58	0
54	MG	2A	3139	1/1	0.95	0.12	65,65,65,65	0
54	MG	1A	3180	1/1	0.95	0.20	36,36,36,36	0
54	MG	1A	3616	1/1	0.95	0.11	45,45,45,45	0
54	MG	1A	3870	1/1	0.95	0.06	66,66,66,66	0
54	MG	2A	3145	1/1	0.95	0.07	69,69,69,69	0
54	MG	2A	3364	1/1	0.95	0.17	45,45,45,45	0
54	MG	2A	3365	1/1	0.95	0.08	63,63,63,63	0
54	MG	2A	3366	1/1	0.95	0.12	56,56,56,56	0
54	MG	2a	3115	1/1	0.95	0.51	69,69,69,69	0
54	MG	1A	3617	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3619	1/1	0.95	0.08	39,39,39,39	0
54	MG	2a	3118	1/1	0.95	0.12	74,74,74,74	0
54	MG	2A	3369	1/1	0.95	0.08	56,56,56,56	0
54	MG	1A	3876	1/1	0.95	0.05	35,35,35,35	0
54	MG	1a	1676	1/1	0.95	0.21	59,59,59,59	0
54	MG	2a	3122	1/1	0.95	0.12	61,61,61,61	0
54	MG	2A	3374	1/1	0.95	0.07	43,43,43,43	0
54	MG	2A	3651	1/1	0.95	0.06	48,48,48,48	0
54	MG	1A	3529	1/1	0.95	0.07	62,62,62,62	0
54	MG	2A	3376	1/1	0.95	0.10	64,64,64,64	0
54	MG	1a	1843	1/1	0.95	0.09	54,54,54,54	0
54	MG	2A	3656	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3728	1/1	0.95	0.24	47,47,47,47	0
54	MG	1A	3134	1/1	0.95	0.16	44,44,44,44	0
54	MG	2A	3659	1/1	0.95	0.15	55,55,55,55	0
54	MG	2a	3135	1/1	0.95	0.10	73,73,73,73	0
54	MG	2A	3384	1/1	0.95	0.09	46,46,46,46	0
54	MG	2a	3137	1/1	0.95	0.08	69,69,69,69	0
54	MG	1a	1680	1/1	0.95	0.19	65,65,65,65	0
54	MG	2A	3663	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	3730	1/1	0.95	0.05	32,32,32,32	0
54	MG	2A	3157	1/1	0.95	0.13	60,60,60,60	0
54	MG	1A	3885	1/1	0.95	0.08	33,33,33,33	0
54	MG	1a	1683	1/1	0.95	0.25	69,69,69,69	0
54	MG	1A	3030	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3626	1/1	0.95	0.21	36,36,36,36	0
54	MG	1A	3141	1/1	0.95	0.28	48,48,48,48	0
54	MG	1A	3369	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3744	1/1	0.95	0.06	59,59,59,59	0
54	MG	1A	3536	1/1	0.95	0.13	61,61,61,61	0
54	MG	1a	1860	1/1	0.95	0.07	59,59,59,59	0
54	MG	1a	1861	1/1	0.95	0.08	58,58,58,58	0
54	MG	1a	1862	1/1	0.95	0.09	62,62,62,62	0
54	MG	2a	3158	1/1	0.95	0.09	69,69,69,69	0
54	MG	1A	3190	1/1	0.95	0.08	54,54,54,54	0
54	MG	2A	3684	1/1	0.95	0.07	41,41,41,41	0
54	MG	2A	3685	1/1	0.95	0.08	67,67,67,67	0
54	MG	1a	1865	1/1	0.95	0.16	76,76,76,76	0
54	MG	1A	3632	1/1	0.95	0.10	34,34,34,34	0
54	MG	2A	3415	1/1	0.95	0.13	55,55,55,55	0
54	MG	1A	3375	1/1	0.95	0.07	49,49,49,49	0
54	MG	2a	3167	1/1	0.95	0.08	60,60,60,60	0
54	MG	1A	3142	1/1	0.95	0.12	41,41,41,41	0
54	MG	1A	3636	1/1	0.95	0.07	29,29,29,29	0
54	MG	2A	3420	1/1	0.95	0.09	70,70,70,70	0
54	MG	2A	3183	1/1	0.95	0.09	46,46,46,46	0
54	MG	1A	3301	1/1	0.95	0.09	47,47,47,47	0
54	MG	2A	3185	1/1	0.95	0.12	63,63,63,63	0
54	MG	1A	3909	1/1	0.95	0.07	58,58,58,58	0
54	MG	1A	3379	1/1	0.95	0.07	52,52,52,52	0
54	MG	2a	3178	1/1	0.95	0.14	63,63,63,63	0
54	MG	2a	3179	1/1	0.95	0.11	78,78,78,78	0
54	MG	2A	3427	1/1	0.95	0.08	65,65,65,65	0
54	MG	1A	3911	1/1	0.95	0.07	25,25,25,25	0
54	MG	1A	3307	1/1	0.95	0.14	45,45,45,45	0
54	MG	1A	3230	1/1	0.95	0.21	50,50,50,50	0
54	MG	2A	3431	1/1	0.95	0.08	61,61,61,61	0
54	MG	1A	3919	1/1	0.95	0.11	35,35,35,35	0
54	MG	2A	3709	1/1	0.95	0.09	46,46,46,46	0
54	MG	1a	1703	1/1	0.95	0.28	58,58,58,58	0
54	MG	1G	201	1/1	0.95	0.05	69,69,69,69	0
54	MG	1A	3080	1/1	0.95	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3715	1/1	0.95	0.10	66,66,66,66	0
54	MG	2a	3191	1/1	0.95	0.18	63,63,63,63	0
54	MG	1A	3045	1/1	0.95	0.09	35,35,35,35	0
54	MG	1A	3931	1/1	0.95	0.06	58,58,58,58	0
54	MG	1A	3765	1/1	0.95	0.07	47,47,47,47	0
54	MG	2A	3721	1/1	0.95	0.06	55,55,55,55	0
54	MG	2A	3722	1/1	0.95	0.16	57,57,57,57	0
54	MG	1A	3936	1/1	0.95	0.09	59,59,59,59	0
54	MG	1A	3312	1/1	0.95	0.31	45,45,45,45	0
54	MG	2A	3200	1/1	0.95	0.07	50,50,50,50	0
54	MG	1e	202	1/1	0.95	0.26	59,59,59,59	0
57	MPD	18	103	8/8	0.95	0.13	31,44,47,48	0
54	MG	1A	3940	1/1	0.95	0.10	60,60,60,60	0
54	MG	1A	3769	1/1	0.95	0.08	41,41,41,41	0
54	MG	1A	3770	1/1	0.95	0.14	42,42,42,42	0
54	MG	1A	3555	1/1	0.95	0.05	30,30,30,30	0
54	MG	2A	3450	1/1	0.95	0.10	53,53,53,53	0
54	MG	1A	3772	1/1	0.95	0.17	58,58,58,58	0
54	MG	2D	309	1/1	0.96	0.15	55,55,55,55	0
54	MG	1A	3324	1/1	0.96	0.21	49,49,49,49	0
54	MG	13	103	1/1	0.96	0.08	49,49,49,49	0
54	MG	1A	3587	1/1	0.96	0.09	47,47,47,47	0
54	MG	2E	302	1/1	0.96	0.11	52,52,52,52	0
54	MG	2A	3254	1/1	0.96	0.25	49,49,49,49	0
54	MG	2A	3255	1/1	0.96	0.05	40,40,40,40	0
54	MG	2E	306	1/1	0.96	0.11	37,37,37,37	0
54	MG	1A	3488	1/1	0.96	0.11	46,46,46,46	0
54	MG	2A	3258	1/1	0.96	0.14	34,34,34,34	0
54	MG	2A	3046	1/1	0.96	0.11	64,64,64,64	0
54	MG	2A	3261	1/1	0.96	0.20	50,50,50,50	0
54	MG	1a	1759	1/1	0.96	0.11	60,60,60,60	0
54	MG	1a	1760	1/1	0.96	0.07	64,64,64,64	0
54	MG	1A	3684	1/1	0.96	0.16	52,52,52,52	0
54	MG	2A	3050	1/1	0.96	0.12	49,49,49,49	0
54	MG	2A	3266	1/1	0.96	0.20	55,55,55,55	0
54	MG	2A	3506	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3039	1/1	0.96	0.10	54,54,54,54	0
54	MG	15	108	1/1	0.96	0.18	66,66,66,66	0
54	MG	2A	3269	1/1	0.96	0.17	61,61,61,61	0
54	MG	17	102	1/1	0.96	0.13	42,42,42,42	0
54	MG	17	104	1/1	0.96	0.15	33,33,33,33	0
54	MG	1A	3400	1/1	0.96	0.12	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	3688	1/1	0.96	0.17	41,41,41,41	0
54	MG	2A	3515	1/1	0.96	0.07	60,60,60,60	0
54	MG	18	101	1/1	0.96	0.12	49,49,49,49	0
54	MG	1A	3074	1/1	0.96	0.07	33,33,33,33	0
54	MG	1A	3214	1/1	0.96	0.08	46,46,46,46	0
54	MG	2V	201	1/1	0.96	0.10	65,65,65,65	0
54	MG	2V	203	1/1	0.96	0.11	61,61,61,61	0
54	MG	1A	3404	1/1	0.96	0.05	33,33,33,33	0
54	MG	1a	1601	1/1	0.96	0.07	46,46,46,46	0
54	MG	2X	101	1/1	0.96	0.11	52,52,52,52	0
54	MG	1A	3984	1/1	0.96	0.06	57,57,57,57	0
54	MG	2A	3524	1/1	0.96	0.11	58,58,58,58	0
54	MG	1A	3052	1/1	0.96	0.21	51,51,51,51	0
54	MG	2A	3283	1/1	0.96	0.14	37,37,37,37	0
54	MG	1A	3497	1/1	0.96	0.10	42,42,42,42	0
54	MG	1A	3177	1/1	0.96	0.15	34,34,34,34	0
54	MG	2A	3069	1/1	0.96	0.16	44,44,44,44	0
54	MG	2A	3070	1/1	0.96	0.09	60,60,60,60	0
54	MG	1A	3267	1/1	0.96	0.12	58,58,58,58	0
54	MG	2A	3533	1/1	0.96	0.10	45,45,45,45	0
54	MG	1A	3698	1/1	0.96	0.08	49,49,49,49	0
54	MG	1A	3408	1/1	0.96	0.06	37,37,37,37	0
54	MG	28	101	1/1	0.96	0.36	68,68,68,68	0
54	MG	1A	3826	1/1	0.96	0.07	26,26,26,26	0
54	MG	1A	3104	1/1	0.96	0.26	39,39,39,39	0
54	MG	1A	3270	1/1	0.96	0.12	38,38,38,38	0
54	MG	1A	3703	1/1	0.96	0.10	50,50,50,50	0
54	MG	1A	3705	1/1	0.96	0.05	53,53,53,53	0
54	MG	1A	3706	1/1	0.96	0.19	49,49,49,49	0
54	MG	1A	3602	1/1	0.96	0.08	50,50,50,50	0
54	MG	1a	1619	1/1	0.96	0.10	60,60,60,60	0
54	MG	1A	3064	1/1	0.96	0.07	42,42,42,42	0
54	MG	2A	3085	1/1	0.96	0.33	53,53,53,53	0
54	MG	1A	3709	1/1	0.96	0.42	42,42,42,42	0
54	MG	1A	3065	1/1	0.96	0.07	37,37,37,37	0
54	MG	1A	3341	1/1	0.96	0.09	52,52,52,52	0
54	MG	1a	1626	1/1	0.96	0.09	65,65,65,65	0
54	MG	2a	3013	1/1	0.96	0.10	61,61,61,61	0
54	MG	2A	3306	1/1	0.96	0.06	42,42,42,42	0
54	MG	1a	1627	1/1	0.96	0.05	55,55,55,55	0
54	MG	1A	3607	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3274	1/1	0.96	0.20	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	3018	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3276	1/1	0.96	0.06	55,55,55,55	0
54	MG	1A	3185	1/1	0.96	0.27	41,41,41,41	0
54	MG	1A	3844	1/1	0.96	0.05	40,40,40,40	0
54	MG	1A	3845	1/1	0.96	0.09	50,50,50,50	0
54	MG	2A	3559	1/1	0.96	0.12	38,38,38,38	0
54	MG	2A	3560	1/1	0.96	0.15	41,41,41,41	0
54	MG	1A	3846	1/1	0.96	0.07	47,47,47,47	0
54	MG	2A	3099	1/1	0.96	0.12	51,51,51,51	0
54	MG	1A	3847	1/1	0.96	0.25	56,56,56,56	0
54	MG	1A	3346	1/1	0.96	0.12	32,32,32,32	0
54	MG	1A	3850	1/1	0.96	0.11	53,53,53,53	0
54	MG	1A	3423	1/1	0.96	0.09	35,35,35,35	0
54	MG	2A	3105	1/1	0.96	0.06	45,45,45,45	0
54	MG	1A	3278	1/1	0.96	0.23	47,47,47,47	0
54	MG	1A	3083	1/1	0.96	0.24	41,41,41,41	0
54	MG	1a	1642	1/1	0.96	0.09	65,65,65,65	0
54	MG	2a	3036	1/1	0.96	0.10	46,46,46,46	0
54	MG	1A	3857	1/1	0.96	0.11	47,47,47,47	0
54	MG	1A	3350	1/1	0.96	0.05	32,32,32,32	0
54	MG	2A	3112	1/1	0.96	0.26	65,65,65,65	0
54	MG	1A	3859	1/1	0.96	0.08	69,69,69,69	0
54	MG	2A	3577	1/1	0.96	0.15	59,59,59,59	0
54	MG	1A	3351	1/1	0.96	0.10	16,16,16,16	0
54	MG	1a	1647	1/1	0.96	0.20	61,61,61,61	0
54	MG	1A	3618	1/1	0.96	0.07	56,56,56,56	0
54	MG	2A	3582	1/1	0.96	0.07	64,64,64,64	0
54	MG	1a	1650	1/1	0.96	0.22	59,59,59,59	0
54	MG	1A	3431	1/1	0.96	0.06	28,28,28,28	0
54	MG	2A	3119	1/1	0.96	0.11	54,54,54,54	0
54	MG	2A	3338	1/1	0.96	0.05	38,38,38,38	0
54	MG	1a	1823	1/1	0.96	0.07	78,78,78,78	0
54	MG	2A	3588	1/1	0.96	0.08	61,61,61,61	0
54	MG	2A	3589	1/1	0.96	0.10	41,41,41,41	0
54	MG	1A	3023	1/1	0.96	0.16	36,36,36,36	0
54	MG	1a	1825	1/1	0.96	0.09	67,67,67,67	0
54	MG	1A	3866	1/1	0.96	0.06	49,49,49,49	0
54	MG	1A	3530	1/1	0.96	0.09	25,25,25,25	0
54	MG	2A	3344	1/1	0.96	0.12	55,55,55,55	0
54	MG	2a	3058	1/1	0.96	0.11	60,60,60,60	0
54	MG	1A	3869	1/1	0.96	0.18	40,40,40,40	0
54	MG	1A	3622	1/1	0.96	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3148	1/1	0.96	0.08	36,36,36,36	0
54	MG	2A	3132	1/1	0.96	0.08	35,35,35,35	0
54	MG	1A	3732	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3735	1/1	0.96	0.07	31,31,31,31	0
54	MG	1A	3736	1/1	0.96	0.08	52,52,52,52	0
54	MG	1A	3532	1/1	0.96	0.05	58,58,58,58	0
54	MG	2A	3138	1/1	0.96	0.07	44,44,44,44	0
54	MG	1a	1836	1/1	0.96	0.08	71,71,71,71	0
54	MG	2A	3140	1/1	0.96	0.07	50,50,50,50	0
54	MG	1B	217	1/1	0.96	0.07	47,47,47,47	0
54	MG	2A	3615	1/1	0.96	0.08	45,45,45,45	0
54	MG	1A	3285	1/1	0.96	0.18	54,54,54,54	0
54	MG	1a	1666	1/1	0.96	0.06	74,74,74,74	0
54	MG	2a	3074	1/1	0.96	0.06	65,65,65,65	0
54	MG	1a	1667	1/1	0.96	0.18	64,64,64,64	0
54	MG	1A	3739	1/1	0.96	0.12	40,40,40,40	0
54	MG	1A	3884	1/1	0.96	0.10	38,38,38,38	0
54	MG	1B	222	1/1	0.96	0.06	59,59,59,59	0
54	MG	1A	3085	1/1	0.96	0.26	41,41,41,41	0
54	MG	1A	3437	1/1	0.96	0.08	30,30,30,30	0
54	MG	1A	3290	1/1	0.96	0.12	54,54,54,54	0
54	MG	1B	227	1/1	0.96	0.07	57,57,57,57	0
54	MG	1A	3631	1/1	0.96	0.23	52,52,52,52	0
54	MG	1A	3359	1/1	0.96	0.10	51,51,51,51	0
54	MG	2A	3373	1/1	0.96	0.13	49,49,49,49	0
54	MG	1D	301	1/1	0.96	0.29	39,39,39,39	0
54	MG	1D	303	1/1	0.96	0.14	43,43,43,43	0
54	MG	1D	305	1/1	0.96	0.11	58,58,58,58	0
54	MG	2A	3159	1/1	0.96	0.13	49,49,49,49	0
54	MG	2A	3379	1/1	0.96	0.12	39,39,39,39	0
54	MG	1A	3749	1/1	0.96	0.09	49,49,49,49	0
54	MG	1a	1857	1/1	0.96	0.05	60,60,60,60	0
54	MG	1A	3192	1/1	0.96	0.16	40,40,40,40	0
54	MG	1a	1859	1/1	0.96	0.08	67,67,67,67	0
54	MG	1A	3752	1/1	0.96	0.12	53,53,53,53	0
54	MG	2a	3097	1/1	0.96	0.23	56,56,56,56	0
54	MG	1A	3634	1/1	0.96	0.06	52,52,52,52	0
54	MG	2A	3389	1/1	0.96	0.07	41,41,41,41	0
54	MG	2A	3391	1/1	0.96	0.06	47,47,47,47	0
54	MG	2A	3392	1/1	0.96	0.16	65,65,65,65	0
54	MG	2A	3168	1/1	0.96	0.06	54,54,54,54	0
54	MG	1A	3086	1/1	0.96	0.23	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	3442	1/1	0.96	0.10	32,32,32,32	0
54	MG	1A	3362	1/1	0.96	0.10	54,54,54,54	0
54	MG	1a	1866	1/1	0.96	0.07	44,44,44,44	0
54	MG	2A	3174	1/1	0.96	0.07	51,51,51,51	0
54	MG	2A	3175	1/1	0.96	0.17	48,48,48,48	0
54	MG	1D	319	1/1	0.96	0.14	61,61,61,61	0
54	MG	2A	3402	1/1	0.96	0.06	39,39,39,39	0
54	MG	2A	3177	1/1	0.96	0.10	65,65,65,65	0
54	MG	1A	3364	1/1	0.96	0.06	52,52,52,52	0
54	MG	1A	3907	1/1	0.96	0.08	63,63,63,63	0
54	MG	2A	3407	1/1	0.96	0.10	60,60,60,60	0
54	MG	1A	3293	1/1	0.96	0.12	41,41,41,41	0
54	MG	1A	3642	1/1	0.96	0.09	63,63,63,63	0
54	MG	1A	3366	1/1	0.96	0.10	37,37,37,37	0
54	MG	1F	303	1/1	0.96	0.17	36,36,36,36	0
54	MG	2A	3670	1/1	0.96	0.15	70,70,70,70	0
54	MG	1F	306	1/1	0.96	0.12	31,31,31,31	0
54	MG	2A	3672	1/1	0.96	0.10	57,57,57,57	0
54	MG	1F	310	1/1	0.96	0.07	31,31,31,31	0
54	MG	2A	3418	1/1	0.96	0.16	66,66,66,66	0
54	MG	1F	311	1/1	0.96	0.24	53,53,53,53	0
54	MG	1A	3151	1/1	0.96	0.11	48,48,48,48	0
54	MG	2A	3678	1/1	0.96	0.10	43,43,43,43	0
54	MG	1A	3913	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3915	1/1	0.96	0.09	29,29,29,29	0
54	MG	1A	3916	1/1	0.96	0.05	34,34,34,34	0
54	MG	1A	3766	1/1	0.96	0.05	57,57,57,57	0
54	MG	1A	3553	1/1	0.96	0.34	38,38,38,38	0
54	MG	2a	3134	1/1	0.96	0.20	67,67,67,67	0
54	MG	1G	203	1/1	0.96	0.07	60,60,60,60	0
54	MG	1A	3295	1/1	0.96	0.12	64,64,64,64	0
54	MG	1A	3049	1/1	0.96	0.16	60,60,60,60	0
54	MG	1A	3927	1/1	0.96	0.07	45,45,45,45	0
54	MG	1A	3454	1/1	0.96	0.06	19,19,19,19	0
54	MG	1A	3123	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3935	1/1	0.96	0.07	37,37,37,37	0
54	MG	2A	3692	1/1	0.96	0.11	51,51,51,51	0
54	MG	1g	201	1/1	0.96	0.31	75,75,75,75	0
54	MG	1A	3651	1/1	0.96	0.16	51,51,51,51	0
54	MG	2a	3146	1/1	0.96	0.13	65,65,65,65	0
54	MG	2a	3147	1/1	0.96	0.05	68,68,68,68	0
54	MG	1A	3558	1/1	0.96	0.07	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3149	1/1	0.96	0.10	61,61,61,61	0
54	MG	2A	3696	1/1	0.96	0.07	57,57,57,57	0
54	MG	1P	202	1/1	0.96	0.17	42,42,42,42	0
54	MG	1A	3456	1/1	0.96	0.08	47,47,47,47	0
54	MG	1A	3372	1/1	0.96	0.08	29,29,29,29	0
54	MG	1Q	202	1/1	0.96	0.04	34,34,34,34	0
54	MG	1A	3241	1/1	0.96	0.12	39,39,39,39	0
54	MG	2A	3209	1/1	0.96	0.24	54,54,54,54	0
54	MG	2A	3445	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3566	1/1	0.96	0.08	39,39,39,39	0
54	MG	1A	3302	1/1	0.96	0.10	37,37,37,37	0
54	MG	1A	3303	1/1	0.96	0.09	51,51,51,51	0
54	MG	1y	201	1/1	0.96	0.09	70,70,70,70	0
54	MG	2a	3163	1/1	0.96	0.16	52,52,52,52	0
54	MG	1A	3785	1/1	0.96	0.06	42,42,42,42	0
54	MG	1A	3786	1/1	0.96	0.06	30,30,30,30	0
54	MG	2A	3712	1/1	0.96	0.07	63,63,63,63	0
54	MG	1A	3242	1/1	0.96	0.28	38,38,38,38	0
54	MG	2A	3714	1/1	0.96	0.06	65,65,65,65	0
54	MG	2A	3002	1/1	0.96	0.06	56,56,56,56	0
54	MG	2A	3456	1/1	0.96	0.09	46,46,46,46	0
54	MG	1A	3951	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3124	1/1	0.96	0.06	37,37,37,37	0
54	MG	2A	3720	1/1	0.96	0.07	57,57,57,57	0
54	MG	1A	3953	1/1	0.96	0.06	70,70,70,70	0
54	MG	1U	205	1/1	0.96	0.22	44,44,44,44	0
54	MG	1A	3050	1/1	0.96	0.12	46,46,46,46	0
54	MG	2A	3014	1/1	0.96	0.12	39,39,39,39	0
54	MG	1A	3090	1/1	0.96	0.09	44,44,44,44	0
54	MG	2A	3016	1/1	0.96	0.09	52,52,52,52	0
54	MG	1A	3127	1/1	0.96	0.06	48,48,48,48	0
54	MG	1a	1733	1/1	0.96	0.08	52,52,52,52	0
54	MG	1a	1734	1/1	0.96	0.07	41,41,41,41	0
54	MG	1A	3313	1/1	0.96	0.08	45,45,45,45	0
54	MG	2A	3470	1/1	0.96	0.06	39,39,39,39	0
54	MG	2A	3471	1/1	0.96	0.10	63,63,63,63	0
54	MG	1a	1737	1/1	0.96	0.06	60,60,60,60	0
54	MG	2A	3025	1/1	0.96	0.15	58,58,58,58	0
54	MG	2A	3026	1/1	0.96	0.11	40,40,40,40	0
54	MG	1A	3069	1/1	0.96	0.10	40,40,40,40	0
54	MG	2A	3028	1/1	0.96	0.10	52,52,52,52	0
54	MG	1A	3317	1/1	0.96	0.26	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	3252	1/1	0.96	0.33	44,44,44,44	0
54	MG	2f	201	1/1	0.96	0.05	54,54,54,54	0
54	MG	1A	3167	1/1	0.96	0.06	41,41,41,41	0
54	MG	2k	201	1/1	0.96	0.12	63,63,63,63	0
54	MG	2A	3240	1/1	0.96	0.27	41,41,41,41	0
54	MG	10	104	1/1	0.96	0.13	58,58,58,58	0
55	HGR	1A	4022	36/36	0.96	0.08	23,32,37,43	0
54	MG	1A	3207	1/1	0.96	0.09	56,56,56,56	0
56	ZIT	2A	3731	52/52	0.96	0.10	33,45,64,67	0
54	MG	1A	3480	1/1	0.96	0.09	60,60,60,60	0
54	MG	1A	3058	1/1	0.96	0.15	54,54,54,54	0
54	MG	1A	3801	1/1	0.96	0.07	31,31,31,31	0
54	MG	2D	303	1/1	0.96	0.38	49,49,49,49	0
54	MG	1A	3059	1/1	0.96	0.14	27,27,27,27	0
54	MG	1A	3584	1/1	0.96	0.06	52,52,52,52	0
54	MG	1A	3486	1/1	0.96	0.06	33,33,33,33	0
54	MG	13	101	1/1	0.96	0.13	42,42,42,42	0
54	MG	2D	308	1/1	0.96	0.06	45,45,45,45	0
59	ZN	14	102	1/1	0.96	0.09	113,113,113,113	0
54	MG	2A	3167	1/1	0.97	0.14	46,46,46,46	0
54	MG	1U	201	1/1	0.97	0.16	44,44,44,44	0
54	MG	2A	3361	1/1	0.97	0.05	31,31,31,31	0
54	MG	1A	3824	1/1	0.97	0.05	47,47,47,47	0
54	MG	2A	3363	1/1	0.97	0.08	65,65,65,65	0
54	MG	1e	203	1/1	0.97	0.06	61,61,61,61	0
54	MG	1U	203	1/1	0.97	0.25	40,40,40,40	0
54	MG	1A	3513	1/1	0.97	0.04	63,63,63,63	0
54	MG	1V	201	1/1	0.97	0.24	35,35,35,35	0
54	MG	1A	3606	1/1	0.97	0.06	25,25,25,25	0
54	MG	1A	3515	1/1	0.97	0.06	47,47,47,47	0
54	MG	2A	3370	1/1	0.97	0.10	55,55,55,55	0
54	MG	1A	3828	1/1	0.97	0.36	38,38,38,38	0
54	MG	1A	3003	1/1	0.97	0.04	31,31,31,31	0
54	MG	1W	203	1/1	0.97	0.07	40,40,40,40	0
54	MG	1l	201	1/1	0.97	0.18	67,67,67,67	0
54	MG	1A	3429	1/1	0.97	0.07	35,35,35,35	0
54	MG	2A	3592	1/1	0.97	0.05	59,59,59,59	0
54	MG	1A	3979	1/1	0.97	0.06	59,59,59,59	0
54	MG	1A	3215	1/1	0.97	0.12	43,43,43,43	0
54	MG	1A	3016	1/1	0.97	0.28	38,38,38,38	0
54	MG	1A	3833	1/1	0.97	0.08	36,36,36,36	0
54	MG	1o	102	1/1	0.97	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	10	105	1/1	0.97	0.07	55,55,55,55	0
54	MG	1A	3053	1/1	0.97	0.17	38,38,38,38	0
54	MG	1A	3522	1/1	0.97	0.07	61,61,61,61	0
54	MG	1A	3523	1/1	0.97	0.08	56,56,56,56	0
54	MG	2A	3602	1/1	0.97	0.10	47,47,47,47	0
54	MG	1A	3718	1/1	0.97	0.07	38,38,38,38	0
54	MG	2A	3604	1/1	0.97	0.06	56,56,56,56	0
54	MG	2A	3606	1/1	0.97	0.06	61,61,61,61	0
54	MG	1A	3091	1/1	0.97	0.14	40,40,40,40	0
54	MG	1A	3024	1/1	0.97	0.03	22,22,22,22	0
54	MG	1A	3435	1/1	0.97	0.07	35,35,35,35	0
54	MG	2A	3611	1/1	0.97	0.05	40,40,40,40	0
54	MG	1A	3283	1/1	0.97	0.15	46,46,46,46	0
54	MG	2A	3613	1/1	0.97	0.07	40,40,40,40	0
54	MG	1A	3284	1/1	0.97	0.05	44,44,44,44	0
54	MG	2a	3031	1/1	0.97	0.13	65,65,65,65	0
54	MG	2A	3010	1/1	0.97	0.06	40,40,40,40	0
54	MG	1A	3171	1/1	0.97	0.23	41,41,41,41	0
54	MG	2A	3013	1/1	0.97	0.07	57,57,57,57	0
54	MG	1A	3288	1/1	0.97	0.23	44,44,44,44	0
54	MG	15	102	1/1	0.97	0.12	47,47,47,47	0
54	MG	15	104	1/1	0.97	0.24	39,39,39,39	0
54	MG	2A	3403	1/1	0.97	0.09	38,38,38,38	0
54	MG	2A	3017	1/1	0.97	0.30	41,41,41,41	0
54	MG	2A	3204	1/1	0.97	0.19	60,60,60,60	0
54	MG	2A	3624	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3037	1/1	0.97	0.09	54,54,54,54	0
54	MG	2A	3626	1/1	0.97	0.05	28,28,28,28	0
54	MG	2A	3019	1/1	0.97	0.15	47,47,47,47	0
54	MG	1A	3625	1/1	0.97	0.34	47,47,47,47	0
54	MG	1A	3996	1/1	0.97	0.14	41,41,41,41	0
54	MG	1A	3094	1/1	0.97	0.28	35,35,35,35	0
54	MG	1A	3363	1/1	0.97	0.07	28,28,28,28	0
54	MG	17	103	1/1	0.97	0.25	40,40,40,40	0
54	MG	1a	1754	1/1	0.97	0.05	57,57,57,57	0
54	MG	1A	3443	1/1	0.97	0.06	30,30,30,30	0
54	MG	1A	3537	1/1	0.97	0.06	28,28,28,28	0
54	MG	2A	3029	1/1	0.97	0.13	32,32,32,32	0
54	MG	2A	3637	1/1	0.97	0.07	65,65,65,65	0
54	MG	1A	3854	1/1	0.97	0.13	38,38,38,38	0
54	MG	1A	3855	1/1	0.97	0.11	43,43,43,43	0
54	MG	1A	3444	1/1	0.97	0.05	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	4004	1/1	0.97	0.08	18,18,18,18	0
54	MG	1A	3540	1/1	0.97	0.04	35,35,35,35	0
54	MG	1a	1763	1/1	0.97	0.04	49,49,49,49	0
54	MG	1A	3176	1/1	0.97	0.08	49,49,49,49	0
54	MG	1A	4007	1/1	0.97	0.05	59,59,59,59	0
54	MG	1A	3072	1/1	0.97	0.21	38,38,38,38	0
54	MG	1A	3543	1/1	0.97	0.09	48,48,48,48	0
54	MG	1a	1769	1/1	0.97	0.06	58,58,58,58	0
54	MG	1A	3740	1/1	0.97	0.07	55,55,55,55	0
54	MG	2A	3228	1/1	0.97	0.31	45,45,45,45	0
54	MG	1A	3863	1/1	0.97	0.05	37,37,37,37	0
54	MG	1A	3545	1/1	0.97	0.05	50,50,50,50	0
54	MG	1A	3007	1/1	0.97	0.05	38,38,38,38	0
54	MG	1A	3026	1/1	0.97	0.19	40,40,40,40	0
54	MG	1a	1611	1/1	0.97	0.22	55,55,55,55	0
54	MG	1A	3135	1/1	0.97	0.24	43,43,43,43	0
54	MG	1A	3640	1/1	0.97	0.13	56,56,56,56	0
54	MG	2A	3443	1/1	0.97	0.08	44,44,44,44	0
54	MG	2A	3664	1/1	0.97	0.06	46,46,46,46	0
54	MG	2A	3665	1/1	0.97	0.04	28,28,28,28	0
54	MG	1a	1614	1/1	0.97	0.12	58,58,58,58	0
54	MG	2A	3237	1/1	0.97	0.18	52,52,52,52	0
54	MG	1A	3233	1/1	0.97	0.26	40,40,40,40	0
54	MG	1A	3872	1/1	0.97	0.05	39,39,39,39	0
54	MG	1A	3873	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	3182	1/1	0.97	0.11	44,44,44,44	0
54	MG	1A	3551	1/1	0.97	0.09	61,61,61,61	0
54	MG	2A	3451	1/1	0.97	0.19	65,65,65,65	0
54	MG	1A	3753	1/1	0.97	0.06	49,49,49,49	0
54	MG	1A	3644	1/1	0.97	0.08	34,34,34,34	0
54	MG	1A	3136	1/1	0.97	0.06	53,53,53,53	0
54	MG	2A	3246	1/1	0.97	0.14	49,49,49,49	0
54	MG	1A	3236	1/1	0.97	0.23	37,37,37,37	0
54	MG	1a	1625	1/1	0.97	0.15	54,54,54,54	0
54	MG	1A	3137	1/1	0.97	0.31	36,36,36,36	0
54	MG	1A	3457	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3304	1/1	0.97	0.22	52,52,52,52	0
54	MG	1A	3306	1/1	0.97	0.11	35,35,35,35	0
54	MG	1a	1794	1/1	0.97	0.07	62,62,62,62	0
54	MG	1A	3461	1/1	0.97	0.07	47,47,47,47	0
54	MG	1A	3239	1/1	0.97	0.29	47,47,47,47	0
54	MG	2A	3688	1/1	0.97	0.06	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3561	1/1	0.97	0.04	40,40,40,40	0
54	MG	2A	3071	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3767	1/1	0.97	0.08	50,50,50,50	0
54	MG	2A	3260	1/1	0.97	0.17	50,50,50,50	0
54	MG	1a	1634	1/1	0.97	0.09	43,43,43,43	0
54	MG	1A	3562	1/1	0.97	0.19	47,47,47,47	0
54	MG	1A	3240	1/1	0.97	0.16	48,48,48,48	0
54	MG	1B	219	1/1	0.97	0.07	40,40,40,40	0
54	MG	2A	3475	1/1	0.97	0.12	64,64,64,64	0
54	MG	1A	3564	1/1	0.97	0.25	57,57,57,57	0
54	MG	1A	3384	1/1	0.97	0.06	30,30,30,30	0
54	MG	1A	3188	1/1	0.97	0.28	45,45,45,45	0
54	MG	1B	223	1/1	0.97	0.06	65,65,65,65	0
54	MG	2A	3702	1/1	0.97	0.10	62,62,62,62	0
54	MG	1A	3467	1/1	0.97	0.05	28,28,28,28	0
54	MG	1A	3774	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3906	1/1	0.97	0.05	62,62,62,62	0
54	MG	2A	3084	1/1	0.97	0.10	49,49,49,49	0
54	MG	1A	3076	1/1	0.97	0.10	35,35,35,35	0
54	MG	2A	3708	1/1	0.97	0.07	43,43,43,43	0
54	MG	1A	3311	1/1	0.97	0.08	52,52,52,52	0
54	MG	1a	1812	1/1	0.97	0.15	72,72,72,72	0
54	MG	1A	3040	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3105	1/1	0.97	0.28	40,40,40,40	0
54	MG	2A	3279	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3472	1/1	0.97	0.07	54,54,54,54	0
54	MG	1D	304	1/1	0.97	0.10	43,43,43,43	0
54	MG	1A	3020	1/1	0.97	0.29	41,41,41,41	0
54	MG	1a	1653	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3914	1/1	0.97	0.04	54,54,54,54	0
54	MG	1D	309	1/1	0.97	0.04	47,47,47,47	0
54	MG	2a	3132	1/1	0.97	0.12	60,60,60,60	0
54	MG	1D	310	1/1	0.97	0.11	33,33,33,33	0
54	MG	2A	3497	1/1	0.97	0.06	56,56,56,56	0
54	MG	2A	3097	1/1	0.97	0.04	56,56,56,56	0
54	MG	1A	3781	1/1	0.97	0.06	50,50,50,50	0
54	MG	1D	312	1/1	0.97	0.08	45,45,45,45	0
54	MG	2a	3139	1/1	0.97	0.12	73,73,73,73	0
54	MG	2A	3100	1/1	0.97	0.16	50,50,50,50	0
54	MG	1A	3193	1/1	0.97	0.19	45,45,45,45	0
54	MG	1a	1660	1/1	0.97	0.08	68,68,68,68	0
54	MG	1A	3917	1/1	0.97	0.08	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1828	1/1	0.97	0.05	70,70,70,70	0
54	MG	1A	3668	1/1	0.97	0.06	49,49,49,49	0
54	MG	1A	3669	1/1	0.97	0.08	60,60,60,60	0
54	MG	1A	3194	1/1	0.97	0.12	52,52,52,52	0
54	MG	1A	3921	1/1	0.97	0.04	21,21,21,21	0
54	MG	1A	3923	1/1	0.97	0.17	41,41,41,41	0
54	MG	1A	3925	1/1	0.97	0.05	53,53,53,53	0
54	MG	1A	3671	1/1	0.97	0.09	40,40,40,40	0
54	MG	1A	3061	1/1	0.97	0.08	52,52,52,52	0
54	MG	1E	307	1/1	0.97	0.10	26,26,26,26	0
54	MG	1A	3929	1/1	0.97	0.08	55,55,55,55	0
54	MG	1E	309	1/1	0.97	0.06	54,54,54,54	0
54	MG	1E	310	1/1	0.97	0.08	56,56,56,56	0
54	MG	1F	302	1/1	0.97	0.21	38,38,38,38	0
54	MG	1a	1675	1/1	0.97	0.11	70,70,70,70	0
54	MG	1A	3930	1/1	0.97	0.06	64,64,64,64	0
54	MG	2A	3122	1/1	0.97	0.15	54,54,54,54	0
54	MG	1F	305	1/1	0.97	0.11	40,40,40,40	0
54	MG	1A	3478	1/1	0.97	0.09	50,50,50,50	0
54	MG	1F	308	1/1	0.97	0.21	60,60,60,60	0
54	MG	2A	3127	1/1	0.97	0.23	53,53,53,53	0
54	MG	1F	309	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3081	1/1	0.97	0.18	38,38,38,38	0
54	MG	1A	3082	1/1	0.97	0.06	42,42,42,42	0
54	MG	2A	3320	1/1	0.97	0.22	49,49,49,49	0
54	MG	1A	3112	1/1	0.97	0.10	32,32,32,32	0
54	MG	1A	3021	1/1	0.97	0.15	40,40,40,40	0
54	MG	1F	314	1/1	0.97	0.06	54,54,54,54	0
54	MG	2A	3134	1/1	0.97	0.12	77,77,77,77	0
54	MG	1A	3401	1/1	0.97	0.07	33,33,33,33	0
54	MG	2a	3175	1/1	0.97	0.05	67,67,67,67	0
54	MG	2A	3539	1/1	0.97	0.06	59,59,59,59	0
54	MG	1A	3031	1/1	0.97	0.10	20,20,20,20	0
54	MG	1A	3032	1/1	0.97	0.23	65,65,65,65	0
54	MG	1A	3682	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3154	1/1	0.97	0.22	40,40,40,40	0
54	MG	1A	3155	1/1	0.97	0.10	36,36,36,36	0
54	MG	2A	3331	1/1	0.97	0.05	67,67,67,67	0
54	MG	1A	3264	1/1	0.97	0.05	47,47,47,47	0
54	MG	2A	3142	1/1	0.97	0.06	43,43,43,43	0
54	MG	2A	3334	1/1	0.97	0.06	49,49,49,49	0
54	MG	1A	3117	1/1	0.97	0.23	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1864	1/1	0.97	0.05	60,60,60,60	0
54	MG	1A	3332	1/1	0.97	0.12	37,37,37,37	0
54	MG	1A	3266	1/1	0.97	0.10	51,51,51,51	0
54	MG	1A	3118	1/1	0.97	0.08	41,41,41,41	0
54	MG	1A	3336	1/1	0.97	0.40	47,47,47,47	0
54	MG	1A	3120	1/1	0.97	0.31	38,38,38,38	0
54	MG	1A	3269	1/1	0.97	0.16	42,42,42,42	0
54	MG	1A	3810	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3162	1/1	0.97	0.27	41,41,41,41	0
54	MG	1P	205	1/1	0.97	0.07	38,38,38,38	0
54	MG	1Q	201	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	3271	1/1	0.97	0.06	50,50,50,50	0
54	MG	2V	202	1/1	0.97	0.13	54,54,54,54	0
54	MG	1A	3813	1/1	0.97	0.06	46,46,46,46	0
56	ZIT	1A	4023	52/52	0.97	0.09	20,37,57,63	0
54	MG	2W	201	1/1	0.97	0.26	49,49,49,49	0
54	MG	1A	3343	1/1	0.97	0.11	29,29,29,29	0
54	MG	1A	3699	1/1	0.97	0.05	42,42,42,42	0
54	MG	1A	3163	1/1	0.97	0.07	46,46,46,46	0
54	MG	1A	3033	1/1	0.97	0.13	44,44,44,44	0
54	MG	2A	3567	1/1	0.97	0.08	59,59,59,59	0
54	MG	1A	3510	1/1	0.97	0.06	52,52,52,52	0
54	MG	1A	3213	1/1	0.97	0.09	55,55,55,55	0
54	MG	1A	3704	1/1	0.97	0.08	61,61,61,61	0
54	MG	1A	3275	1/1	0.97	0.38	37,37,37,37	0
54	MG	2A	3166	1/1	0.97	0.11	52,52,52,52	0
54	MG	2A	3650	1/1	0.98	0.09	57,57,57,57	0
54	MG	2A	3125	1/1	0.98	0.15	40,40,40,40	0
54	MG	1a	1724	1/1	0.98	0.07	68,68,68,68	0
54	MG	2A	3653	1/1	0.98	0.10	63,63,63,63	0
54	MG	1A	3255	1/1	0.98	0.10	35,35,35,35	0
54	MG	1A	4021	1/1	0.98	0.06	58,58,58,58	0
54	MG	1A	3784	1/1	0.98	0.06	48,48,48,48	0
54	MG	1A	3144	1/1	0.98	0.12	41,41,41,41	0
54	MG	1A	3175	1/1	0.98	0.12	35,35,35,35	0
54	MG	1A	3690	1/1	0.98	0.10	60,60,60,60	0
54	MG	2A	3660	1/1	0.98	0.07	46,46,46,46	0
54	MG	1A	3145	1/1	0.98	0.04	37,37,37,37	0
54	MG	1A	3905	1/1	0.98	0.04	45,45,45,45	0
54	MG	1A	3524	1/1	0.98	0.04	26,26,26,26	0
54	MG	1A	3693	1/1	0.98	0.04	67,67,67,67	0
54	MG	1a	1735	1/1	0.98	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	3370	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	3146	1/1	0.98	0.12	36,36,36,36	0
54	MG	1A	3178	1/1	0.98	0.15	33,33,33,33	0
54	MG	1B	212	1/1	0.98	0.07	48,48,48,48	0
54	MG	1A	3373	1/1	0.98	0.09	32,32,32,32	0
54	MG	2A	3307	1/1	0.98	0.18	55,55,55,55	0
54	MG	1A	3121	1/1	0.98	0.07	25,25,25,25	0
54	MG	1g	202	1/1	0.98	0.06	63,63,63,63	0
54	MG	1A	3314	1/1	0.98	0.07	25,25,25,25	0
54	MG	1A	3448	1/1	0.98	0.06	47,47,47,47	0
54	MG	1A	3315	1/1	0.98	0.13	40,40,40,40	0
54	MG	2A	3677	1/1	0.98	0.07	41,41,41,41	0
54	MG	1a	1603	1/1	0.98	0.09	51,51,51,51	0
54	MG	2A	3149	1/1	0.98	0.05	44,44,44,44	0
54	MG	1A	3100	1/1	0.98	0.12	52,52,52,52	0
54	MG	1a	1747	1/1	0.98	0.07	39,39,39,39	0
54	MG	1A	3046	1/1	0.98	0.07	16,16,16,16	0
54	MG	1A	3381	1/1	0.98	0.05	22,22,22,22	0
54	MG	1A	3102	1/1	0.98	0.29	35,35,35,35	0
54	MG	1A	3383	1/1	0.98	0.08	42,42,42,42	0
54	MG	1A	3183	1/1	0.98	0.10	34,34,34,34	0
54	MG	1A	3924	1/1	0.98	0.04	48,48,48,48	0
54	MG	1A	3385	1/1	0.98	0.05	35,35,35,35	0
54	MG	1A	3220	1/1	0.98	0.07	32,32,32,32	0
54	MG	1A	3624	1/1	0.98	0.21	38,38,38,38	0
54	MG	1A	3928	1/1	0.98	0.04	65,65,65,65	0
54	MG	1A	3221	1/1	0.98	0.16	28,28,28,28	0
54	MG	2A	3003	1/1	0.98	0.05	42,42,42,42	0
54	MG	1D	302	1/1	0.98	0.04	53,53,53,53	0
54	MG	1A	3712	1/1	0.98	0.12	43,43,43,43	0
54	MG	2A	3006	1/1	0.98	0.08	46,46,46,46	0
54	MG	1A	3544	1/1	0.98	0.04	34,34,34,34	0
54	MG	2A	3008	1/1	0.98	0.05	46,46,46,46	0
54	MG	1A	3388	1/1	0.98	0.08	52,52,52,52	0
54	MG	1D	306	1/1	0.98	0.04	44,44,44,44	0
54	MG	2A	3171	1/1	0.98	0.05	47,47,47,47	0
54	MG	2A	3518	1/1	0.98	0.04	58,58,58,58	0
54	MG	1A	3934	1/1	0.98	0.10	60,60,60,60	0
54	MG	2A	3012	1/1	0.98	0.05	30,30,30,30	0
54	MG	1A	3715	1/1	0.98	0.04	38,38,38,38	0
54	MG	2A	3522	1/1	0.98	0.05	39,39,39,39	0
54	MG	1A	3184	1/1	0.98	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3085	1/1	0.98	0.25	60,60,60,60	0
54	MG	1A	3323	1/1	0.98	0.06	26,26,26,26	0
54	MG	1A	3938	1/1	0.98	0.09	44,44,44,44	0
54	MG	1A	3939	1/1	0.98	0.09	55,55,55,55	0
54	MG	1D	314	1/1	0.98	0.07	49,49,49,49	0
54	MG	1A	3103	1/1	0.98	0.05	56,56,56,56	0
54	MG	2A	3020	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3941	1/1	0.98	0.08	67,67,67,67	0
54	MG	1A	3013	1/1	0.98	0.06	20,20,20,20	0
54	MG	1A	3818	1/1	0.98	0.06	46,46,46,46	0
54	MG	1A	3187	1/1	0.98	0.16	43,43,43,43	0
54	MG	1A	3226	1/1	0.98	0.12	43,43,43,43	0
54	MG	2A	3719	1/1	0.98	0.11	47,47,47,47	0
54	MG	1E	301	1/1	0.98	0.18	38,38,38,38	0
54	MG	1A	3722	1/1	0.98	0.04	44,44,44,44	0
54	MG	1E	303	1/1	0.98	0.06	35,35,35,35	0
54	MG	1A	3001	1/1	0.98	0.04	38,38,38,38	0
54	MG	1a	1784	1/1	0.98	0.17	64,64,64,64	0
54	MG	1E	305	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3823	1/1	0.98	0.05	42,42,42,42	0
54	MG	1A	3019	1/1	0.98	0.23	32,32,32,32	0
54	MG	1A	3229	1/1	0.98	0.05	41,41,41,41	0
54	MG	1A	3130	1/1	0.98	0.04	35,35,35,35	0
54	MG	1A	3028	1/1	0.98	0.25	40,40,40,40	0
54	MG	1A	3279	1/1	0.98	0.10	33,33,33,33	0
54	MG	1A	3157	1/1	0.98	0.23	44,44,44,44	0
54	MG	1F	304	1/1	0.98	0.25	40,40,40,40	0
54	MG	1A	3559	1/1	0.98	0.08	40,40,40,40	0
54	MG	1a	1649	1/1	0.98	0.15	61,61,61,61	0
54	MG	1A	3158	1/1	0.98	0.36	46,46,46,46	0
54	MG	1F	307	1/1	0.98	0.11	39,39,39,39	0
54	MG	1A	3338	1/1	0.98	0.08	33,33,33,33	0
54	MG	2B	210	1/1	0.98	0.36	57,57,57,57	0
54	MG	1A	3733	1/1	0.98	0.04	45,45,45,45	0
54	MG	1A	3734	1/1	0.98	0.06	75,75,75,75	0
54	MG	1A	3339	1/1	0.98	0.03	34,34,34,34	0
54	MG	1A	3075	1/1	0.98	0.05	37,37,37,37	0
54	MG	1A	3109	1/1	0.98	0.13	48,48,48,48	0
54	MG	1A	3063	1/1	0.98	0.05	41,41,41,41	0
54	MG	2A	3378	1/1	0.98	0.05	50,50,50,50	0
54	MG	2A	3051	1/1	0.98	0.06	42,42,42,42	0
54	MG	2A	3380	1/1	0.98	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3381	1/1	0.98	0.07	33,33,33,33	0
54	MG	1A	3482	1/1	0.98	0.04	55,55,55,55	0
54	MG	1A	3409	1/1	0.98	0.06	26,26,26,26	0
54	MG	1F	317	1/1	0.98	0.07	51,51,51,51	0
54	MG	1A	3741	1/1	0.98	0.06	30,30,30,30	0
54	MG	2A	3386	1/1	0.98	0.06	41,41,41,41	0
54	MG	2a	3133	1/1	0.98	0.07	62,62,62,62	0
54	MG	1A	3742	1/1	0.98	0.06	34,34,34,34	0
54	MG	1A	3484	1/1	0.98	0.04	54,54,54,54	0
54	MG	1A	3410	1/1	0.98	0.06	27,27,27,27	0
54	MG	2E	301	1/1	0.98	0.07	60,60,60,60	0
54	MG	2A	3059	1/1	0.98	0.04	46,46,46,46	0
54	MG	1A	3972	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3745	1/1	0.98	0.19	38,38,38,38	0
54	MG	1N	201	1/1	0.98	0.10	48,48,48,48	0
54	MG	2A	3578	1/1	0.98	0.06	63,63,63,63	0
54	MG	1A	3238	1/1	0.98	0.14	36,36,36,36	0
54	MG	1A	3286	1/1	0.98	0.06	34,34,34,34	0
54	MG	2F	304	1/1	0.98	0.17	49,49,49,49	0
54	MG	1A	3976	1/1	0.98	0.03	27,27,27,27	0
54	MG	2A	3066	1/1	0.98	0.06	51,51,51,51	0
54	MG	1A	3287	1/1	0.98	0.23	40,40,40,40	0
54	MG	1A	3415	1/1	0.98	0.10	31,31,31,31	0
54	MG	1A	3750	1/1	0.98	0.05	25,25,25,25	0
54	MG	1a	1821	1/1	0.98	0.05	65,65,65,65	0
54	MG	1A	3029	1/1	0.98	0.05	47,47,47,47	0
54	MG	1A	3164	1/1	0.98	0.16	38,38,38,38	0
54	MG	1A	3418	1/1	0.98	0.06	29,29,29,29	0
54	MG	1A	3042	1/1	0.98	0.07	30,30,30,30	0
54	MG	1A	3755	1/1	0.98	0.06	64,64,64,64	0
54	MG	2A	3410	1/1	0.98	0.08	51,51,51,51	0
54	MG	1A	3043	1/1	0.98	0.12	26,26,26,26	0
54	MG	1Q	204	1/1	0.98	0.06	42,42,42,42	0
54	MG	1Q	205	1/1	0.98	0.09	50,50,50,50	0
54	MG	1A	3860	1/1	0.98	0.10	37,37,37,37	0
54	MG	1A	3662	1/1	0.98	0.09	34,34,34,34	0
54	MG	1A	3243	1/1	0.98	0.17	32,32,32,32	0
54	MG	1A	3759	1/1	0.98	0.07	28,28,28,28	0
54	MG	1A	3760	1/1	0.98	0.11	36,36,36,36	0
54	MG	1A	3138	1/1	0.98	0.26	36,36,36,36	0
54	MG	1A	3500	1/1	0.98	0.06	36,36,36,36	0
54	MG	1A	3867	1/1	0.98	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3096	1/1	0.98	0.05	21,21,21,21	0
54	MG	1A	3355	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3203	1/1	0.98	0.06	54,54,54,54	0
54	MG	1a	1841	1/1	0.98	0.05	66,66,66,66	0
54	MG	1U	204	1/1	0.98	0.19	32,32,32,32	0
54	MG	2A	3610	1/1	0.98	0.04	53,53,53,53	0
54	MG	1A	3871	1/1	0.98	0.07	35,35,35,35	0
54	MG	1U	206	1/1	0.98	0.15	37,37,37,37	0
54	MG	1a	1697	1/1	0.98	0.13	52,52,52,52	0
54	MG	1A	3426	1/1	0.98	0.04	43,43,43,43	0
54	MG	2A	3257	1/1	0.98	0.14	28,28,28,28	0
54	MG	1V	203	1/1	0.98	0.17	48,48,48,48	0
54	MG	1A	3297	1/1	0.98	0.07	20,20,20,20	0
54	MG	1A	3506	1/1	0.98	0.06	63,63,63,63	0
54	MG	1A	3507	1/1	0.98	0.08	35,35,35,35	0
54	MG	1A	3428	1/1	0.98	0.03	34,34,34,34	0
54	MG	1W	202	1/1	0.98	0.21	48,48,48,48	0
54	MG	1A	3247	1/1	0.98	0.34	39,39,39,39	0
54	MG	2A	3442	1/1	0.98	0.07	42,42,42,42	0
54	MG	1W	204	1/1	0.98	0.08	53,53,53,53	0
54	MG	1a	1856	1/1	0.98	0.04	56,56,56,56	0
54	MG	1A	3299	1/1	0.98	0.09	35,35,35,35	0
54	MG	2A	3106	1/1	0.98	0.10	37,37,37,37	0
54	MG	1A	3248	1/1	0.98	0.13	38,38,38,38	0
54	MG	10	101	1/1	0.98	0.10	46,46,46,46	0
54	MG	1A	3140	1/1	0.98	0.05	54,54,54,54	0
54	MG	1A	3883	1/1	0.98	0.04	50,50,50,50	0
54	MG	1A	3514	1/1	0.98	0.07	46,46,46,46	0
54	MG	2A	3274	1/1	0.98	0.06	45,45,45,45	0
54	MG	1A	3055	1/1	0.98	0.25	41,41,41,41	0
54	MG	1A	3044	1/1	0.98	0.07	38,38,38,38	0
54	MG	1A	4012	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3887	1/1	0.98	0.06	47,47,47,47	0
54	MG	1A	3015	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3889	1/1	0.98	0.06	60,60,60,60	0
54	MG	11	103	1/1	0.98	0.05	49,49,49,49	0
54	MG	1A	3518	1/1	0.98	0.05	47,47,47,47	0
54	MG	1A	3600	1/1	0.98	0.05	53,53,53,53	0
54	MG	2A	3121	1/1	0.98	0.05	43,43,43,43	0
54	MG	2A	3285	1/1	0.98	0.09	38,38,38,38	0
54	MG	1A	3254	1/1	0.98	0.52	48,48,48,48	0
54	MG	1A	3782	1/1	0.98	0.04	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1875	1/1	0.98	0.04	56,56,56,56	0
59	ZN	2Y	202	1/1	0.98	0.04	92,92,92,92	0
59	ZN	24	501	1/1	0.98	0.10	128,128,128,128	0
59	ZN	29	501	1/1	0.98	0.04	70,70,70,70	0
59	ZN	2n	501	1/1	0.98	0.05	95,95,95,95	0
60	SF4	2d	501	8/8	0.98	0.05	72,83,85,87	0
54	MG	1R	201	1/1	0.99	0.10	41,41,41,41	0
54	MG	1R	202	1/1	0.99	0.14	43,43,43,43	0
54	MG	1A	3263	1/1	0.99	0.08	32,32,32,32	0
54	MG	1A	3119	1/1	0.99	0.14	34,34,34,34	0
54	MG	1A	3348	1/1	0.99	0.09	28,28,28,28	0
54	MG	2A	3408	1/1	0.99	0.08	51,51,51,51	0
54	MG	1A	3374	1/1	0.99	0.03	22,22,22,22	0
54	MG	1A	3459	1/1	0.99	0.03	33,33,33,33	0
54	MG	1A	3966	1/1	0.99	0.06	50,50,50,50	0
54	MG	2A	3413	1/1	0.99	0.04	43,43,43,43	0
54	MG	1a	1855	1/1	0.99	0.03	52,52,52,52	0
54	MG	1T	201	1/1	0.99	0.04	63,63,63,63	0
54	MG	1A	3494	1/1	0.99	0.03	32,32,32,32	0
54	MG	1A	3005	1/1	0.99	0.14	28,28,28,28	0
54	MG	2A	3346	1/1	0.99	0.10	42,42,42,42	0
54	MG	1A	3326	1/1	0.99	0.04	28,28,28,28	0
54	MG	2a	3154	1/1	0.99	0.05	54,54,54,54	0
54	MG	2A	3648	1/1	0.99	0.03	34,34,34,34	0
54	MG	1A	3305	1/1	0.99	0.11	43,43,43,43	0
54	MG	1A	3378	1/1	0.99	0.04	19,19,19,19	0
54	MG	1A	3006	1/1	0.99	0.03	27,27,27,27	0
54	MG	1A	3678	1/1	0.99	0.03	45,45,45,45	0
54	MG	1A	3922	1/1	0.99	0.07	47,47,47,47	0
54	MG	1A	3231	1/1	0.99	0.19	39,39,39,39	0
54	MG	2A	3426	1/1	0.99	0.03	66,66,66,66	0
54	MG	1V	202	1/1	0.99	0.19	39,39,39,39	0
54	MG	1F	301	1/1	0.99	0.06	37,37,37,37	0
54	MG	1a	1868	1/1	0.99	0.04	54,54,54,54	0
54	MG	1A	3794	1/1	0.99	0.06	33,33,33,33	0
54	MG	1A	3466	1/1	0.99	0.05	29,29,29,29	0
54	MG	1A	3122	1/1	0.99	0.08	33,33,33,33	0
54	MG	1A	3250	1/1	0.99	0.12	36,36,36,36	0
54	MG	1A	3879	1/1	0.99	0.03	51,51,51,51	0
54	MG	1a	1622	1/1	0.99	0.04	56,56,56,56	0
54	MG	1A	3609	1/1	0.99	0.05	51,51,51,51	0
54	MG	1A	3881	1/1	0.99	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3111	1/1	0.99	0.19	32,32,32,32	0
54	MG	1A	3685	1/1	0.99	0.11	38,38,38,38	0
54	MG	2a	3176	1/1	0.99	0.14	56,56,56,56	0
54	MG	1a	1749	1/1	0.99	0.07	41,41,41,41	0
54	MG	1A	3575	1/1	0.99	0.06	36,36,36,36	0
54	MG	1A	3333	1/1	0.99	0.07	24,24,24,24	0
54	MG	1A	3095	1/1	0.99	0.05	47,47,47,47	0
54	MG	1A	3174	1/1	0.99	0.06	50,50,50,50	0
54	MG	1A	3508	1/1	0.99	0.08	33,33,33,33	0
54	MG	1A	3473	1/1	0.99	0.03	55,55,55,55	0
54	MG	1a	1756	1/1	0.99	0.08	59,59,59,59	0
54	MG	1A	3414	1/1	0.99	0.07	20,20,20,20	0
54	MG	1A	3161	1/1	0.99	0.14	41,41,41,41	0
54	MG	2A	3525	1/1	0.99	0.04	65,65,65,65	0
54	MG	1A	3018	1/1	0.99	0.21	27,27,27,27	0
54	MG	1A	3445	1/1	0.99	0.08	45,45,45,45	0
54	MG	1A	3852	1/1	0.99	0.06	41,41,41,41	0
54	MG	2E	303	1/1	0.99	0.04	55,55,55,55	0
54	MG	2A	3605	1/1	0.99	0.04	41,41,41,41	0
54	MG	1A	3089	1/1	0.99	0.07	45,45,45,45	0
54	MG	1A	3946	1/1	0.99	0.05	62,62,62,62	0
54	MG	2A	3455	1/1	0.99	0.03	40,40,40,40	0
54	MG	2F	301	1/1	0.99	0.17	43,43,43,43	0
54	MG	1A	3390	1/1	0.99	0.03	27,27,27,27	0
54	MG	1A	3206	1/1	0.99	0.13	38,38,38,38	0
54	MG	1A	3296	1/1	0.99	0.10	23,23,23,23	0
54	MG	1A	3899	1/1	0.99	0.03	37,37,37,37	0
54	MG	2A	3460	1/1	0.99	0.04	56,56,56,56	0
54	MG	1a	1768	1/1	0.99	0.04	52,52,52,52	0
54	MG	15	101	1/1	0.99	0.14	31,31,31,31	0
54	MG	1A	3900	1/1	0.99	0.03	51,51,51,51	0
54	MG	15	103	1/1	0.99	0.18	34,34,34,34	0
54	MG	2A	3390	1/1	0.99	0.04	35,35,35,35	0
54	MG	1A	3901	1/1	0.99	0.09	46,46,46,46	0
54	MG	1A	3115	1/1	0.99	0.12	37,37,37,37	0
54	MG	2A	3393	1/1	0.99	0.08	45,45,45,45	0
54	MG	1D	308	1/1	0.99	0.03	23,23,23,23	0
54	MG	1A	3903	1/1	0.99	0.04	51,51,51,51	0
54	MG	1A	3904	1/1	0.99	0.04	35,35,35,35	0
54	MG	17	101	1/1	0.99	0.05	38,38,38,38	0
59	ZN	15	109	1/1	0.99	0.05	48,48,48,48	0
59	ZN	16	501	1/1	0.99	0.05	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	ZN	19	103	1/1	0.99	0.03	46,46,46,46	0
59	ZN	1n	103	1/1	0.99	0.03	67,67,67,67	0
54	MG	1A	3009	1/1	0.99	0.06	37,37,37,37	0
54	MG	1A	3209	1/1	0.99	0.14	38,38,38,38	0
59	ZN	26	501	1/1	0.99	0.03	66,66,66,66	0
54	MG	1A	3048	1/1	0.99	0.02	29,29,29,29	0
54	MG	1A	3908	1/1	0.99	0.06	55,55,55,55	0
60	SF4	1d	305	8/8	0.99	0.04	63,70,75,78	0
54	MG	1A	3079	1/1	0.99	0.12	36,36,36,36	0
54	MG	2A	3412	1/1	1.00	0.04	38,38,38,38	0
54	MG	1B	213	1/1	1.00	0.03	48,48,48,48	0
54	MG	1A	3849	1/1	1.00	0.03	26,26,26,26	0
59	ZN	1Y	202	1/1	1.00	0.03	63,63,63,63	0
54	MG	2A	3576	1/1	1.00	0.02	27,27,27,27	0
54	MG	2A	3647	1/1	1.00	0.06	36,36,36,36	0
54	MG	1A	3637	1/1	1.00	0.09	34,34,34,34	0
54	MG	1A	3525	1/1	1.00	0.02	23,23,23,23	0
54	MG	1A	3977	1/1	1.00	0.03	36,36,36,36	0
54	MG	2A	3514	1/1	1.00	0.04	43,43,43,43	0
54	MG	1A	3485	1/1	1.00	0.03	35,35,35,35	0
59	ZN	25	104	1/1	1.00	0.03	54,54,54,54	0
54	MG	1A	3933	1/1	1.00	0.02	53,53,53,53	0
54	MG	1A	3539	1/1	1.00	0.02	45,45,45,45	0
54	MG	1A	3839	1/1	1.00	0.05	49,49,49,49	0
54	MG	1A	3352	1/1	1.00	0.07	38,38,38,38	0
54	MG	1A	3491	1/1	1.00	0.08	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.