



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:37 PM UTC

PDB ID : 8VTY / pdb_00008vty
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with ciprofloxacin and protein Y at 2.60Å resolution
Authors : Aleksandrova, E.V.; Ma, C.-X.; Klepacki, D.; Alizadeh, F.; Vazquez-Laslop, N.; Liang, J.-H.; Polikanov, Y.S.; Mankin, A.S.
Deposited on : 2024-01-27
Resolution : 2.60 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

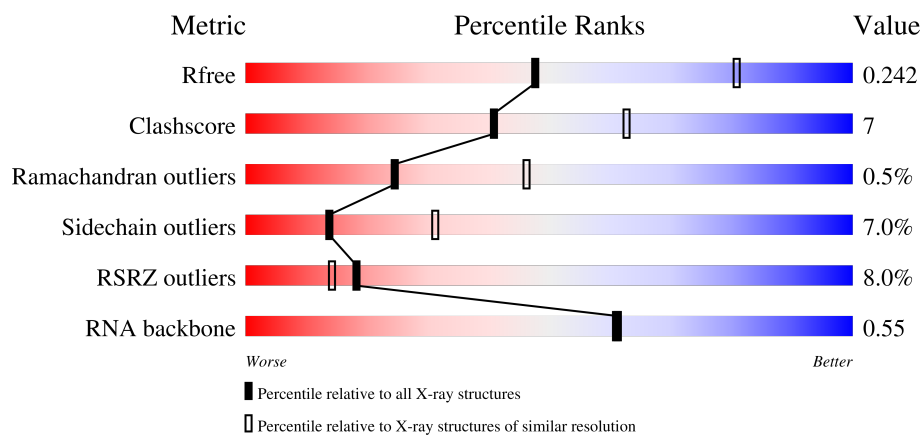
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	5% 69% 25% • •
1	2A	2915	6% 66% 27% 6% •
2	1B	121	2% 80% 18% • •

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Mol	Chain	Length	Quality of chain
2	2B	121	5% 59% 37% ..
3	1D	276	% 83% 15% .
3	2D	276	% 83% 13% .
4	1E	206	% 78% 17% ..
4	2E	206	% 76% 19% ..
5	1F	210	% 77% 16% ..
5	2F	210	73% 20% ..
6	1G	182	7% 74% 22% ..
6	2G	182	25% 52% 44% ..
7	1H	180	4% 76% 21% ..
7	2H	180	18% 61% 33% ..
8	1I	148	7% 78% 17% ..
8	2I	148	3% 77% 20% ..
9	1N	140	% 83% 13% .
9	2N	140	2% 78% 21% .
10	1O	122	84% 16%
10	2O	122	84% 16%
11	1P	150	% 81% 17% ..
11	2P	150	% 82% 13% ..
12	1Q	141	87% 11% .
12	2Q	141	4% 82% 16% .
13	1R	118	80% 19% .
13	2R	118	79% 19% .
14	1S	112	% 78% 18% ..
14	2S	112	19% 69% 28% ..

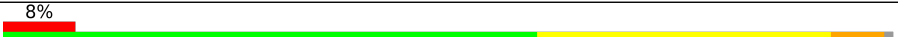
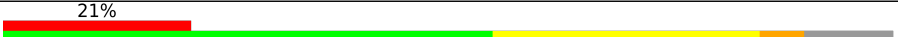
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Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25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

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3641	-	-	-	X
54	MG	1A	3996	-	-	-	X
54	MG	1a	1794	-	-	-	X
54	MG	2A	3190	-	-	-	X
54	MG	2A	3409	-	-	-	X
54	MG	2a	3079	-	-	-	X
54	MG	2a	3160	-	-	-	X

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 297563 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	1056	Total	Mg	0	0
			1056	1056		
54	1B	29	Total	Mg	0	0
			29	29		
54	1D	18	Total	Mg	0	0
			18	18		
54	1E	9	Total	Mg	0	0
			9	9		
54	1F	19	Total	Mg	0	0
			19	19		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	3	Total	Mg	0	0
			3	3		
54	1N	5	Total	Mg	0	0
			5	5		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	6	Total	Mg	0	0
			6	6		
54	1Q	5	Total	Mg	0	0
			5	5		
54	1R	6	Total	Mg	0	0
			6	6		
54	1T	5	Total	Mg	0	0
			5	5		
54	1U	7	Total	Mg	0	0
			7	7		
54	1V	6	Total	Mg	0	0
			6	6		
54	1W	3	Total	Mg	0	0
			3	3		
54	1Z	1	Total	Mg	0	0
			1	1		
54	10	7	Total	Mg	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	11	5	Total 5	Mg 5	0	0
54	13	4	Total 4	Mg 4	0	0
54	14	1	Total 1	Mg 1	0	0
54	15	8	Total 8	Mg 8	0	0
54	17	7	Total 7	Mg 7	0	0
54	18	3	Total 3	Mg 3	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	277	Total 277	Mg 277	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	5	Total 5	Mg 5	0	0
54	1e	2	Total 2	Mg 2	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	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	3	Total 3	Mg 3	0	0
54	1o	1	Total 1	Mg 1	0	0
54	1t	1	Total 1	Mg 1	0	0

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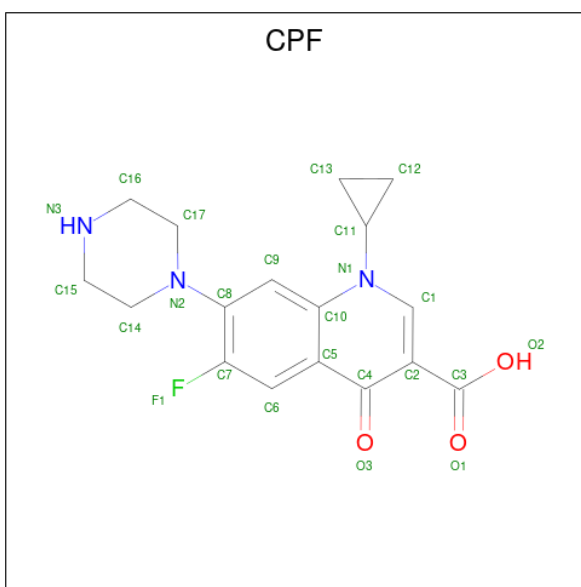
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1y	4	Total 4	Mg 4	0	0
54	2A	741	Total 741	Mg 741	0	0
54	2B	18	Total 18	Mg 18	0	0
54	2D	12	Total 12	Mg 12	0	0
54	2E	7	Total 7	Mg 7	0	0
54	2F	4	Total 4	Mg 4	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2N	1	Total 1	Mg 1	0	0
54	2O	2	Total 2	Mg 2	0	0
54	2Q	3	Total 3	Mg 3	0	0
54	2R	3	Total 3	Mg 3	0	0
54	2T	3	Total 3	Mg 3	0	0
54	2V	3	Total 3	Mg 3	0	0
54	2W	3	Total 3	Mg 3	0	0
54	2X	1	Total 1	Mg 1	0	0
54	2Y	1	Total 1	Mg 1	0	0
54	20	3	Total 3	Mg 3	0	0
54	21	1	Total 1	Mg 1	0	0
54	23	2	Total 2	Mg 2	0	0
54	25	1	Total 1	Mg 1	0	0
54	27	1	Total 1	Mg 1	0	0

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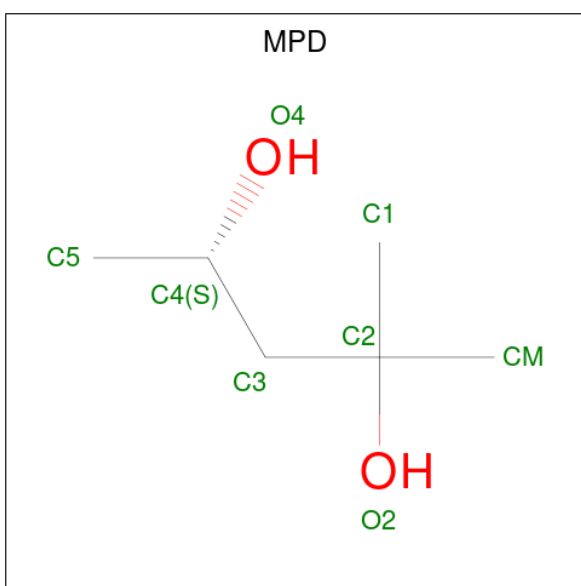
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	28	2	Total 2	Mg 2	0	0
54	2a	195	Total 195	Mg 195	0	0
54	2d	1	Total 1	Mg 1	0	0
54	2e	1	Total 1	Mg 1	0	0
54	2f	2	Total 2	Mg 2	0	0
54	2j	1	Total 1	Mg 1	0	0
54	2k	1	Total 1	Mg 1	0	0
54	2n	1	Total 1	Mg 1	0	0
54	2o	1	Total 1	Mg 1	0	0
54	2p	1	Total 1	Mg 1	0	0
54	2r	1	Total 1	Mg 1	0	0
54	2t	1	Total 1	Mg 1	0	0

- Molecule 55 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDR OQUINOLINE-3-CARBOXYLIC ACID (CCD ID: CPF) (formula: C₁₇H₁₈FN₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	1A	1	Total	C	F	N	O	0	0
			24	17	1	3	3		
55	2A	1	Total	C	F	N	O	0	0
			24	17	1	3	3		

- Molecule 56 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



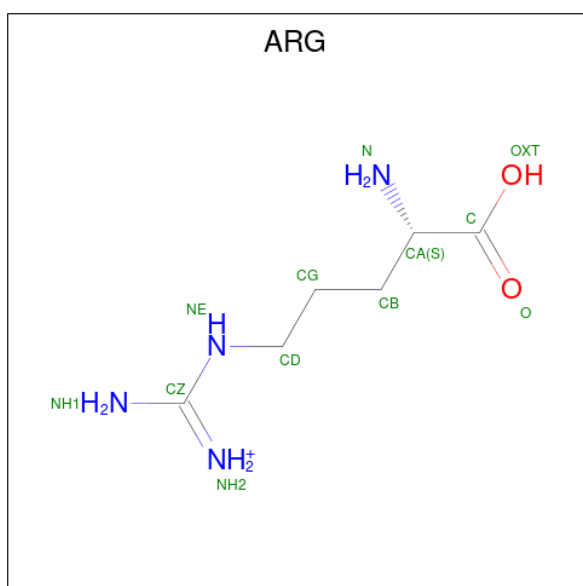
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	1A	1	Total	C	O	0	0
			8	6	2		
56	1O	1	Total	C	O	0	0
			8	6	2		

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

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



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

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

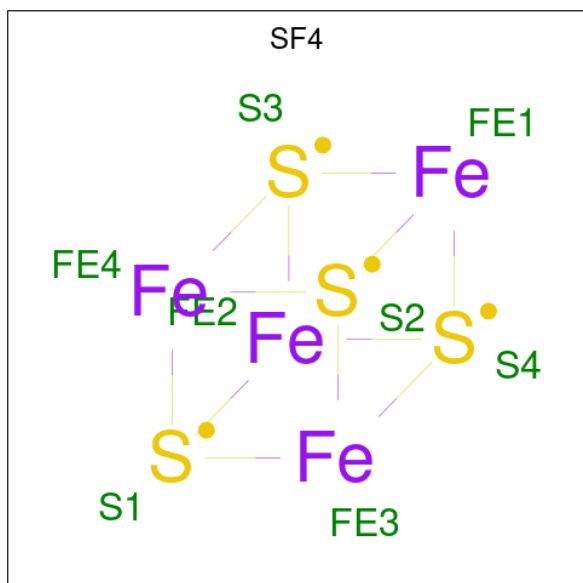
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

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



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

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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3927	Total	O	0	0
			3927	3927		
60	1B	89	Total	O	0	0
			89	89		
60	1D	110	Total	O	0	0
			110	110		
60	1E	72	Total	O	0	0
			72	72		
60	1F	67	Total	O	0	0
			67	67		
60	1G	16	Total	O	0	0
			16	16		
60	1H	14	Total	O	0	0
			14	14		
60	1I	5	Total	O	0	0
			5	5		
60	1N	52	Total	O	0	0
			52	52		
60	1O	25	Total	O	0	0
			25	25		
60	1P	65	Total	O	0	0
			65	65		
60	1Q	41	Total	O	0	0
			41	41		
60	1R	32	Total	O	0	0
			32	32		
60	1S	8	Total	O	0	0
			8	8		
60	1T	36	Total	O	0	0
			36	36		
60	1U	43	Total	O	0	0
			43	43		
60	1V	36	Total	O	0	0
			36	36		
60	1W	28	Total	O	0	0
			28	28		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1X	26	Total 26	O 26	0	0
60	1Y	17	Total 17	O 17	0	0
60	1Z	11	Total 11	O 11	0	0
60	10	25	Total 25	O 25	0	0
60	11	28	Total 28	O 28	0	0
60	12	13	Total 13	O 13	0	0
60	13	25	Total 25	O 25	0	0
60	14	3	Total 3	O 3	0	0
60	15	28	Total 28	O 28	0	0
60	16	20	Total 20	O 20	0	0
60	17	13	Total 13	O 13	0	0
60	18	28	Total 28	O 28	0	0
60	19	8	Total 8	O 8	0	0
60	1a	496	Total 496	O 496	0	0
60	1b	1	Total 1	O 1	0	0
60	1c	1	Total 1	O 1	0	0
60	1d	9	Total 9	O 9	0	0
60	1e	10	Total 10	O 10	0	0
60	1f	1	Total 1	O 1	0	0
60	1h	1	Total 1	O 1	0	0
60	1j	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1k	1	Total 1	O 1	0	0
60	1l	4	Total 4	O 4	0	0
60	1o	4	Total 4	O 4	0	0
60	1p	1	Total 1	O 1	0	0
60	1y	5	Total 5	O 5	0	0
60	2A	2249	Total 2249	O 2249	0	0
60	2B	42	Total 42	O 42	0	0
60	2D	47	Total 47	O 47	0	0
60	2E	28	Total 28	O 28	0	0
60	2F	23	Total 23	O 23	0	0
60	2G	4	Total 4	O 4	0	0
60	2H	1	Total 1	O 1	0	0
60	2N	6	Total 6	O 6	0	0
60	2O	15	Total 15	O 15	0	0
60	2P	21	Total 21	O 21	0	0
60	2Q	18	Total 18	O 18	0	0
60	2R	22	Total 22	O 22	0	0
60	2S	2	Total 2	O 2	0	0
60	2T	12	Total 12	O 12	0	0
60	2U	16	Total 16	O 16	0	0
60	2V	8	Total 8	O 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2W	19	Total 19	O 19	0	0
60	2X	8	Total 8	O 8	0	0
60	2Y	4	Total 4	O 4	0	0
60	2Z	8	Total 8	O 8	0	0
60	20	10	Total 10	O 10	0	0
60	21	17	Total 17	O 17	0	0
60	22	2	Total 2	O 2	0	0
60	23	2	Total 2	O 2	0	0
60	25	7	Total 7	O 7	0	0
60	26	6	Total 6	O 6	0	0
60	27	9	Total 9	O 9	0	0
60	28	15	Total 15	O 15	0	0
60	2a	404	Total 404	O 404	0	0
60	2d	3	Total 3	O 3	0	0
60	2e	3	Total 3	O 3	0	0
60	2f	3	Total 3	O 3	0	0
60	2j	2	Total 2	O 2	0	0
60	2l	5	Total 5	O 5	0	0
60	2o	2	Total 2	O 2	0	0
60	2p	1	Total 1	O 1	0	0
60	2q	1	Total 1	O 1	0	0

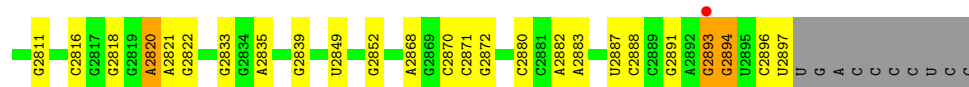
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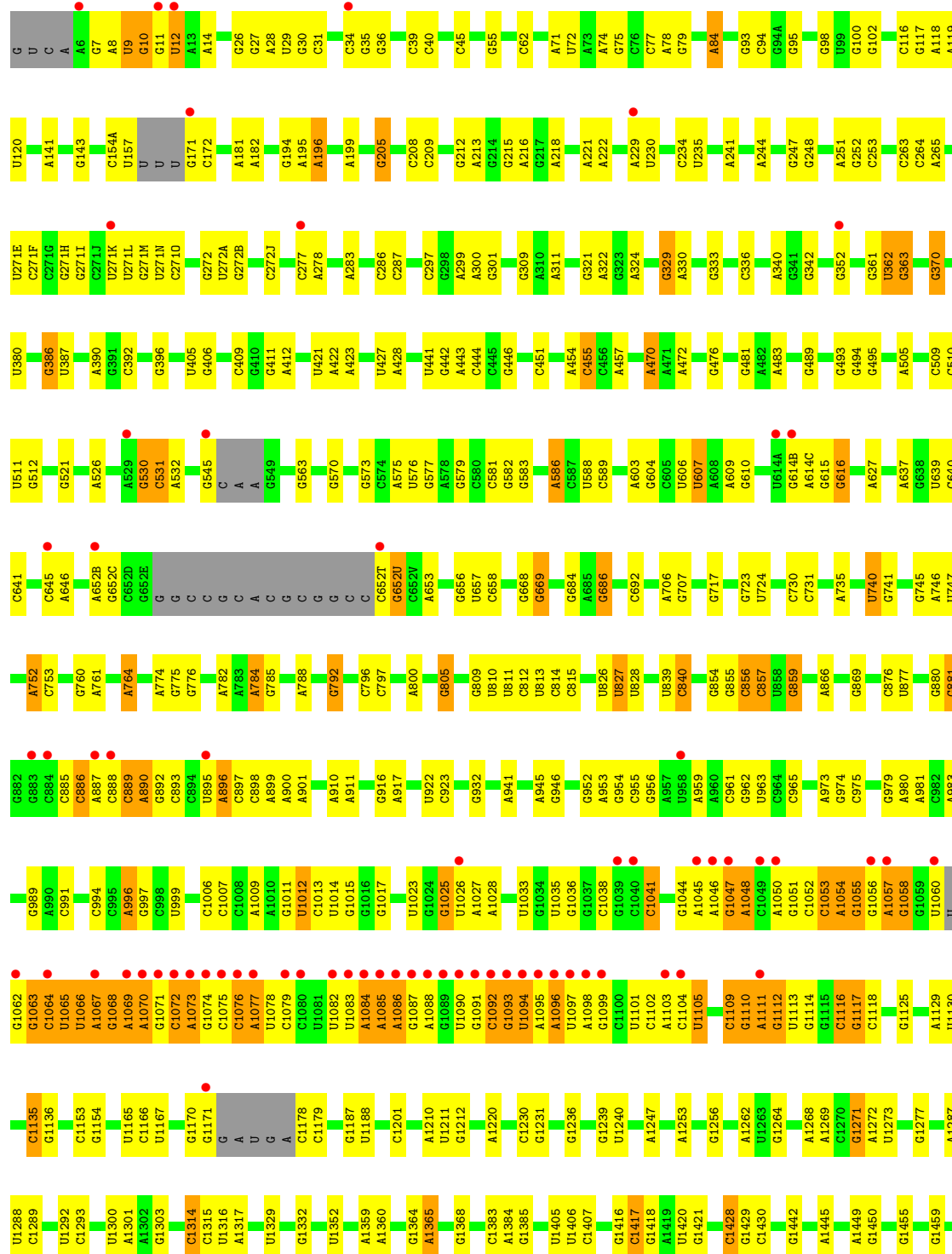
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60	2t	3	Total 3	O 3	0	0
60	2u	1	Total 1	O 1	0	0
60	2y	1	Total 1	O 1	0	0

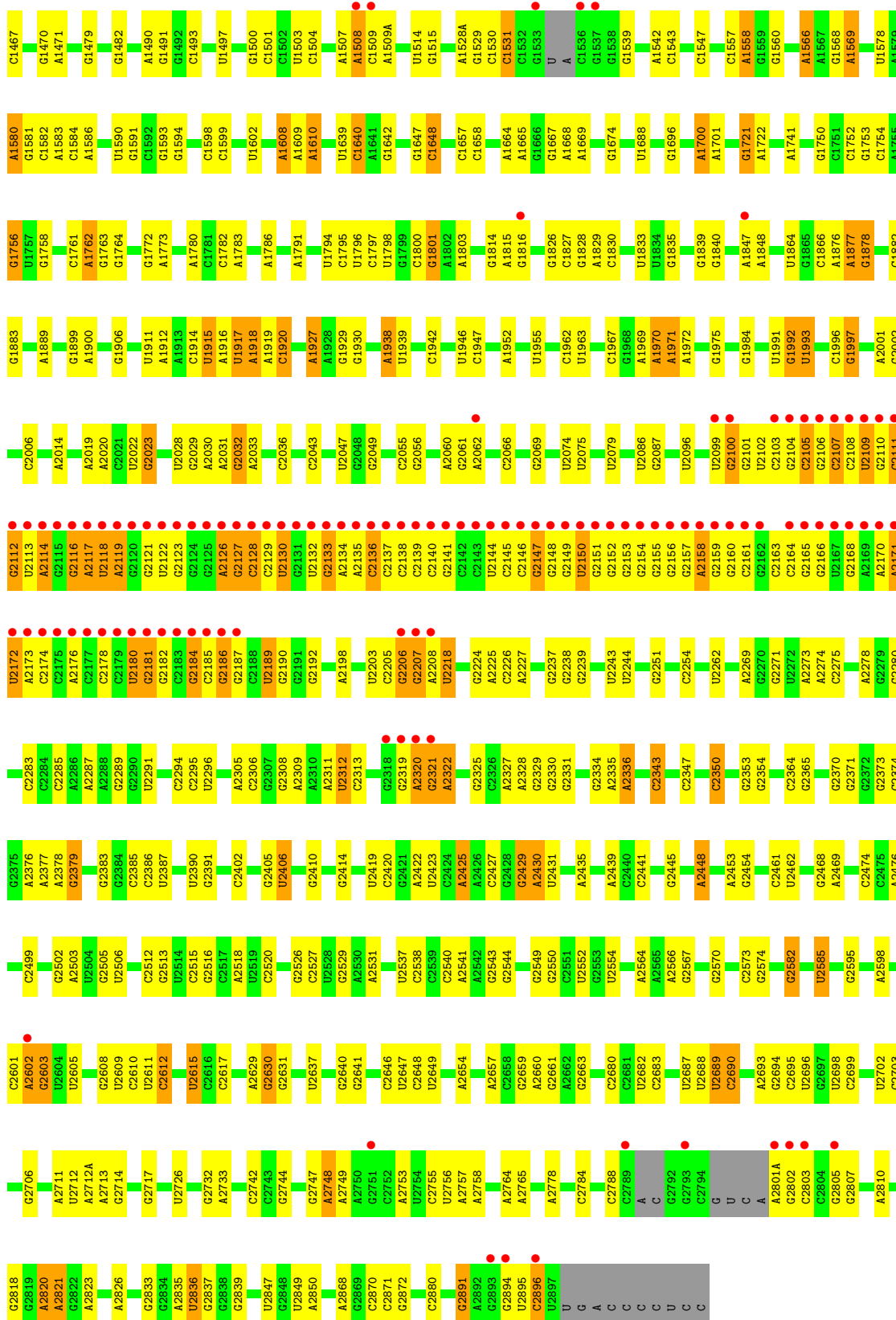
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U2554	U2554	A2426	A2305	C2178	A2117	A2014	A1877	C1754	A1569	G1448	A1301	G1164
G2557	G2557	G2427	A2306	U2179	U2118	A2019	G1878	A1755	A1571	G1450	G1303	U1165
C2558	C2558	G2428	G2308	G2182	G2120	A2020	A1889	G1756	U1578	G1452	C1315	C1166
U2563	U2563	G2429	A2309	G2183	G2121	G2021	A1890	U1762	U1579	U1453	C1320	G1170
A2564	A2564	A2430	A2310	G2184	U2122	G2022	A1900	G1763	A1580	G1455	A1321	G1171
G2565	G2565	U2431	A2312	C2185	G2123	G2023	G1906	G1764	A1581	G1459	G1332	G1173
G2567	G2567	A2435	G2313	G2186	G2125	G2024	U1911	U1765	C1582	G1460	G1333	U1175
A2572	A2572	G2439	G2314	C2187	A2126	A2030	U1912	C1767	C1584	G1465	U1340	G1176
C2573	C2573	C2440	G2315	U2189	C2127	G2032	A1913	U1768	A1586	C1467	G1334	A1177
G2586	G2586	C2441	G2316	G2190	C2128	A2033	A1914	A1773	A1587	U1466	U1345	C1178
C2586	C2586	C2442	G2319	G2191	U2130	G2038	U1915	U1778	C1588	G1470	C1345	C1187
A2590	A2590	G2444	A2320	G2192	U2131	C2039	U1916	U1779	G1593	A1471	U1352	U1188
C2591	C2591	G2445	G2325	G2193	G2133	C2043	U1917	A1780	G1594	G1482	G1356	G1203
G2592	G2592	G2446	G2326	A2198	A2135	G2049	A1918	C1781	A1608	G1486	A1358	A1210
A2602	A2602	A2448	G2327	G2206	C2136	C2055	U1919	G1782	A1609	G1487	A1359	U1211
G2603	G2603	U2449	A2328	G2207	C2137	G2056	G1920	A1783	A1610	C1493	G1364	A1220
U2604	U2604	A2450	G2329	A2208	C2138	C2065	U1921	U1784	A1614	G1500	A1365	G1239
U2605	U2605	A2453	G2330	U2218	C2139	G2066	G1929	A1785	A1641	C1506	G1371	U1240
G2608	G2608	C2464	G2331	G2224	C2140	G2069	U1931	A1786	G1642	A1507	U1372	G1250
U2609	U2609	G2464	A2335	A2225	C2141	U2074	U1932	C1790	A1508	C1509	A1378	C1251
C2610	C2610	G2468	A2336	C2226	C2142	U2075	A1932	A1791	A1509	C1510	A1379	G1252
U2611	U2611	A2469	G2345	U2232	U2144	U2086	G1933	G1795	A1510	G1511	G1380	A1253
C2612	C2612	G2470	G2346	G2238	C2145	C2096	G1934	U1796	G1512	C1513	G1381	G1256
G2617	G2617	A2476	G2347	G2239	C2146	U2099	A1936	C1797	U1518	U1405	A1268	A1269
G2618	G2618	C2498	U2348	G2239	G2148	U2099	U1937	G1817	G1519	U1406	C1270	G1271
A2629	A2629	G2499	G2349	U2243	C2149	G2100	A1938	G1826	A1528A	G1416	A1272	U1273
G2630	G2630	C2502	C2350	U2244	U2150	C2103	U1939	A1829	G1532	C1417	U1274	A1287
A2639	A2639	U2504	G2364	G2251	G2153	G2104	A1942	G1833	G	U	U1288	C1289
C2646	C2646	G2505	G2365	C2258	G2154	G2105	A1943	U1839	U	A	C1290	G1291
U2647	U2647	U2506	A2377	C2259	G2155	G2106	U1955	G1843	A1700	C1421	C1428	U1292
C2648	C2648	G2507	A2378	A2268	G2157	C2107	U1956	A1701	G1702	G1429	C1430	C1293
U2649	U2649	G2508	C2381	G2271	A2158	U2099	C1957	G1703	G1537	A1542	U1431	G1296
U2650	U2650	A2518	G2382	G2277	G2159	U2099	U1962	A1847	C	C1543	C1430	U1431
C2651	C2651	C2520	G2383	G2278	G2160	G2100	U1963	G1865	G1537	A1554	G1296	C1297
A2654	A2654	G2526	C2385	G2279	G2162	C2103	G1964	C1866	G1537	A1558	G1442	
C2681	C2681	U2529	G2389	C2283	G2163	G2104	C1967					
U2682	U2682	G2535	U2390	C2286	G2164	G2105	G1968					
G2687	G2687	U2535	A2393	A2287	G2165	G2106	A1969					
U2688	U2688	G2548	C2404	A2288	G2166	G2107	A1970					
G2802	G2802	G2549	G2405	G2289	U2167	C2108	A1971					
C2803	C2803	G2550	U2406	G2290	A2169	U2109	A1972					
C2804	C2804	C2551	U2417	U2291	A2170	G2110	A1992					
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G2807	G2807			U2296	A2173	G2112	C1996					
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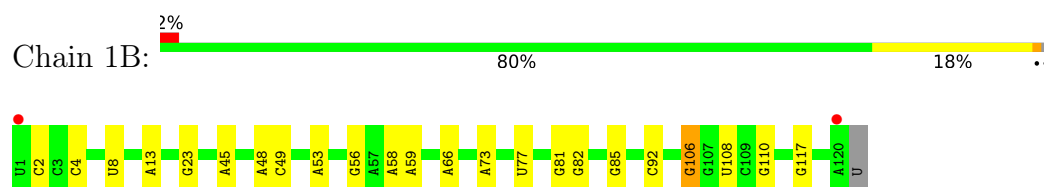


• Molecule 1: 23S Ribosomal RNA

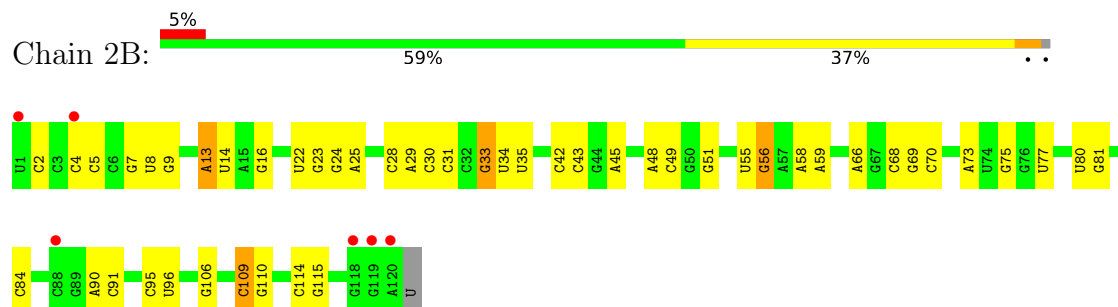




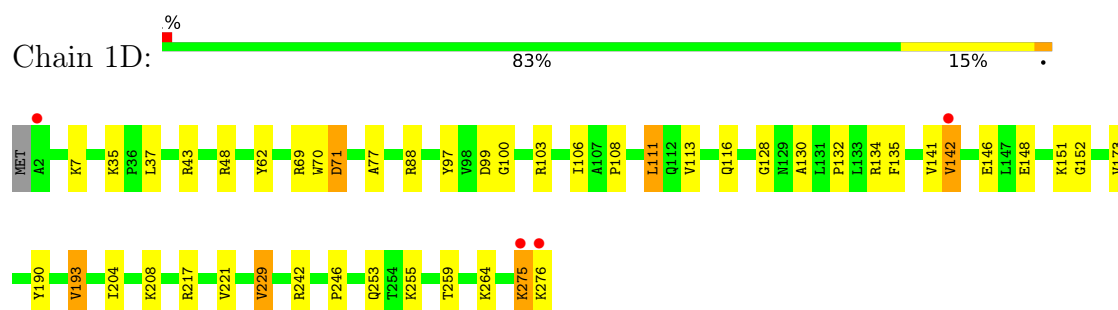
- Molecule 2: 5S Ribosomal RNA



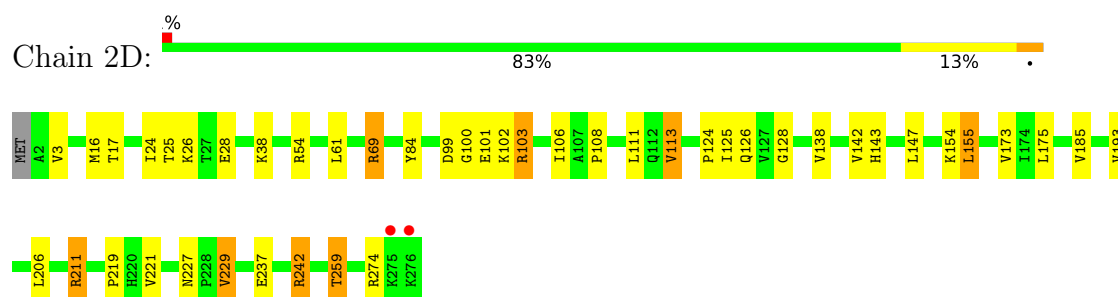
- Molecule 2: 5S Ribosomal RNA



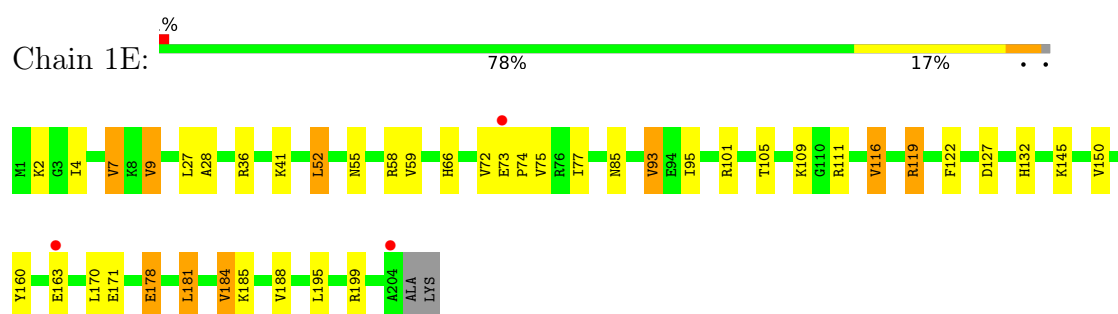
- Molecule 3: 50S ribosomal protein L2



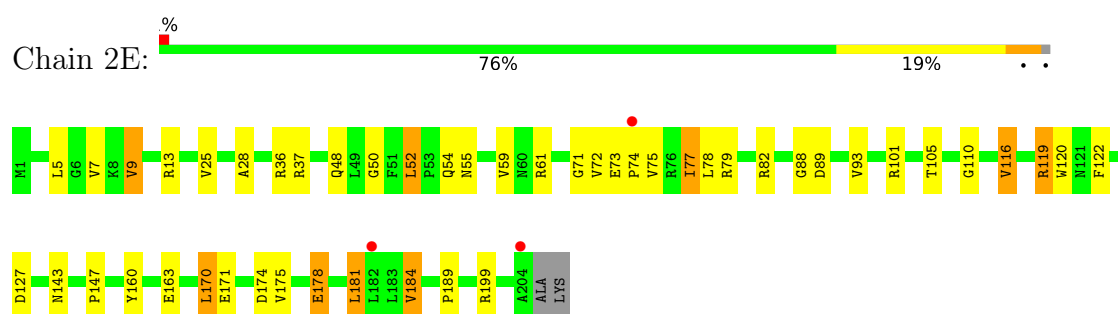
- Molecule 3: 50S ribosomal protein L2



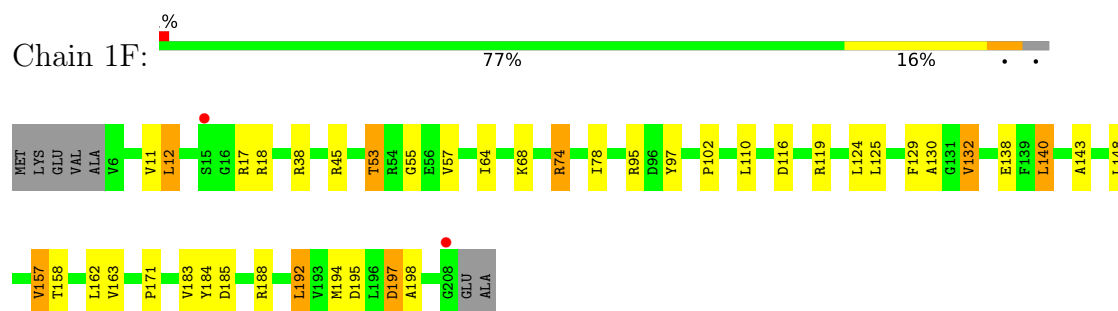
- Molecule 4: 50S ribosomal protein L3



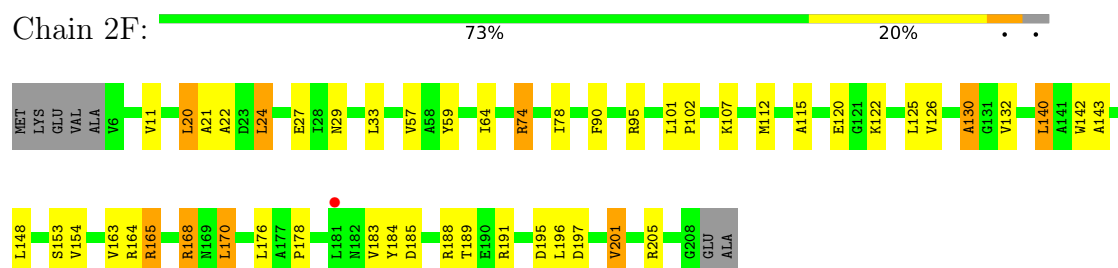
- Molecule 4: 50S ribosomal protein L3



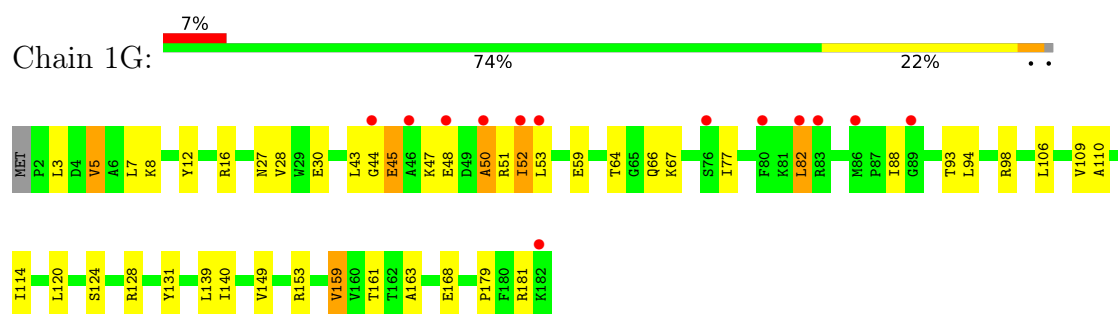
- Molecule 5: 50S ribosomal protein L4



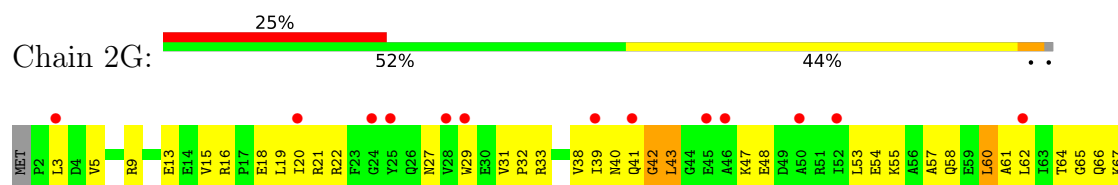
- Molecule 5: 50S ribosomal protein L4

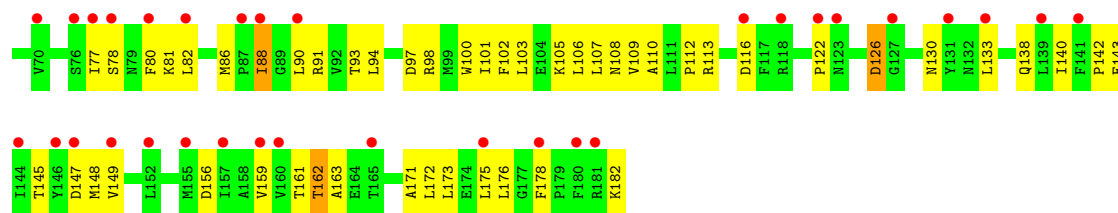


- Molecule 6: 50S ribosomal protein L5

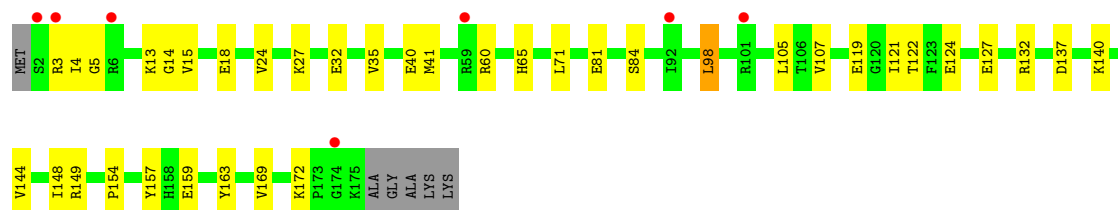
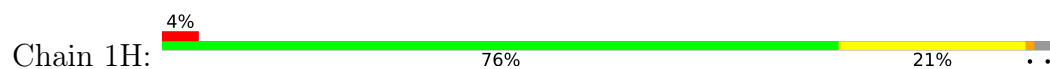


- Molecule 6: 50S ribosomal protein L5

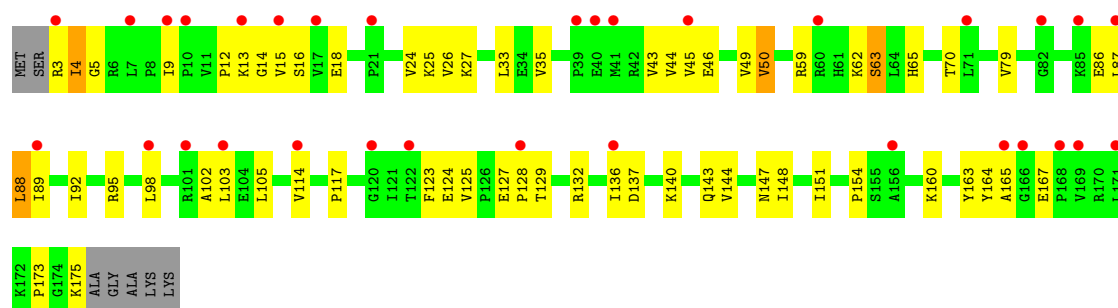




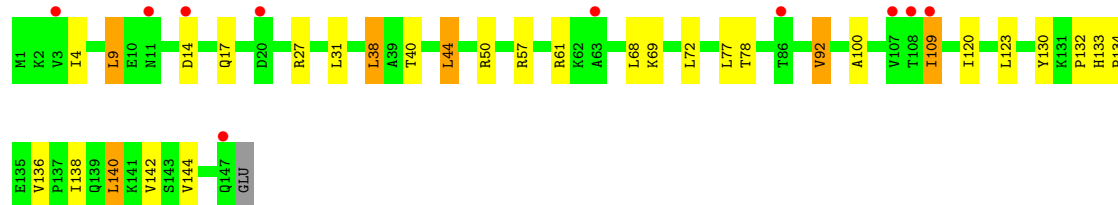
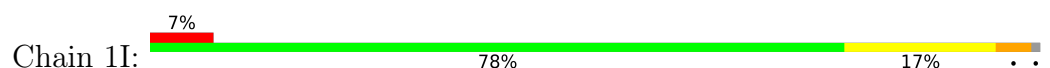
• Molecule 7: 50S ribosomal protein L6



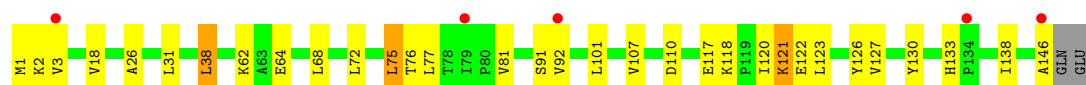
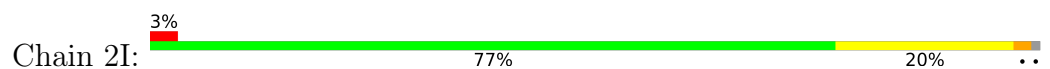
• Molecule 7: 50S ribosomal protein L6



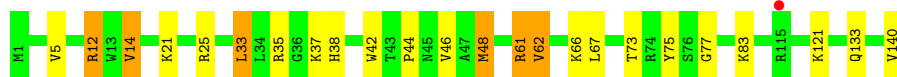
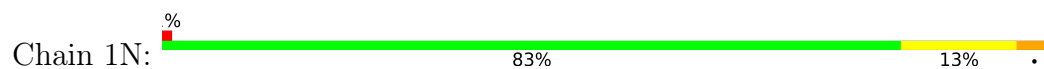
• Molecule 8: 50S ribosomal protein L9



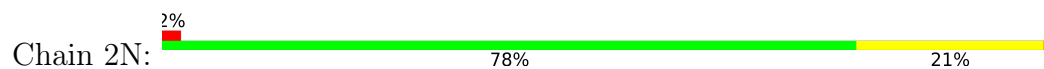
• Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



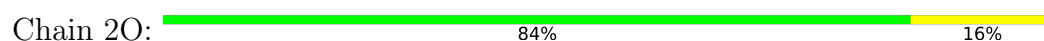
- Molecule 9: 50S ribosomal protein L13



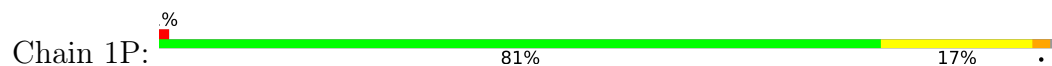
- Molecule 10: 50S ribosomal protein L14



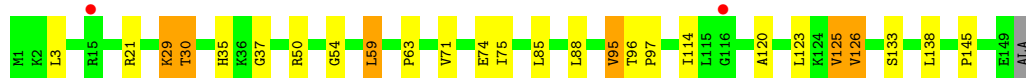
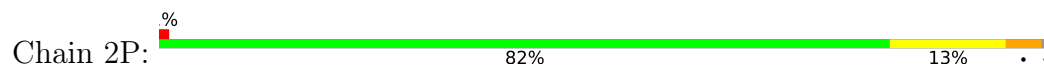
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



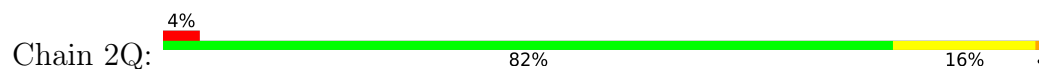
- Molecule 11: 50S ribosomal protein L15



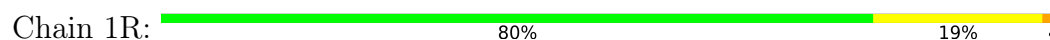
- Molecule 12: 50S ribosomal protein L16



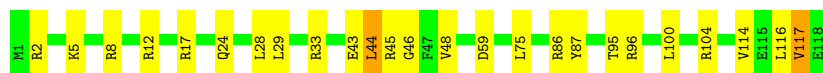
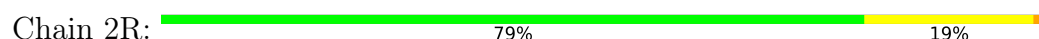
- Molecule 12: 50S ribosomal protein L16



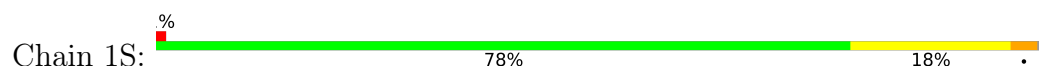
- Molecule 13: 50S ribosomal protein L17



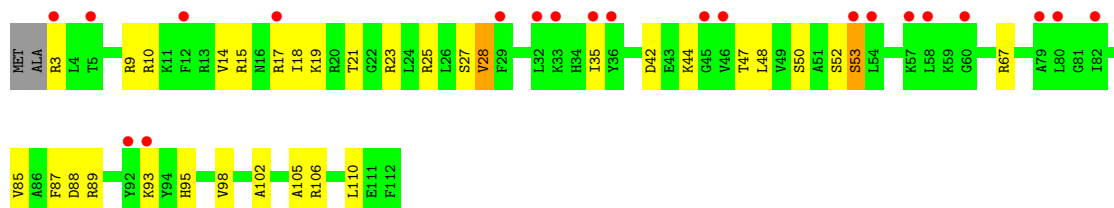
- Molecule 13: 50S ribosomal protein L17



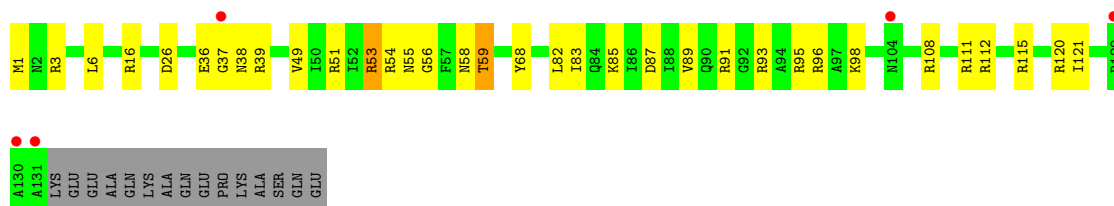
- Molecule 14: 50S ribosomal protein L18



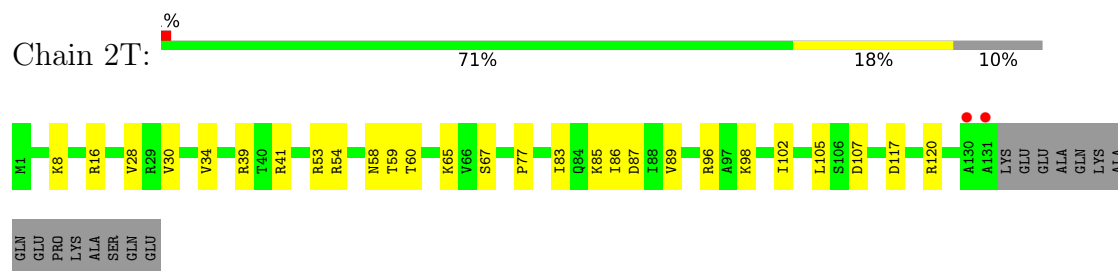
- Molecule 14: 50S ribosomal protein L18



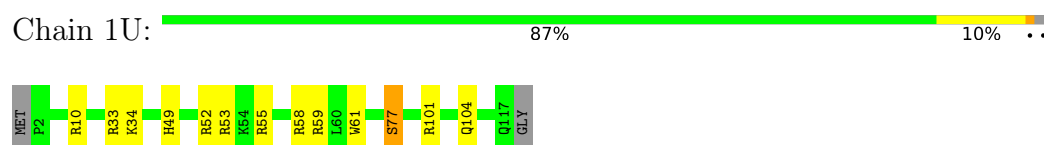
- Molecule 15: 50S ribosomal protein L19



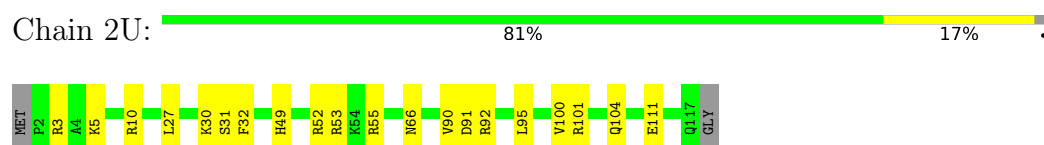
- Molecule 15: 50S ribosomal protein L19



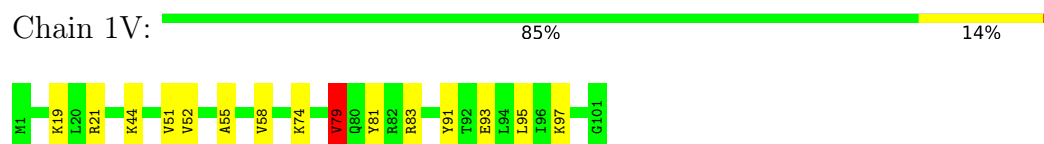
- Molecule 16: 50S ribosomal protein L20



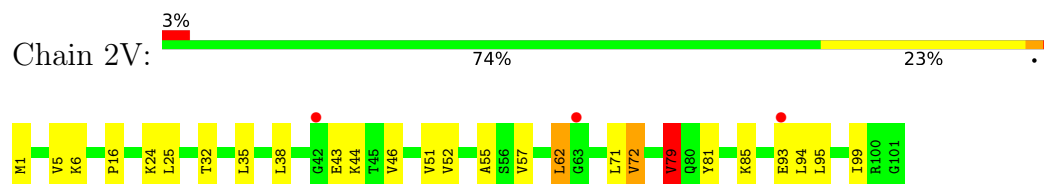
- Molecule 16: 50S ribosomal protein L20



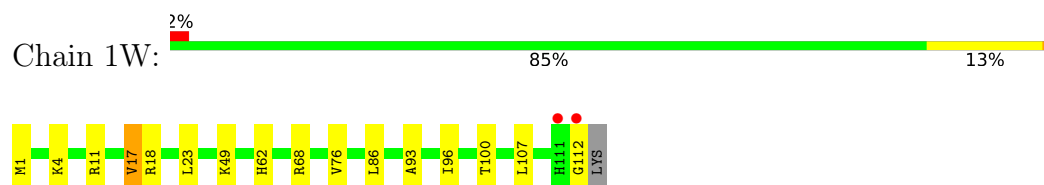
- Molecule 17: 50S ribosomal protein L21



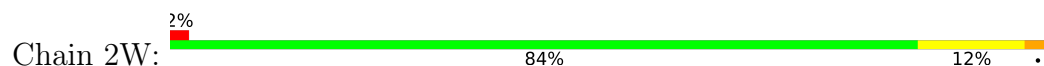
- Molecule 17: 50S ribosomal protein L21

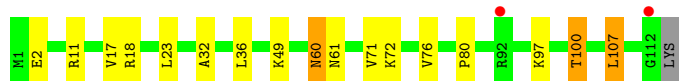


- Molecule 18: 50S ribosomal protein L22

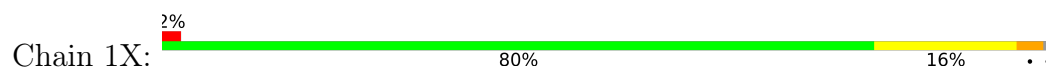


- Molecule 18: 50S ribosomal protein L22

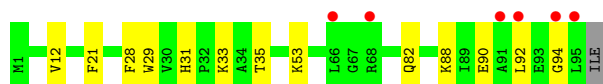
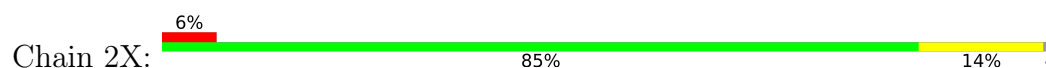




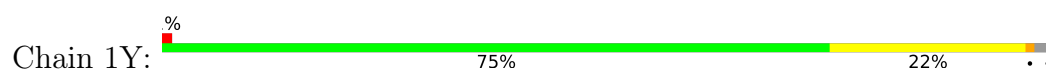
- Molecule 19: 50S ribosomal protein L23



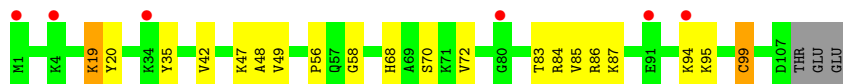
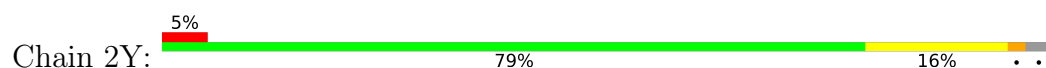
- Molecule 19: 50S ribosomal protein L23



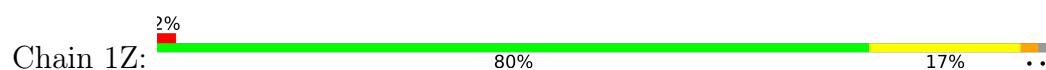
- Molecule 20: 50S ribosomal protein L24



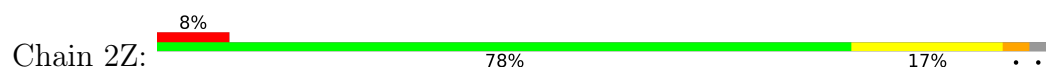
- Molecule 20: 50S ribosomal protein L24

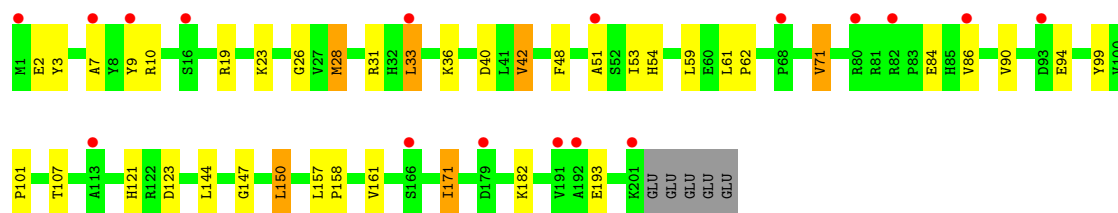


- Molecule 21: 50S ribosomal protein L25

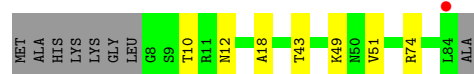
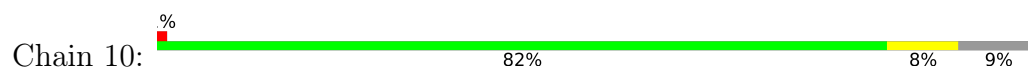


- Molecule 21: 50S ribosomal protein L25

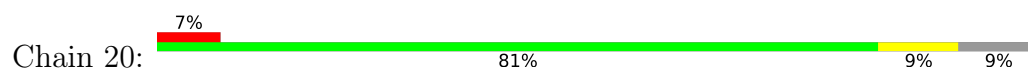




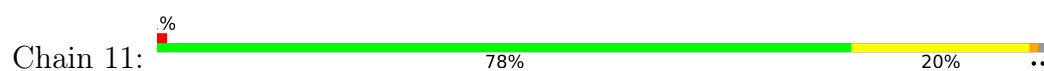
- Molecule 22: 50S ribosomal protein L27



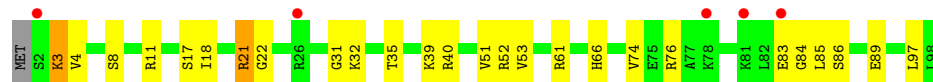
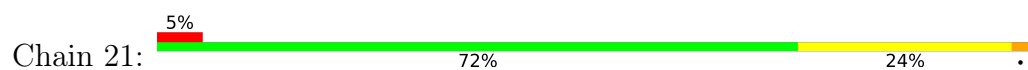
- Molecule 22: 50S ribosomal protein L27



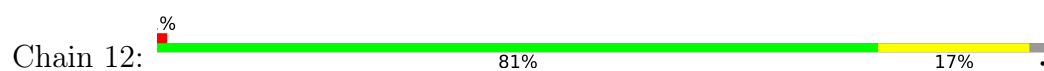
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

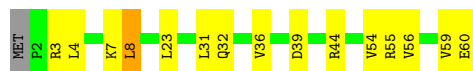


- Molecule 24: 50S ribosomal protein L29

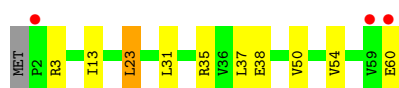
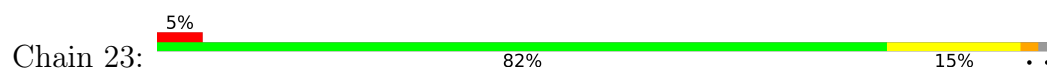




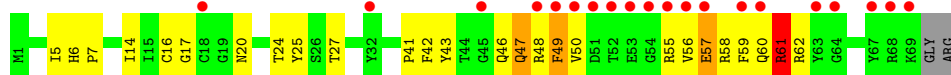
- Molecule 25: 50S ribosomal protein L30



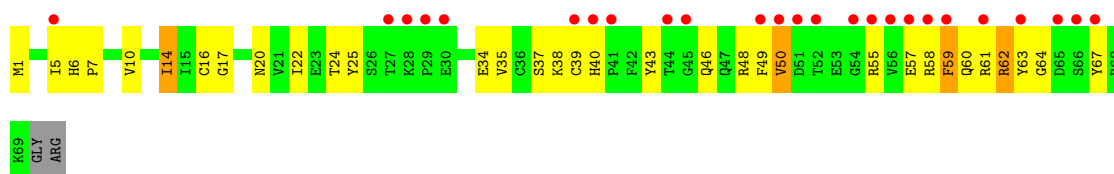
- Molecule 25: 50S ribosomal protein L30



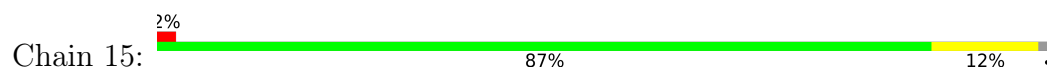
- Molecule 26: 50S ribosomal protein L31



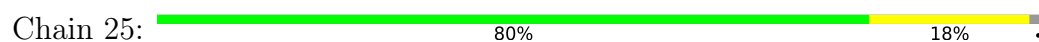
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



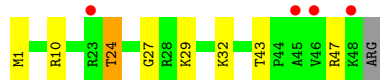
• Molecule 28: 50S ribosomal protein L33

Chain 16:  89% 9% .

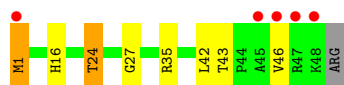
• Molecule 28: 50S ribosomal protein L33

Chain 26:  76% 19% . .

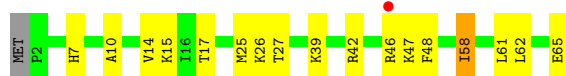
• Molecule 29: 50S ribosomal protein L34

Chain 17:  8% 82% 14% . .

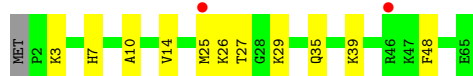
• Molecule 29: 50S ribosomal protein L34

Chain 27:  10% 82% 12% . .

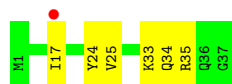
• Molecule 30: 50S ribosomal protein L35

Chain 18:  2% 72% 25% . .

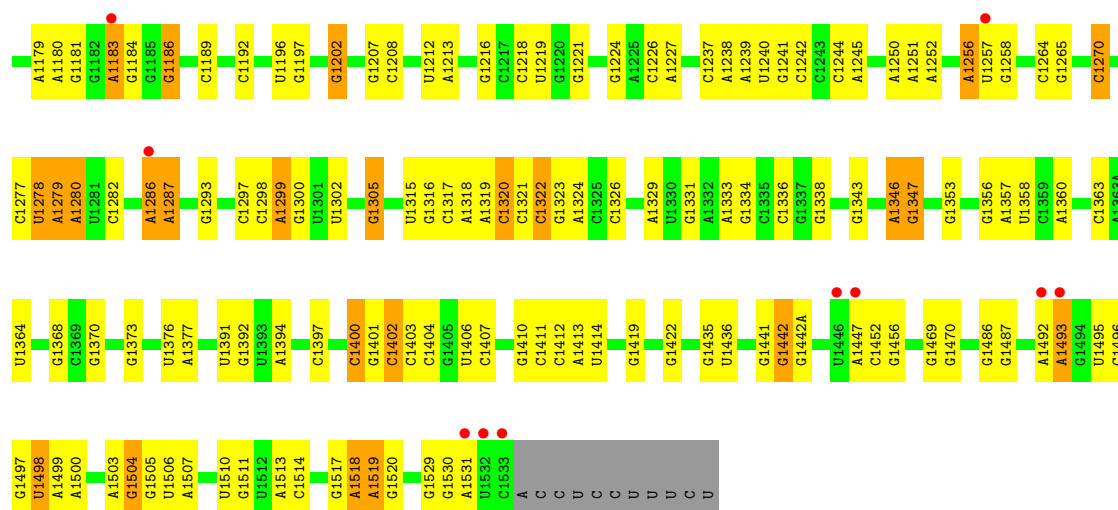
• Molecule 30: 50S ribosomal protein L35

Chain 28:  3% 82% 17% .

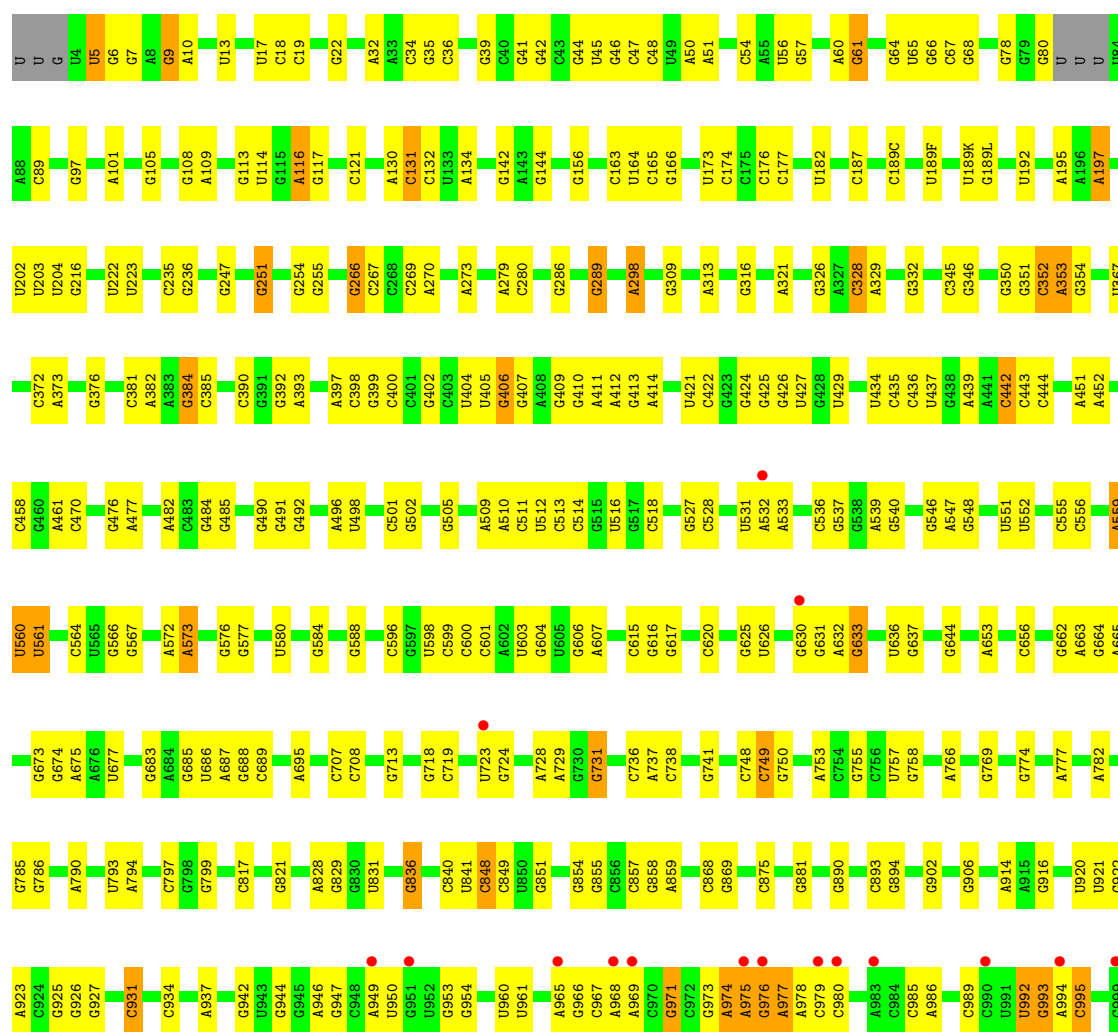
• Molecule 31: 50S ribosomal protein L36

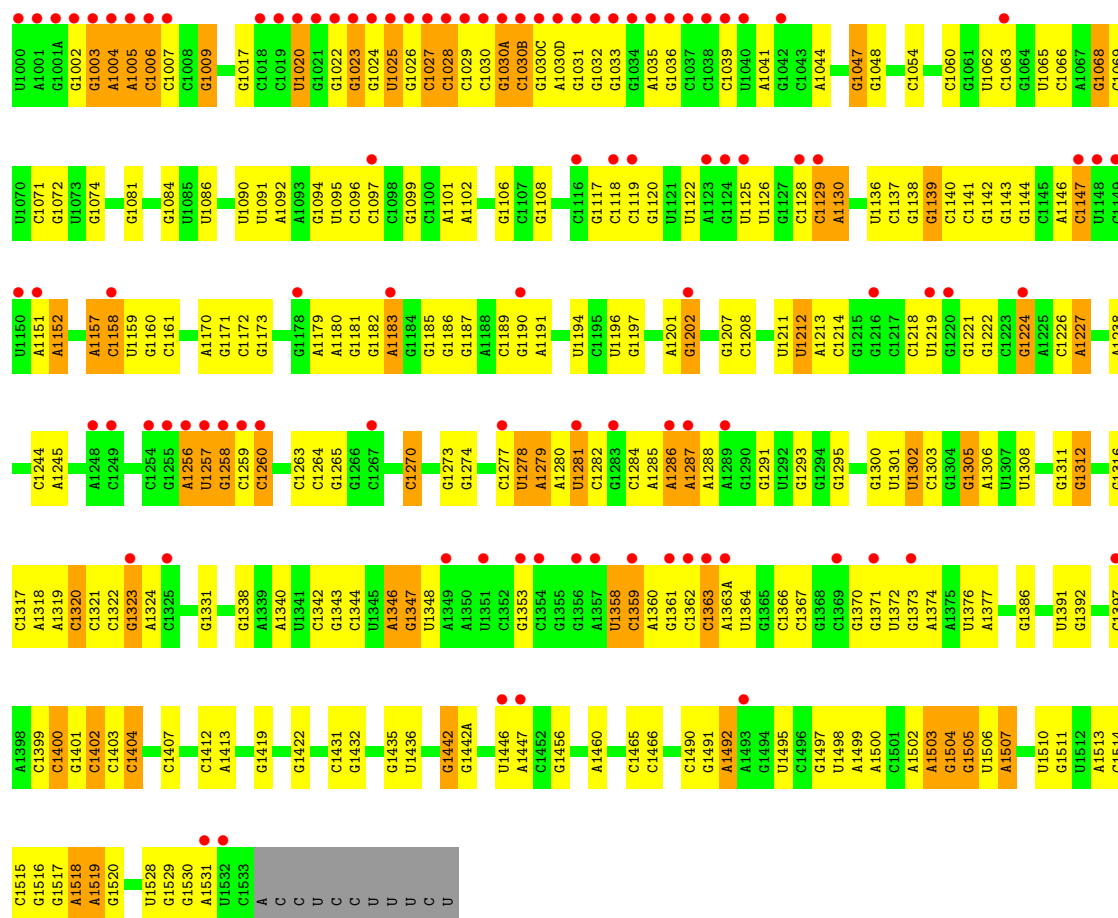
Chain 19:  3% 84% 16%

- 

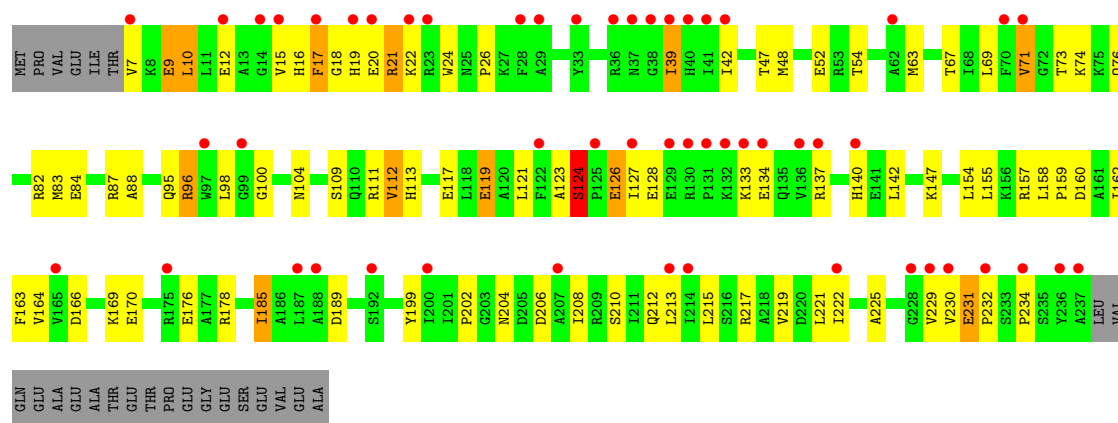


• Molecule 32: 16S Ribosomal RNA

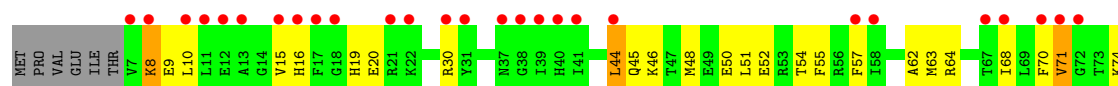


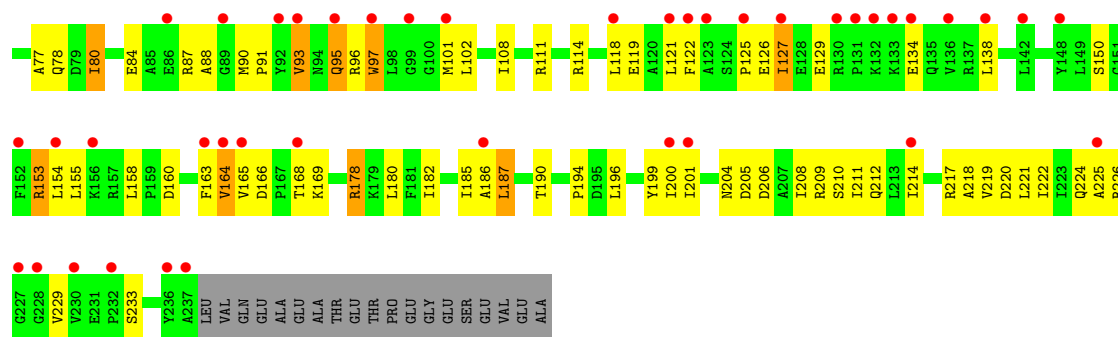


• Molecule 33: 30S ribosomal protein S2

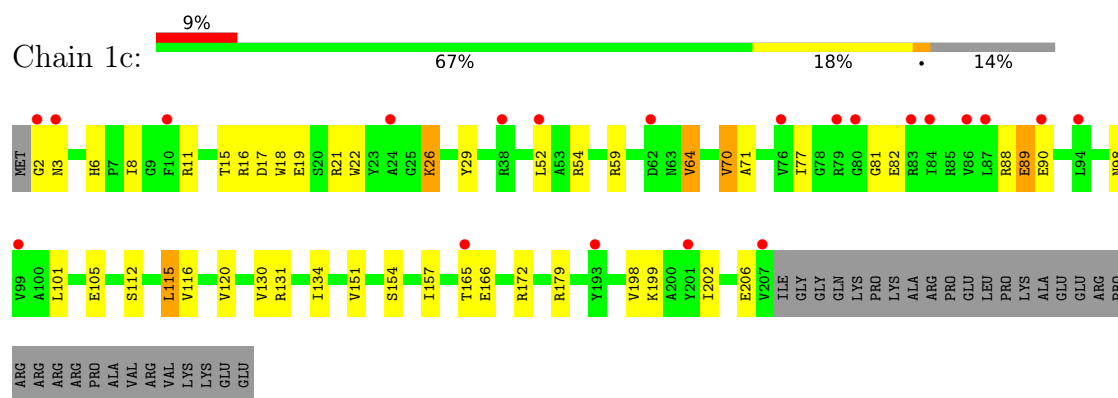


• Molecule 33: 30S ribosomal protein S2

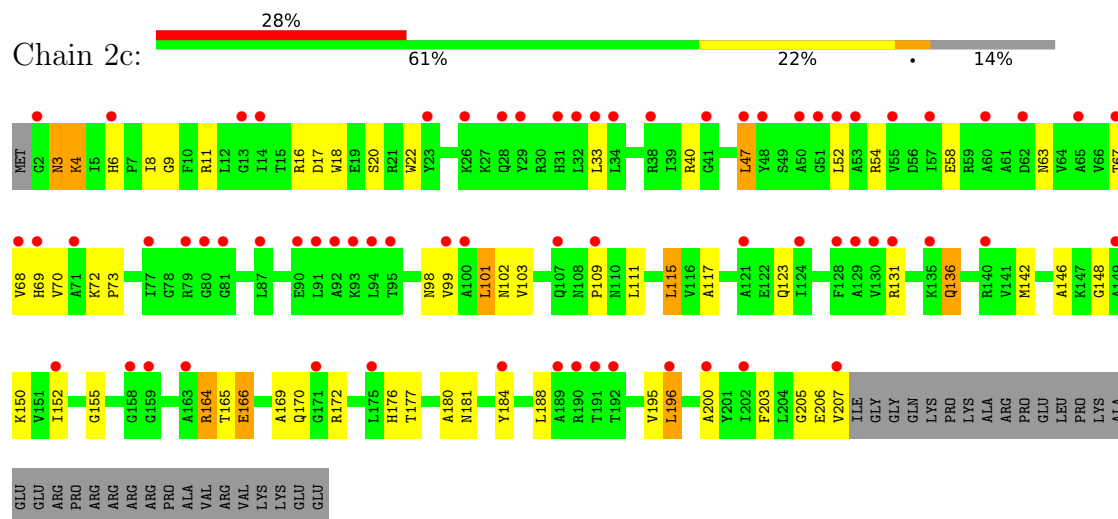




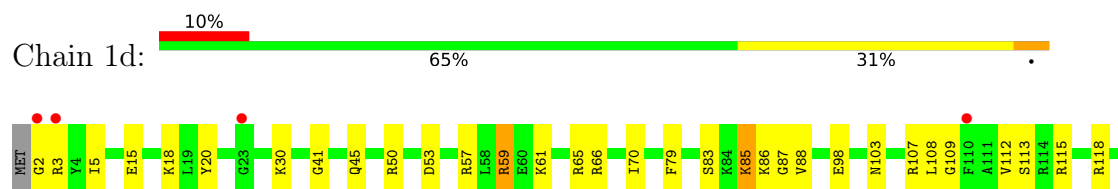
• Molecule 34: 30S ribosomal protein S3

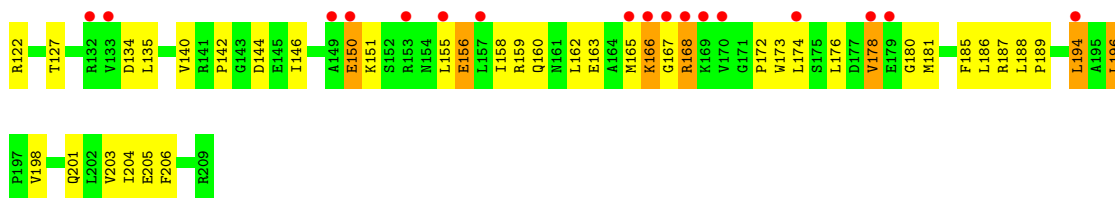


• Molecule 34: 30S ribosomal protein S3

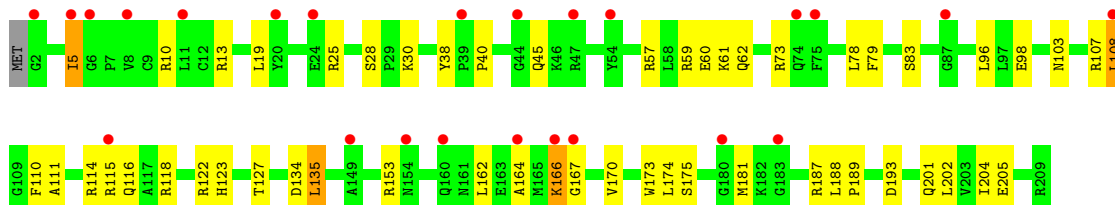
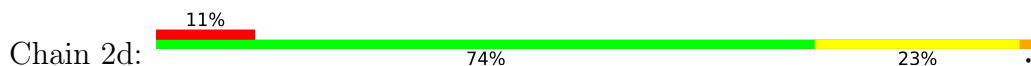


• Molecule 35: 30S ribosomal protein S4

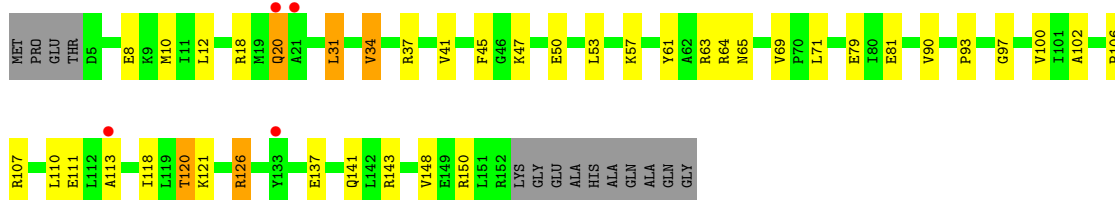




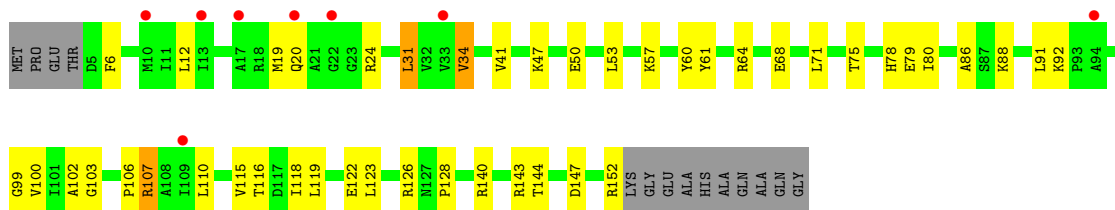
- Molecule 35: 30S ribosomal protein S4



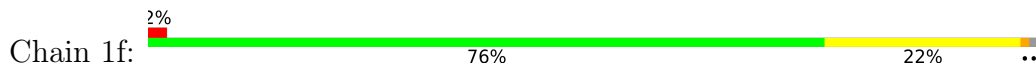
- Molecule 36: 30S ribosomal protein S5



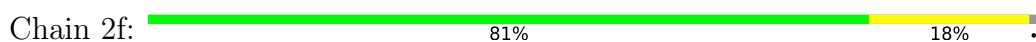
- Molecule 36: 30S ribosomal protein S5

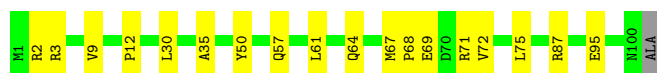


- Molecule 37: 30S ribosomal protein S6

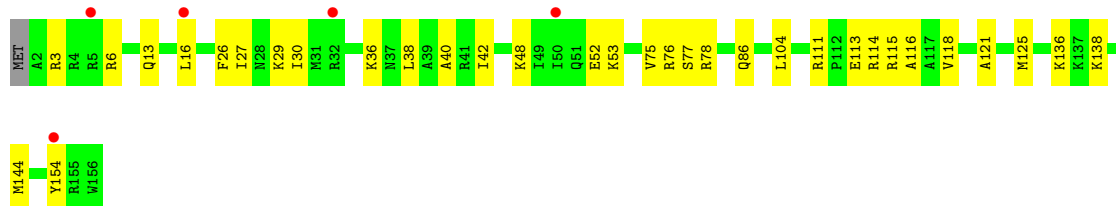
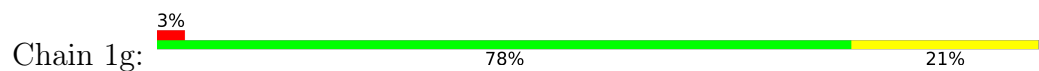


- Molecule 37: 30S ribosomal protein S6

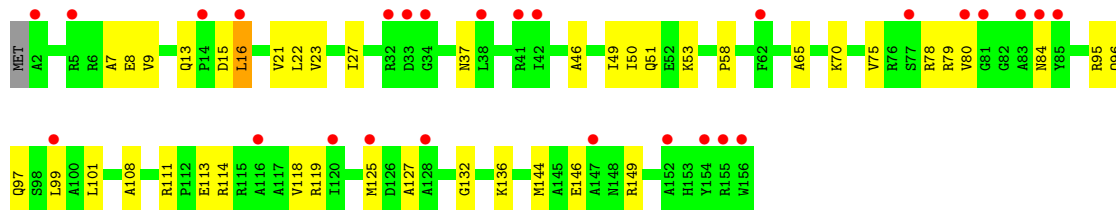
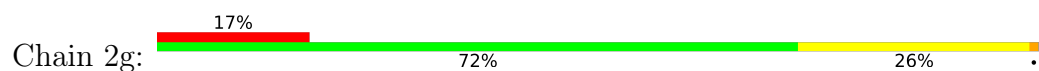




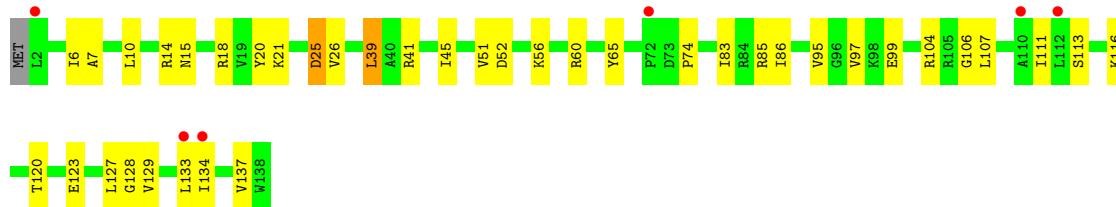
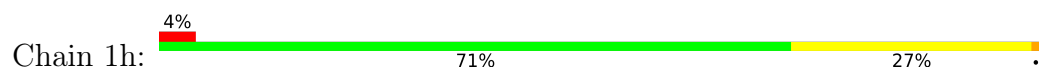
- Molecule 38: 30S ribosomal protein S7



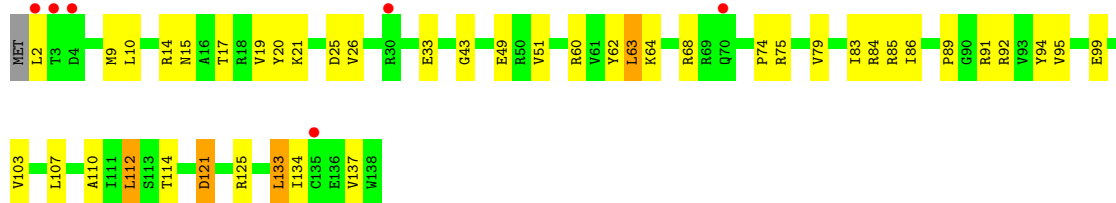
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

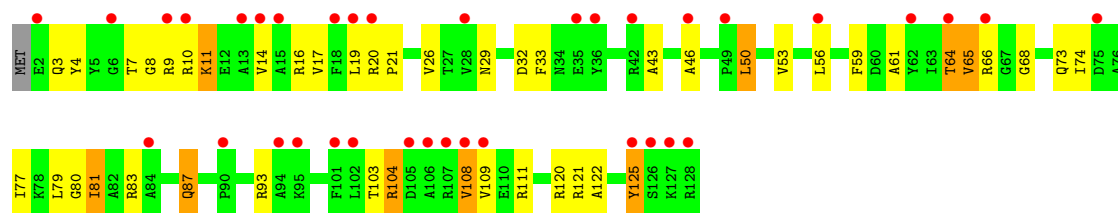


- Molecule 39: 30S ribosomal protein S8

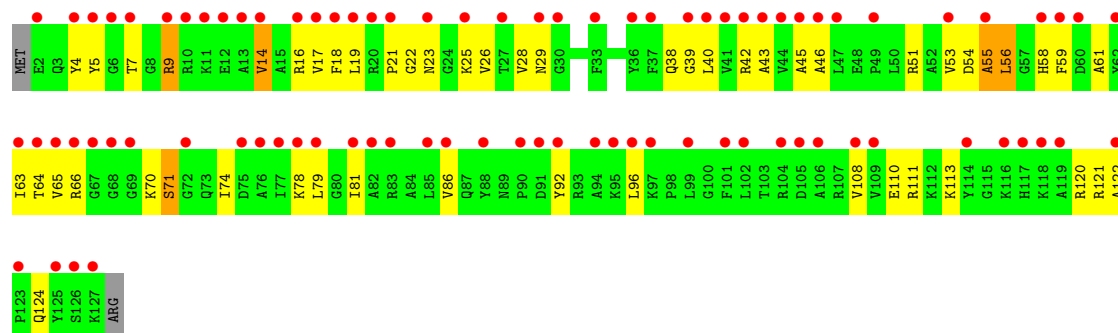


- Molecule 40: 30S ribosomal protein S9

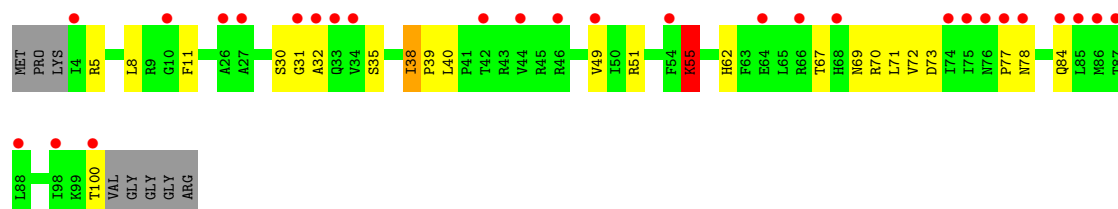




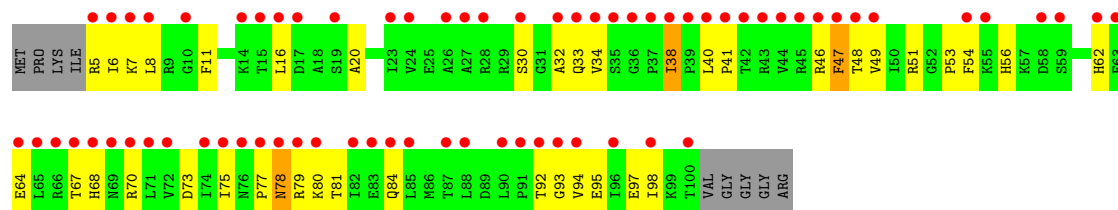
• Molecule 40: 30S ribosomal protein S9



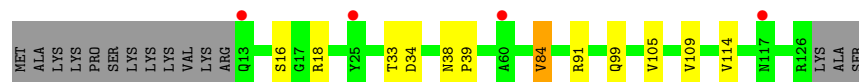
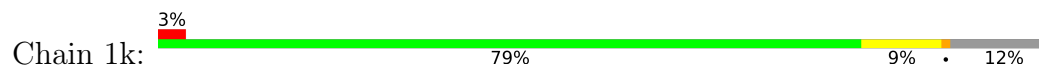
• Molecule 41: 30S ribosomal protein S10



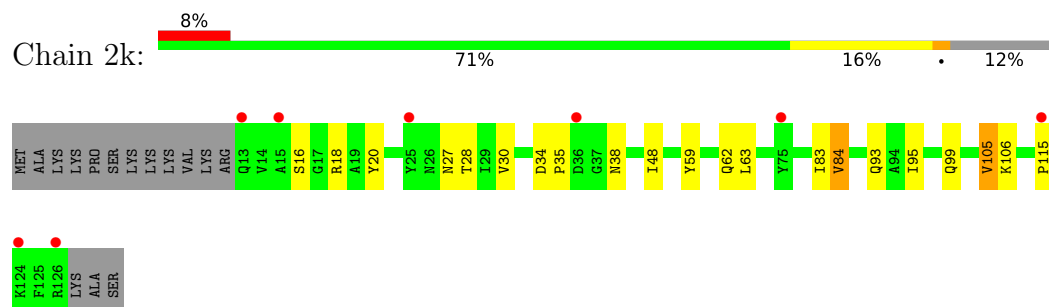
• Molecule 41: 30S ribosomal protein S10



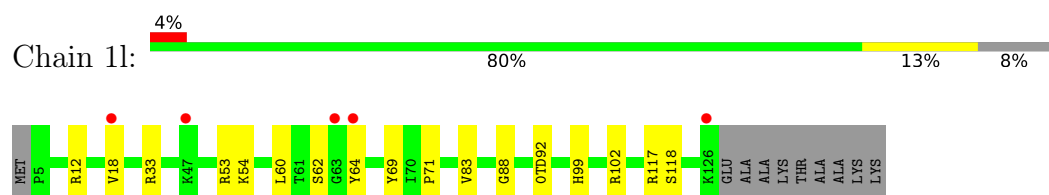
• Molecule 42: 30S ribosomal protein S11



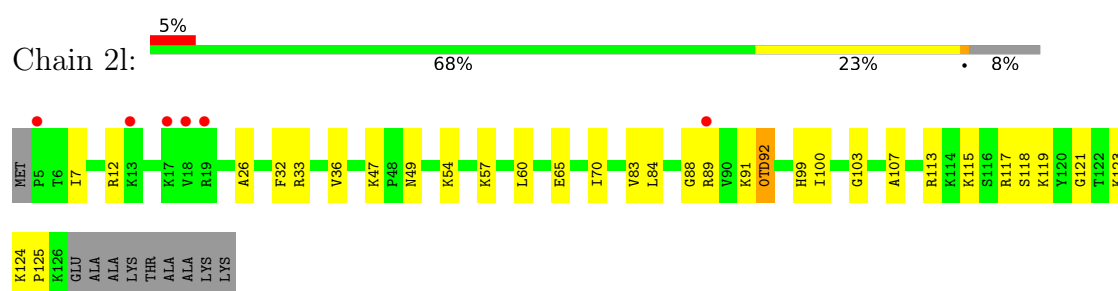
- Molecule 42: 30S ribosomal protein S11



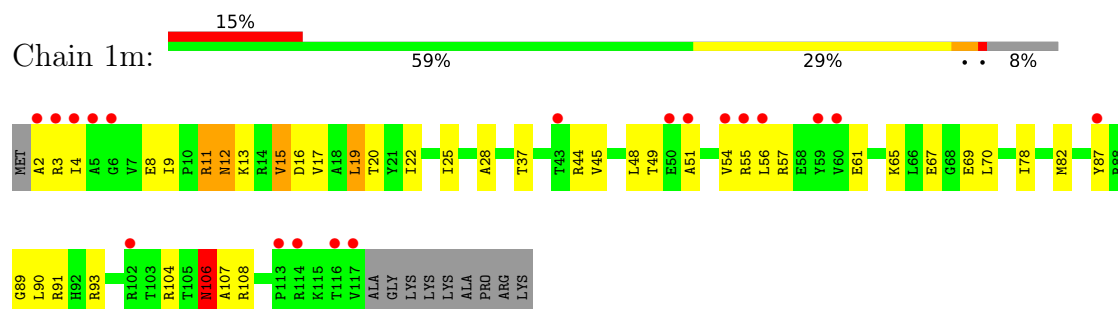
- Molecule 43: 30S ribosomal protein S12



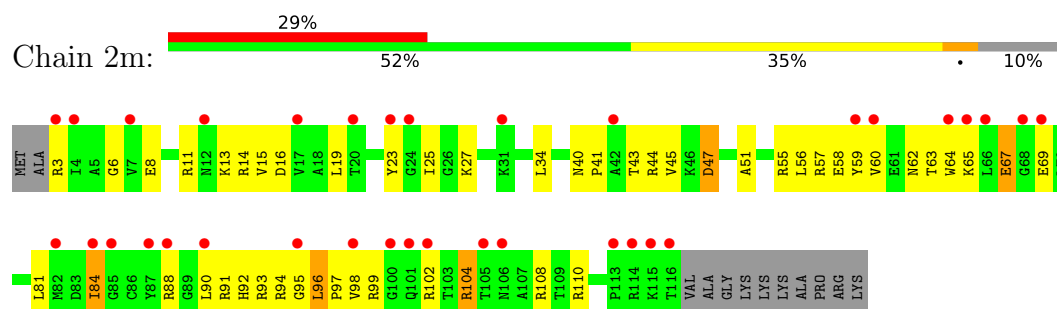
- Molecule 43: 30S ribosomal protein S12



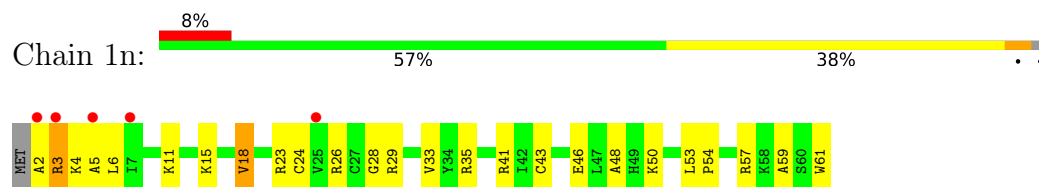
- Molecule 44: 30S ribosomal protein S13



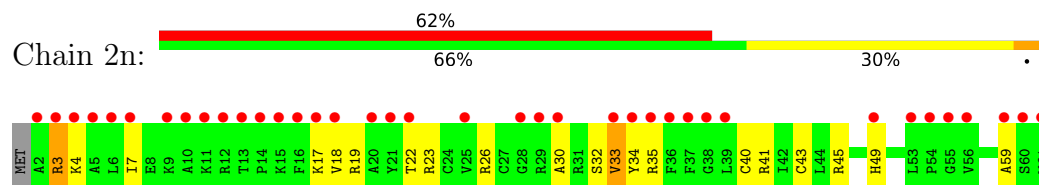
- Molecule 44: 30S ribosomal protein S13



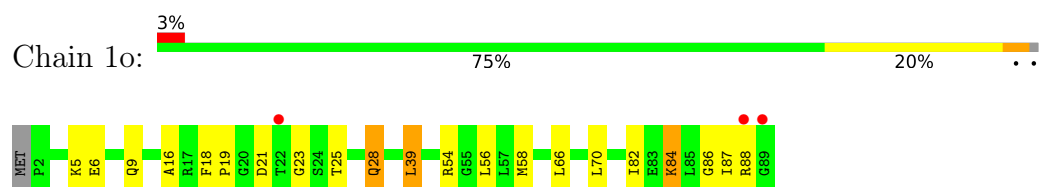
- Molecule 45: 30S ribosomal protein S14 type Z



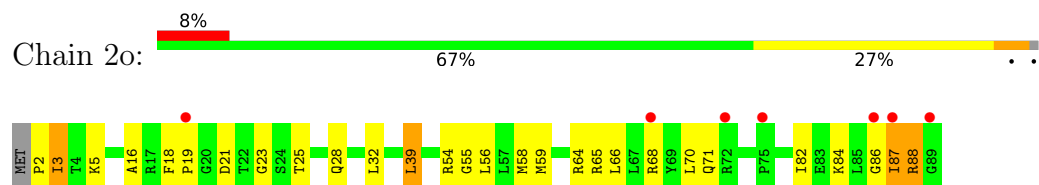
- Molecule 45: 30S ribosomal protein S14 type Z



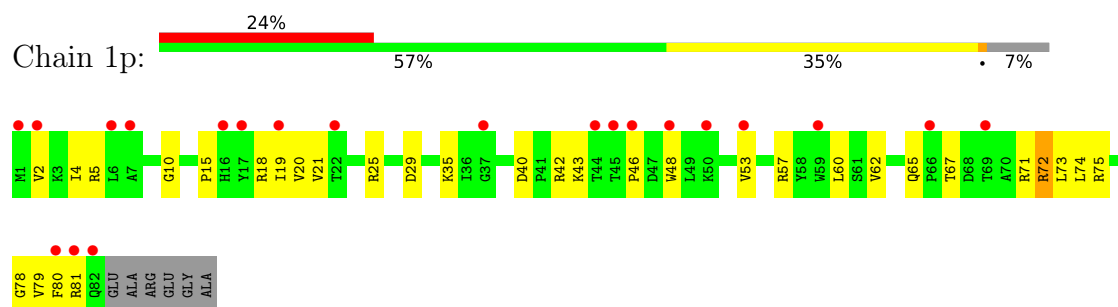
- Molecule 46: 30S ribosomal protein S15



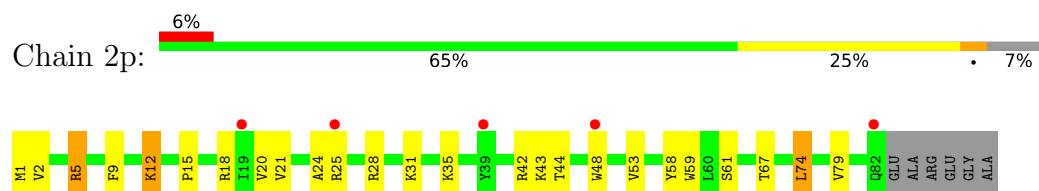
- Molecule 46: 30S ribosomal protein S15



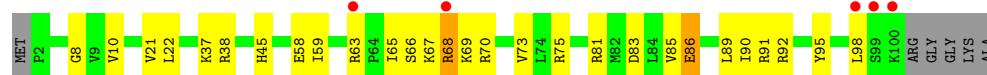
- Molecule 47: 30S ribosomal protein S16



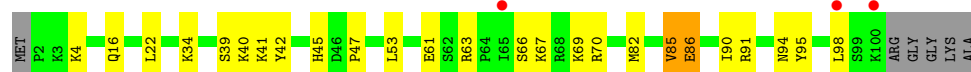
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



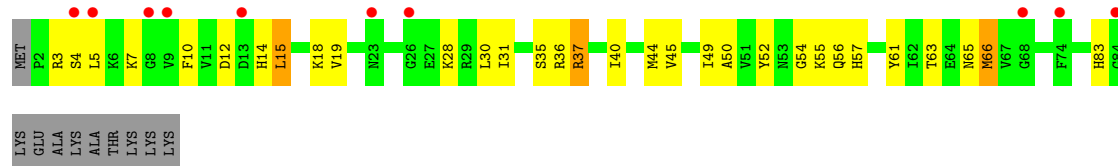
- Molecule 49: 30S ribosomal protein S18



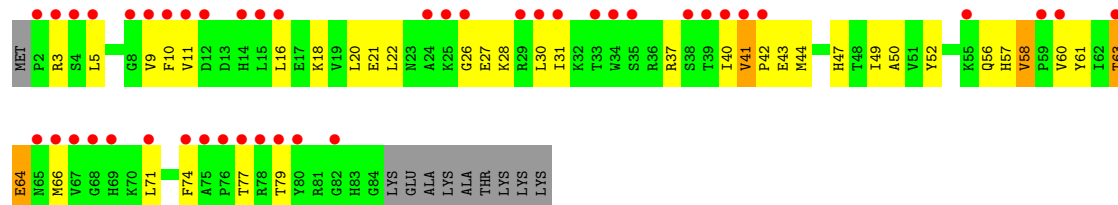
- Molecule 49: 30S ribosomal protein S18



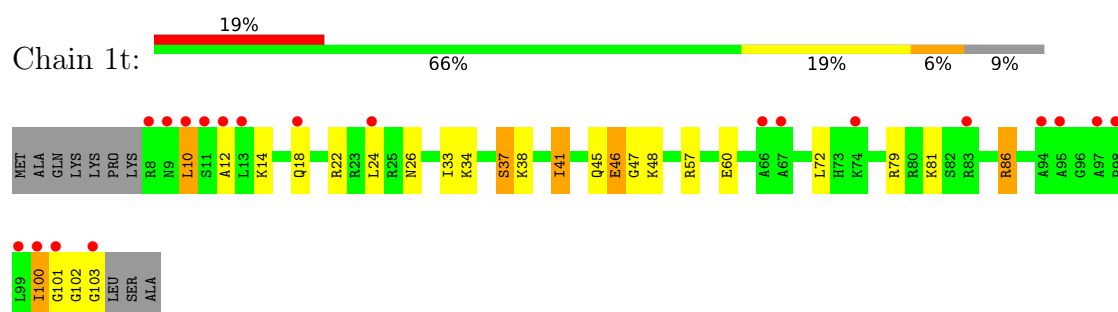
- Molecule 50: 30S ribosomal protein S19



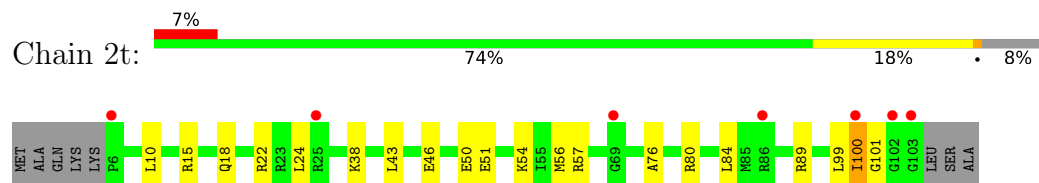
- Molecule 50: 30S ribosomal protein S19



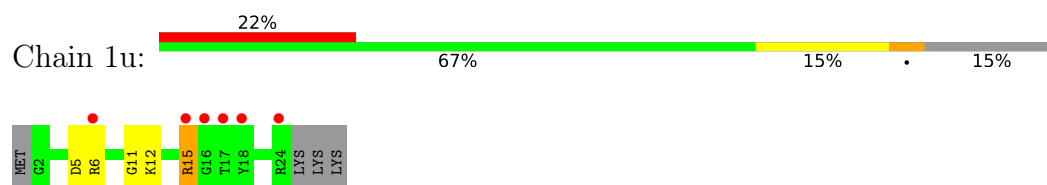
- Molecule 51: 30S ribosomal protein S20



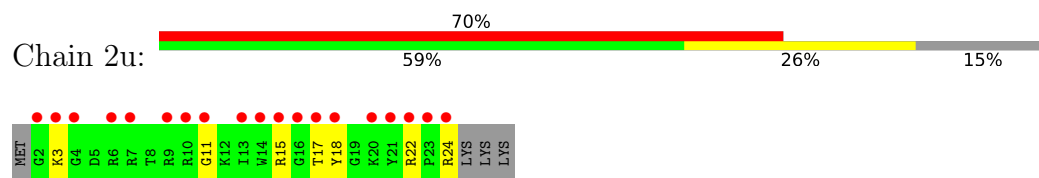
- Molecule 51: 30S ribosomal protein S20



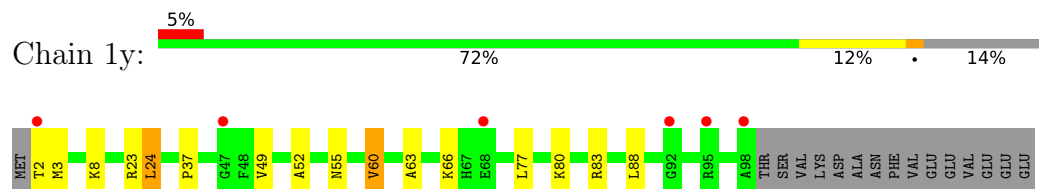
- Molecule 52: 30S ribosomal protein Thx



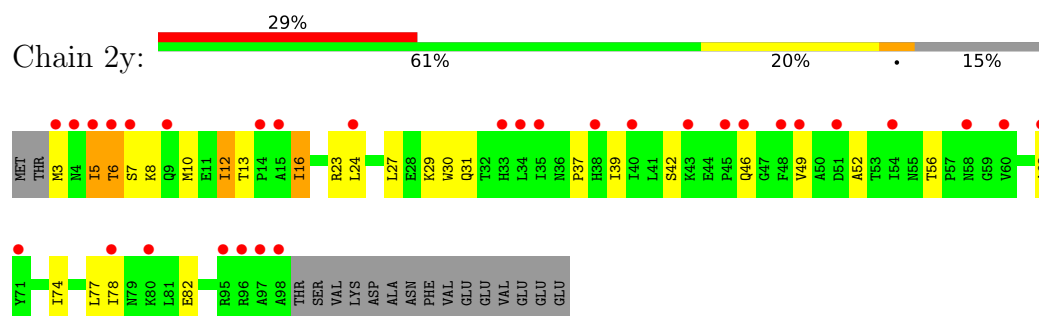
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 53: Ribosome-associated inhibitor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.90Å 449.76Å 620.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.00 – 2.60 122.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (122.00-2.60) 99.8 (122.00-2.60)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.203 , 0.241 0.205 , 0.242	Depositor DCC
R_{free} test set	88927 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	297563	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 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.19	0/69031	0.36	0/107754
1	2A	0.16	0/68903	0.34	0/107552
2	1B	0.15	0/2876	0.31	0/4486
2	2B	0.13	0/2878	0.27	0/4490
3	1D	0.19	0/2181	0.43	0/2940
3	2D	0.15	0/2186	0.41	0/2944
4	1E	0.17	0/1592	0.41	0/2149
4	2E	0.16	0/1592	0.39	0/2149
5	1F	0.17	0/1619	0.38	0/2193
5	2F	0.15	0/1615	0.41	0/2188
6	1G	0.14	0/1451	0.37	0/1961
6	2G	0.14	0/1449	0.35	0/1957
7	1H	0.15	0/1356	0.36	0/1834
7	2H	0.14	0/1350	0.37	0/1826
8	1I	0.15	0/1109	0.38	0/1512
8	2I	0.13	0/1091	0.36	0/1490
9	1N	0.16	0/1148	0.37	0/1547
9	2N	0.13	0/1144	0.33	0/1543
10	1O	0.17	0/943	0.40	0/1269
10	2O	0.15	0/943	0.37	0/1269
11	1P	0.18	0/1152	0.41	0/1533
11	2P	0.15	0/1152	0.42	0/1533
12	1Q	0.17	0/1143	0.40	0/1527
12	2Q	0.13	0/1143	0.35	0/1527
13	1R	0.17	0/982	0.40	0/1312
13	2R	0.15	0/982	0.39	0/1312
14	1S	0.15	0/887	0.37	0/1180
14	2S	0.14	0/880	0.38	0/1172
15	1T	0.17	0/1105	0.43	0/1477
15	2T	0.15	0/1097	0.39	0/1468
16	1U	0.18	0/977	0.38	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.13	0/977	0.34	0/1301
17	1V	0.16	0/786	0.38	0/1053
17	2V	0.14	0/782	0.34	0/1049
18	1W	0.18	0/897	0.38	0/1205
18	2W	0.15	0/897	0.35	0/1205
19	1X	0.17	0/764	0.41	0/1025
19	2X	0.14	0/764	0.39	0/1025
20	1Y	0.17	0/823	0.44	0/1099
20	2Y	0.13	0/823	0.37	0/1100
21	1Z	0.14	0/1620	0.34	0/2200
21	2Z	0.13	0/1590	0.36	0/2162
22	10	0.18	0/616	0.45	0/821
22	20	0.15	0/616	0.41	0/821
23	11	0.17	0/761	0.38	0/1013
23	21	0.16	0/766	0.36	0/1018
24	12	0.15	0/590	0.37	0/781
24	22	0.14	0/594	0.38	0/785
25	13	0.17	0/474	0.41	0/635
25	23	0.13	0/469	0.34	0/630
26	14	0.18	0/559	0.54	0/754
26	24	0.22	0/549	0.58	2/741 (0.3%)
27	15	0.17	0/473	0.44	0/639
27	25	0.18	0/469	0.42	0/635
28	16	0.17	0/460	0.40	0/613
28	26	0.15	0/456	0.35	0/608
29	17	0.20	0/426	0.43	0/561
29	27	0.19	0/426	0.45	0/561
30	18	0.17	0/525	0.39	0/691
30	28	0.14	0/525	0.35	0/691
31	19	0.17	0/310	0.41	0/407
31	29	0.15	0/310	0.36	0/407
32	1a	0.14	0/35795	0.31	0/55864
32	2a	0.14	0/35890	0.31	0/56012
33	1b	0.15	0/1876	0.41	0/2533
33	2b	0.17	0/1860	0.41	0/2518
34	1c	0.14	0/1582	0.37	0/2137
34	2c	0.15	0/1566	0.36	0/2119
35	1d	0.14	0/1695	0.38	0/2274
35	2d	0.14	0/1698	0.37	0/2277
36	1e	0.15	0/1149	0.39	0/1548
36	2e	0.14	0/1149	0.37	0/1548
37	1f	0.14	0/827	0.35	0/1120
37	2f	0.13	0/829	0.35	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.13	0/1254	0.33	0/1683
38	2g	0.13	0/1248	0.32	0/1676
39	1h	0.13	0/1118	0.36	0/1506
39	2h	0.13	0/1108	0.36	0/1494
40	1i	0.14	0/1005	0.39	0/1351
40	2i	0.15	0/985	0.39	0/1329
41	1j	0.14	0/732	0.35	0/993
41	2j	0.16	0/723	0.40	0/984
42	1k	0.14	0/849	0.36	0/1150
42	2k	0.14	0/848	0.38	0/1149
43	1l	0.14	0/937	0.37	0/1260
43	2l	0.14	0/937	0.37	0/1260
44	1m	0.15	0/924	0.41	0/1242
44	2m	0.16	0/905	0.47	1/1217 (0.1%)
45	1n	0.13	0/501	0.36	0/664
45	2n	0.14	0/501	0.36	0/664
46	1o	0.14	0/739	0.33	0/985
46	2o	0.14	0/739	0.36	0/985
47	1p	0.15	0/697	0.44	0/939
47	2p	0.13	0/693	0.39	0/935
48	1q	0.14	0/836	0.36	0/1117
48	2q	0.14	0/836	0.37	0/1117
49	1r	0.13	0/560	0.35	0/746
49	2r	0.14	0/560	0.34	0/746
50	1s	0.13	0/663	0.40	0/895
50	2s	0.13	0/660	0.35	0/893
51	1t	0.15	0/734	0.43	0/969
51	2t	0.14	0/736	0.36	0/976
52	1u	0.13	0/203	0.36	0/266
52	2u	0.21	0/203	0.47	0/266
53	1y	0.17	0/776	0.31	0/1048
53	2y	0.12	0/761	0.29	0/1030
All	All	0.16	0/309941	0.35	3/463239 (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

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	24	59	PHE	CA-C-N	5.29	131.22	121.70
26	24	59	PHE	C-N-CA	5.29	131.22	121.70
44	2m	84	ILE	N-CA-C	-5.06	106.66	112.98

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
33	1b	231	GLU	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31207	449	0
1	2A	61758	0	31153	518	0
2	1B	2572	0	1305	12	0
2	2B	2573	0	1306	29	0
3	1D	2131	0	2207	36	0
3	2D	2136	0	2218	34	0
4	1E	1559	0	1618	26	0
4	2E	1559	0	1618	28	0
5	1F	1584	0	1625	26	0
5	2F	1580	0	1619	33	0
6	1G	1426	0	1445	31	0
6	2G	1424	0	1441	54	0
7	1H	1330	0	1407	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	2H	1324	0	1402	39	0
8	1I	1094	0	1127	21	0
8	2I	1076	0	1094	16	0
9	1N	1121	0	1195	15	0
9	2N	1117	0	1184	19	0
10	1O	933	0	996	16	0
10	2O	933	0	996	12	0
11	1P	1135	0	1212	25	0
11	2P	1135	0	1212	17	0
12	1Q	1122	0	1179	10	0
12	2Q	1122	0	1179	17	0
13	1R	968	0	1033	15	0
13	2R	968	0	1033	14	0
14	1S	877	0	938	17	0
14	2S	870	0	923	27	0
15	1T	1091	0	1151	25	0
15	2T	1083	0	1136	17	0
16	1U	959	0	1019	12	0
16	2U	959	0	1019	15	0
17	1V	775	0	841	12	0
17	2V	771	0	830	13	0
18	1W	886	0	940	9	0
18	2W	886	0	940	10	0
19	1X	750	0	814	13	0
19	2X	750	0	814	6	0
20	1Y	810	0	892	13	0
20	2Y	810	0	887	12	0
21	1Z	1587	0	1598	21	0
21	2Z	1557	0	1564	28	0
22	10	608	0	622	6	0
22	20	608	0	622	5	0
23	11	754	0	823	14	0
23	21	759	0	837	17	0
24	12	588	0	643	8	0
24	22	592	0	654	10	0
25	13	469	0	518	8	0
25	23	464	0	514	6	0
26	14	546	0	522	15	0
26	24	536	0	514	25	0
27	15	459	0	476	4	0
27	25	455	0	465	5	0
28	16	453	0	473	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	26	449	0	469	9	0
29	17	418	0	467	9	0
29	27	418	0	467	4	0
30	18	517	0	582	14	0
30	28	517	0	582	8	0
31	19	307	0	335	3	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	335	0
32	2a	32331	0	16338	352	0
33	1b	1842	0	1862	47	0
33	2b	1825	0	1828	61	0
34	1c	1558	0	1557	28	0
34	2c	1542	0	1517	40	0
35	1d	1665	0	1687	56	0
35	2d	1668	0	1703	37	0
36	1e	1133	0	1191	30	0
36	2e	1133	0	1191	27	0
37	1f	814	0	808	14	0
37	2f	816	0	808	13	0
38	1g	1235	0	1249	18	0
38	2g	1229	0	1238	20	0
39	1h	1098	0	1143	24	0
39	2h	1088	0	1126	24	0
40	1i	986	0	990	34	0
40	2i	966	0	953	33	0
41	1j	719	0	672	15	0
41	2j	710	0	661	34	0
42	1k	834	0	838	6	0
42	2k	833	0	836	16	0
43	1l	932	0	981	10	0
43	2l	932	0	981	20	0
44	1m	914	0	954	27	0
44	2m	895	0	920	31	0
45	1n	492	0	529	21	0
45	2n	492	0	529	17	0
46	1o	728	0	760	13	0
46	2o	728	0	760	15	0
47	1p	681	0	697	18	0
47	2p	677	0	686	15	0
48	1q	823	0	891	19	0
48	2q	823	0	891	22	0
49	1r	555	0	618	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	2r	555	0	618	11	0
50	1s	648	0	658	24	0
50	2s	645	0	635	31	0
51	1t	732	0	809	15	0
51	2t	733	0	795	13	0
52	1u	199	0	208	3	0
52	2u	199	0	208	3	0
53	1y	764	0	786	16	0
53	2y	749	0	757	20	0
54	10	7	0	0	0	0
54	11	5	0	0	0	0
54	13	4	0	0	0	0
54	14	1	0	0	0	0
54	15	8	0	0	0	0
54	17	7	0	0	0	0
54	18	3	0	0	0	0
54	19	2	0	0	0	0
54	1A	1056	0	0	0	0
54	1B	29	0	0	0	0
54	1D	18	0	0	0	0
54	1E	9	0	0	0	0
54	1F	19	0	0	0	0
54	1G	4	0	0	0	0
54	1H	3	0	0	0	0
54	1N	5	0	0	0	0
54	1O	1	0	0	0	0
54	1P	6	0	0	0	0
54	1Q	5	0	0	0	0
54	1R	6	0	0	0	0
54	1T	5	0	0	0	0
54	1U	7	0	0	0	0
54	1V	6	0	0	0	0
54	1W	3	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	277	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	2	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1k	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	1	0	0	0	0
54	1n	3	0	0	0	0
54	1o	1	0	0	0	0
54	1t	1	0	0	0	0
54	1y	4	0	0	0	0
54	20	3	0	0	0	0
54	21	1	0	0	0	0
54	23	2	0	0	0	0
54	25	1	0	0	0	0
54	27	1	0	0	0	0
54	28	2	0	0	0	0
54	2A	741	0	0	0	0
54	2B	18	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	3	0	0	0	0
54	2N	1	0	0	0	0
54	2O	2	0	0	0	0
54	2Q	3	0	0	0	0
54	2R	3	0	0	0	0
54	2T	3	0	0	0	0
54	2V	3	0	0	0	0
54	2W	3	0	0	0	0
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	195	0	0	0	0
54	2d	1	0	0	0	0
54	2e	1	0	0	0	0
54	2f	2	0	0	0	0
54	2j	1	0	0	0	0
54	2k	1	0	0	0	0
54	2n	1	0	0	0	0
54	2o	1	0	0	0	0
54	2p	1	0	0	0	0
54	2r	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	24	0	17	1	0
55	2A	24	0	17	3	0
56	18	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1A	8	0	14	1	0
56	1O	8	0	14	1	0
56	1a	8	0	14	4	0
56	2A	16	0	28	1	0
56	2B	8	0	14	0	0
57	1B	12	0	12	1	0
57	1F	12	0	12	2	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	0	0
59	2d	8	0	0	0	0
60	10	25	0	0	0	0
60	11	28	0	0	0	0
60	12	13	0	0	3	0
60	13	25	0	0	2	0
60	14	3	0	0	0	0
60	15	28	0	0	0	0
60	16	20	0	0	0	0
60	17	13	0	0	0	0
60	18	28	0	0	1	0
60	19	8	0	0	0	0
60	1A	3927	0	0	79	0
60	1B	89	0	0	5	0
60	1D	110	0	0	3	0
60	1E	72	0	0	3	0
60	1F	67	0	0	1	0
60	1G	16	0	0	0	0
60	1H	14	0	0	0	0
60	1I	5	0	0	0	0
60	1N	52	0	0	0	0
60	1O	25	0	0	1	0
60	1P	65	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1Q	41	0	0	1	0
60	1R	32	0	0	1	0
60	1S	8	0	0	1	0
60	1T	36	0	0	2	0
60	1U	43	0	0	3	0
60	1V	36	0	0	0	0
60	1W	28	0	0	1	0
60	1X	26	0	0	1	0
60	1Y	17	0	0	2	0
60	1Z	11	0	0	0	0
60	1a	496	0	0	22	0
60	1b	1	0	0	0	0
60	1c	1	0	0	0	0
60	1d	9	0	0	1	0
60	1e	10	0	0	1	0
60	1f	1	0	0	0	0
60	1h	1	0	0	0	0
60	1j	1	0	0	0	0
60	1k	1	0	0	0	0
60	1l	4	0	0	0	0
60	1o	4	0	0	0	0
60	1p	1	0	0	0	0
60	1y	5	0	0	0	0
60	20	10	0	0	0	0
60	21	17	0	0	2	0
60	22	2	0	0	0	0
60	23	2	0	0	1	0
60	25	7	0	0	0	0
60	26	6	0	0	1	0
60	27	9	0	0	0	0
60	28	15	0	0	0	0
60	2A	2249	0	0	87	0
60	2B	42	0	0	3	0
60	2D	47	0	0	1	0
60	2E	28	0	0	1	0
60	2F	23	0	0	0	0
60	2G	4	0	0	0	0
60	2H	1	0	0	1	0
60	2N	6	0	0	1	0
60	2O	15	0	0	0	0
60	2P	21	0	0	1	0
60	2Q	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2R	22	0	0	2	0
60	2S	2	0	0	0	0
60	2T	12	0	0	0	0
60	2U	16	0	0	3	0
60	2V	8	0	0	0	0
60	2W	19	0	0	0	0
60	2X	8	0	0	0	0
60	2Y	4	0	0	0	0
60	2Z	8	0	0	0	0
60	2a	404	0	0	22	0
60	2d	3	0	0	1	0
60	2e	3	0	0	0	0
60	2f	3	0	0	0	0
60	2j	2	0	0	1	0
60	2l	5	0	0	1	0
60	2o	2	0	0	1	0
60	2p	1	0	0	0	0
60	2q	1	0	0	0	0
60	2r	3	0	0	0	0
60	2t	3	0	0	0	0
60	2u	1	0	0	0	0
60	2y	1	0	0	0	0
All	All	297563	0	194555	3101	0

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

The worst 5 of 3101 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.39	1.19
1:1A:1082:U:O4	1:1A:1086:A:N1	1.97	0.97
32:1a:1086:U:H3	32:1a:1099:G:H22	1.16	0.94
15:1T:55:ASN:H	15:1T:59:THR:HG22	1.35	0.90
1:2A:2319:G:H22	14:2S:3:ARG:HD3	1.37	0.87

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	261 (96%)	12 (4%)	0	100	100
3	2D	273/276 (99%)	262 (96%)	10 (4%)	1 (0%)	30	51
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	46
4	2E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	12	28
5	1F	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24	46
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	46
6	1G	179/182 (98%)	171 (96%)	4 (2%)	4 (2%)	5	10
6	2G	179/182 (98%)	164 (92%)	12 (7%)	3 (2%)	7	15
7	1H	172/180 (96%)	161 (94%)	11 (6%)	0	100	100
7	2H	171/180 (95%)	155 (91%)	16 (9%)	0	100	100
8	1I	145/148 (98%)	132 (91%)	13 (9%)	0	100	100
8	2I	144/148 (97%)	134 (93%)	10 (7%)	0	100	100
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	38
11	2P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18	38
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	28
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	28
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	25
19	2X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	25
20	1Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	2Y	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	1Z	201/206 (98%)	191 (95%)	9 (4%)	1 (0%)	24	46
21	2Z	199/206 (97%)	186 (94%)	13 (6%)	0	100	100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	20	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	25
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1
26	24	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	198 (86%)	26 (11%)	5 (2%)	5	10
33	2b	229/256 (90%)	201 (88%)	22 (10%)	6 (3%)	4	7
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	175 (86%)	28 (14%)	1 (0%)	24	46
35	1d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
35	2d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
36	1e	146/162 (90%)	139 (95%)	7 (5%)	0	100	100
36	2e	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
38	2g	153/156 (98%)	146 (95%)	6 (4%)	1 (1%)	18	38
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
40	1i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16	34
40	2i	124/128 (97%)	109 (88%)	12 (10%)	3 (2%)	4	9
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3	5
41	2j	94/105 (90%)	82 (87%)	9 (10%)	3 (3%)	3	5
42	1k	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
42	2k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	14	30
43	1l	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
43	2l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
44	1m	114/126 (90%)	104 (91%)	8 (7%)	2 (2%)	6	14
44	2m	112/126 (89%)	97 (87%)	12 (11%)	3 (3%)	4	7
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	23
46	2o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	5	9
47	1p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	12	28
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
51	1t	94/106 (89%)	88 (94%)	6 (6%)	0	100	100
51	2t	96/106 (91%)	91 (95%)	5 (5%)	0	100	100
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	2
53	1y	95/113 (84%)	95 (100%)	0	0	100	100
53	2y	94/113 (83%)	92 (98%)	2 (2%)	0	100	100
All	All	11629/12354 (94%)	10978 (94%)	588 (5%)	63 (0%)	24	46

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	1b	21	ARG
33	1b	124	SER
44	1m	67	GLU
44	1m	106	ASN
5	2F	130	ALA

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	31
3	2D	215/218 (99%)	199 (93%)	16 (7%)	13	29
4	1E	164/166 (99%)	150 (92%)	14 (8%)	10	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	152 (93%)	12 (7%)	13	29
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8	18
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	18
6	1G	144/156 (92%)	134 (93%)	10 (7%)	14	32
6	2G	142/156 (91%)	128 (90%)	14 (10%)	7	16
7	1H	144/148 (97%)	134 (93%)	10 (7%)	14	32
7	2H	143/148 (97%)	129 (90%)	14 (10%)	7	17
8	1I	111/124 (90%)	104 (94%)	7 (6%)	16	36
8	2I	108/124 (87%)	100 (93%)	8 (7%)	13	29
9	1N	119/119 (100%)	109 (92%)	10 (8%)	10	23
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	27
10	1O	100/100 (100%)	99 (99%)	1 (1%)	68	86
10	2O	100/100 (100%)	98 (98%)	2 (2%)	48	74
11	1P	115/116 (99%)	110 (96%)	5 (4%)	26	51
11	2P	115/116 (99%)	104 (90%)	11 (10%)	8	17
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	13	30
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	36
13	1R	101/101 (100%)	94 (93%)	7 (7%)	14	32
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9	20
14	1S	87/88 (99%)	79 (91%)	8 (9%)	8	19
14	2S	85/88 (97%)	79 (93%)	6 (7%)	13	31
15	1T	115/127 (91%)	110 (96%)	5 (4%)	26	51
15	2T	113/127 (89%)	109 (96%)	4 (4%)	32	59
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	62
16	2U	93/94 (99%)	90 (97%)	3 (3%)	34	62
17	1V	81/82 (99%)	78 (96%)	3 (4%)	30	57
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	16
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19	40
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	33
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	55
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	14	31
20	2Y	86/91 (94%)	81 (94%)	5 (6%)	18	39
21	1Z	169/179 (94%)	155 (92%)	14 (8%)	10	23
21	2Z	165/179 (92%)	152 (92%)	13 (8%)	11	26
22	10	61/67 (91%)	59 (97%)	2 (3%)	33	61
22	20	61/67 (91%)	60 (98%)	1 (2%)	55	79
23	11	79/83 (95%)	74 (94%)	5 (6%)	16	36
23	21	81/83 (98%)	76 (94%)	5 (6%)	16	36
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	63
24	22	66/67 (98%)	60 (91%)	6 (9%)	9	19
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	26
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	37
26	14	58/63 (92%)	54 (93%)	4 (7%)	14	32
26	24	54/63 (86%)	48 (89%)	6 (11%)	6	12
27	15	51/52 (98%)	49 (96%)	2 (4%)	28	55
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	55
28	16	51/52 (98%)	50 (98%)	1 (2%)	48	74
28	26	50/52 (96%)	48 (96%)	2 (4%)	28	55
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	47
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	17
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	40
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	40
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	65
33	1b	191/220 (87%)	164 (86%)	27 (14%)	3	6
33	2b	187/220 (85%)	163 (87%)	24 (13%)	4	8
34	1c	144/188 (77%)	135 (94%)	9 (6%)	16	36
34	2c	140/188 (74%)	127 (91%)	13 (9%)	8	18
35	1d	171/181 (94%)	155 (91%)	16 (9%)	8	18
35	2d	172/181 (95%)	160 (93%)	12 (7%)	14	31
36	1e	114/123 (93%)	107 (94%)	7 (6%)	17	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	114/123 (93%)	106 (93%)	8 (7%)	14	31
37	1f	85/90 (94%)	79 (93%)	6 (7%)	13	31
37	2f	85/90 (94%)	82 (96%)	3 (4%)	32	59
38	1g	120/127 (94%)	112 (93%)	8 (7%)	15	33
38	2g	119/127 (94%)	109 (92%)	10 (8%)	10	23
39	1h	116/119 (98%)	110 (95%)	6 (5%)	21	44
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	17
40	1i	91/99 (92%)	81 (89%)	10 (11%)	6	13
40	2i	88/99 (89%)	77 (88%)	11 (12%)	4	9
41	1j	68/92 (74%)	64 (94%)	4 (6%)	18	38
41	2j	68/92 (74%)	63 (93%)	5 (7%)	13	29
42	1k	83/99 (84%)	80 (96%)	3 (4%)	31	58
42	2k	83/99 (84%)	79 (95%)	4 (5%)	23	47
43	1l	96/108 (89%)	94 (98%)	2 (2%)	47	73
43	2l	96/108 (89%)	93 (97%)	3 (3%)	35	63
44	1m	90/101 (89%)	82 (91%)	8 (9%)	9	20
44	2m	87/101 (86%)	82 (94%)	5 (6%)	18	40
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	24
45	2n	49/50 (98%)	45 (92%)	4 (8%)	10	24
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21	45
46	2o	78/80 (98%)	70 (90%)	8 (10%)	7	15
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	8
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	15
48	1q	94/97 (97%)	92 (98%)	2 (2%)	47	73
48	2q	94/97 (97%)	91 (97%)	3 (3%)	34	62
49	1r	59/77 (77%)	58 (98%)	1 (2%)	53	78
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	60
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7	15
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7	14
51	1t	71/82 (87%)	62 (87%)	9 (13%)	4	9
51	2t	70/82 (85%)	65 (93%)	5 (7%)	13	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	40
52	2u	18/22 (82%)	18 (100%)	0	100	100
53	1y	82/98 (84%)	80 (98%)	2 (2%)	43	70
53	2y	79/98 (81%)	71 (90%)	8 (10%)	7	15
All	All	9524/10260 (93%)	8854 (93%)	670 (7%)	14	31

5 of 670 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	2W	107	LEU
36	2e	107	ARG
21	2Z	86	VAL
18	2W	100	THR
33	2b	52	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	160	GLN
38	2g	13	GLN
44	2m	62	ASN
38	1g	64	GLN
38	1g	28	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	396 (13%)	27 (0%)
1	2A	2858/2915 (98%)	460 (16%)	32 (1%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	119/121 (98%)	15 (12%)	0
32	1a	1497/1521 (98%)	241 (16%)	0
32	2a	1501/1521 (98%)	254 (16%)	0
All	All	8959/9114 (98%)	1375 (15%)	59 (0%)

5 of 1375 RNA backbone outliers are listed below:

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

5 of 59 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	195	A
1	2A	2601	C
1	2A	827	U
1	2A	2406	U
1	2A	1992	G

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	$\# Z > 2$
1	OMU	1A	2552	54,1	19,22,23	1.24	2 (10%)	25,31,34	1.77	5 (20%)
32	M2G	2a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.85	6 (18%)
1	5MU	1A	1915	54,1	19,22,23	1.47	6 (31%)	27,32,35	2.18	8 (29%)
32	UR3	2a	1498	32	19,22,23	1.00	2 (10%)	26,32,35	1.73	3 (11%)
32	MA6	2a	1518	32	23,26,27	0.40	0	33,38,41	2.03	9 (27%)
32	5MC	1a	1407	32	19,22,23	1.71	3 (15%)	26,32,35	1.14	3 (11%)
32	5MC	2a	967	32	19,22,23	1.79	3 (15%)	26,32,35	1.10	2 (7%)
32	PSU	1a	516	32,54	18,21,22	1.38	2 (11%)	21,30,33	1.97	4 (19%)
1	PSU	1A	2605	1	18,21,22	1.37	3 (16%)	21,30,33	2.03	4 (19%)
1	2MA	1A	2503	54,1	22,25,26	1.50	4 (18%)	32,37,40	2.34	7 (21%)
32	MA6	1a	1519	32	23,26,27	0.42	0	33,38,41	2.03	9 (27%)
32	5MC	1a	1404	32	19,22,23	1.63	3 (15%)	26,32,35	1.09	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PSU	2a	516	32,54	18,21,22	1.36	2 (11%)	21,30,33	2.09	5 (23%)
1	5MU	1A	1939	54,1	19,22,23	1.43	6 (31%)	27,32,35	2.10	6 (22%)
32	G7M	2a	527	32,54	23,26,27	1.52	3 (13%)	34,39,42	1.73	5 (14%)
1	PSU	2A	2605	1	18,21,22	1.32	2 (11%)	21,30,33	2.09	4 (19%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.98	1 (4%)
32	5MC	2a	1400	32	19,22,23	1.66	3 (15%)	26,32,35	1.17	3 (11%)
1	2MA	2A	2503	54,1	22,25,26	1.50	4 (18%)	32,37,40	2.34	8 (25%)
32	5MC	2a	1407	32	19,22,23	1.64	2 (10%)	26,32,35	1.16	3 (11%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	1.98	9 (27%)
32	5MC	1a	967	32	19,22,23	1.67	3 (15%)	26,32,35	1.12	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	0.99	1 (4%)
32	5MC	2a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.12	3 (11%)
32	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.74	3 (11%)
1	OMC	1A	1920	1	19,22,23	0.78	0	25,31,34	0.85	1 (4%)
1	5MC	1A	1962	1	19,22,23	1.78	3 (15%)	26,32,35	1.20	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
1	5MU	2A	1915	1	19,22,23	1.45	4 (21%)	27,32,35	2.20	8 (29%)
1	PSU	1A	1917	54,1	18,21,22	1.36	2 (11%)	21,30,33	1.98	3 (14%)
1	OMU	2A	2552	54,1	19,22,23	1.18	3 (15%)	25,31,34	1.87	5 (20%)
32	2MG	1a	1207	32,54	23,26,27	1.24	2 (8%)	33,38,41	2.36	9 (27%)
32	4OC	2a	1402	32	20,23,24	0.77	0	25,32,35	1.01	1 (4%)
1	OMG	1A	2251	54,1	23,26,27	1.20	3 (13%)	32,38,41	2.00	6 (18%)
32	2MG	2a	1207	32	23,26,27	1.21	2 (8%)	33,38,41	2.21	7 (21%)
32	5MC	1a	1400	32	19,22,23	1.76	3 (15%)	26,32,35	1.14	2 (7%)
1	5MC	2A	1962	54,1	19,22,23	1.61	3 (15%)	26,32,35	1.14	2 (7%)
32	MA6	2a	1519	32	23,26,27	0.41	0	33,38,41	2.09	9 (27%)
1	5MU	2A	1939	1	19,22,23	1.41	5 (26%)	27,32,35	2.16	6 (22%)
1	PSU	1A	1911	1	18,21,22	1.34	2 (11%)	21,30,33	2.05	5 (23%)
43	0TD	1l	92	43	8,9,10	4.52	1 (12%)	6,11,13	6.96	2 (33%)
1	5MC	1A	1942	54,1	19,22,23	1.59	3 (15%)	26,32,35	1.10	2 (7%)
32	G7M	1a	527	32,54	23,26,27	1.52	3 (13%)	34,39,42	1.71	5 (14%)
43	0TD	2l	92	43	8,9,10	4.37	1 (12%)	6,11,13	1.27	1 (16%)
1	OMG	2A	2251	54,1	23,26,27	1.18	3 (13%)	32,38,41	2.02	6 (18%)
32	M2G	1a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.85	6 (18%)
1	5MC	2A	1942	1	19,22,23	1.72	3 (15%)	26,32,35	1.13	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	1.97	3 (14%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1A	2251	54,1	-	0/9/27/28	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	5MC	2A	1962	54,1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	2/11/29/30	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
1	5MC	1A	1942	54,1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,54	-	1/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	3/7/12/14	-
1	OMG	2A	2251	54,1	-	0/9/27/28	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.42	1.69	1.82
43	2l	92	0TD	CB-SB	-12.02	1.70	1.82
32	2a	967	5MC	C5-C4	6.61	1.49	1.44
1	1A	1962	5MC	C5-C4	6.61	1.49	1.44
32	1a	1400	5MC	C5-C4	6.47	1.49	1.44

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-16.76	72.24	102.36
1	1A	2503	2MA	C5-C4-N3	-8.42	118.31	127.18
1	2A	2503	2MA	C5-C4-N3	-8.20	118.55	127.18
32	1a	1207	2MG	C2-N3-C4	7.28	121.11	112.00
32	1a	1498	UR3	C4-N3-C2	-7.03	118.92	124.58

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
1	2A	1915	5MU	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	2A	1915	5MU	O4'-C1'-N1-C6
43	2I	92	0TD	O-C-CA-CB

There are no ring outliers.

19 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1518	MA6	2	0
1	1A	2503	2MA	1	0
32	1a	1519	MA6	2	0
1	1A	1939	5MU	1	0
1	2A	1920	OMC	1	0
32	2a	1400	5MC	1	0
32	1a	1518	MA6	1	0
32	1a	967	5MC	1	0
32	1a	1402	4OC	1	0
32	2a	1404	5MC	2	0
32	1a	1498	UR3	1	0
1	1A	1920	OMC	1	0
1	2A	1915	5MU	1	0
1	1A	1917	PSU	1	0
32	2a	1402	4OC	2	0
32	1a	1400	5MC	2	0
32	2a	1519	MA6	2	0
43	2I	92	0TD	1	0
1	2A	1917	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2572 ligands modelled in this entry, 2559 are monoatomic - leaving 13 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	MPD	18	104	-	7,7,7	0.30	0	9,10,10	0.25	0
57	ARG	1B	230	54	10,11,11	0.76	1 (10%)	9,13,13	0.99	1 (11%)
56	MPD	1a	1878	-	7,7,7	0.40	0	9,10,10	0.40	0
55	CPF	1A	4056	54	27,27,27	2.11	6 (22%)	40,40,40	1.79	11 (27%)
55	CPF	2A	3741	54	27,27,27	2.09	6 (22%)	40,40,40	2.22	13 (32%)
57	ARG	1F	320	-	10,11,11	0.75	1 (10%)	9,13,13	0.87	1 (11%)
56	MPD	2B	219	-	7,7,7	0.31	0	9,10,10	0.23	0
59	SF4	2d	302	35	0,12,12	-	-	-	-	-
56	MPD	1A	4058	-	7,7,7	0.35	0	9,10,10	0.34	0
56	MPD	1O	202	-	7,7,7	0.31	0	9,10,10	0.19	0
56	MPD	2A	3743	-	7,7,7	0.33	0	9,10,10	0.30	0
59	SF4	1d	306	35	0,12,12	-	-	-	-	-
56	MPD	2A	3744	-	7,7,7	0.31	0	9,10,10	0.17	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
56	MPD	18	104	-	-	4/5/5/5	-
57	ARG	1B	230	54	-	2/11/11/11	-
56	MPD	1a	1878	-	-	5/5/5/5	-
55	CPF	1A	4056	54	-	9/12/22/22	0/4/4/4
55	CPF	2A	3741	54	-	6/12/22/22	0/4/4/4
57	ARG	1F	320	-	-	3/11/11/11	-
56	MPD	2B	219	-	-	3/5/5/5	-
59	SF4	2d	302	35	-	-	0/6/5/5
56	MPD	1A	4058	-	-	2/5/5/5	-
56	MPD	1O	202	-	-	2/5/5/5	-
56	MPD	2A	3743	-	-	0/5/5/5	-
59	SF4	1d	306	35	-	-	0/6/5/5
56	MPD	2A	3744	-	-	4/5/5/5	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4056	CPF	C2-C3	-5.59	1.39	1.48
55	2A	3741	CPF	C2-C3	-5.56	1.40	1.48
55	2A	3741	CPF	C5-C4	-4.88	1.38	1.48
55	1A	4056	CPF	C10-N1	-4.71	1.34	1.40
55	1A	4056	CPF	C5-C4	-4.62	1.39	1.48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3741	CPF	F1-C7-C8	6.06	124.15	118.37
55	2A	3741	CPF	C9-C8-N2	-4.45	116.11	122.59
55	2A	3741	CPF	C6-C7-C8	-4.44	119.43	123.35
55	2A	3741	CPF	C7-C8-N2	4.16	125.28	120.42
55	1A	4056	CPF	C2-C1-N1	-4.07	119.54	124.42

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1A	4056	CPF	C1-C2-C3-O2
55	1A	4056	CPF	C4-C2-C3-O2
55	1A	4056	CPF	C1-C2-C3-O1
55	1A	4056	CPF	C4-C2-C3-O1
55	1A	4056	CPF	C7-C8-N2-C17

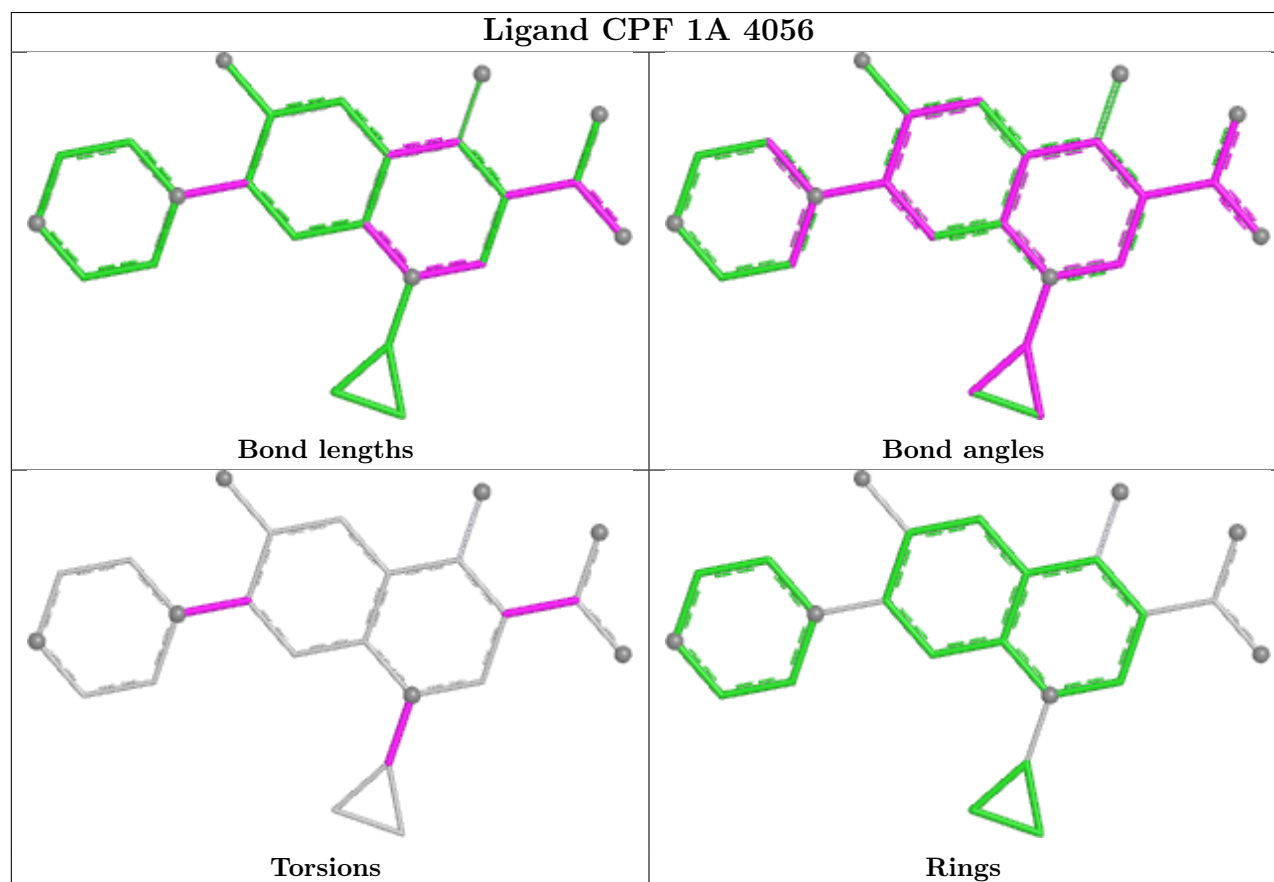
There are no ring outliers.

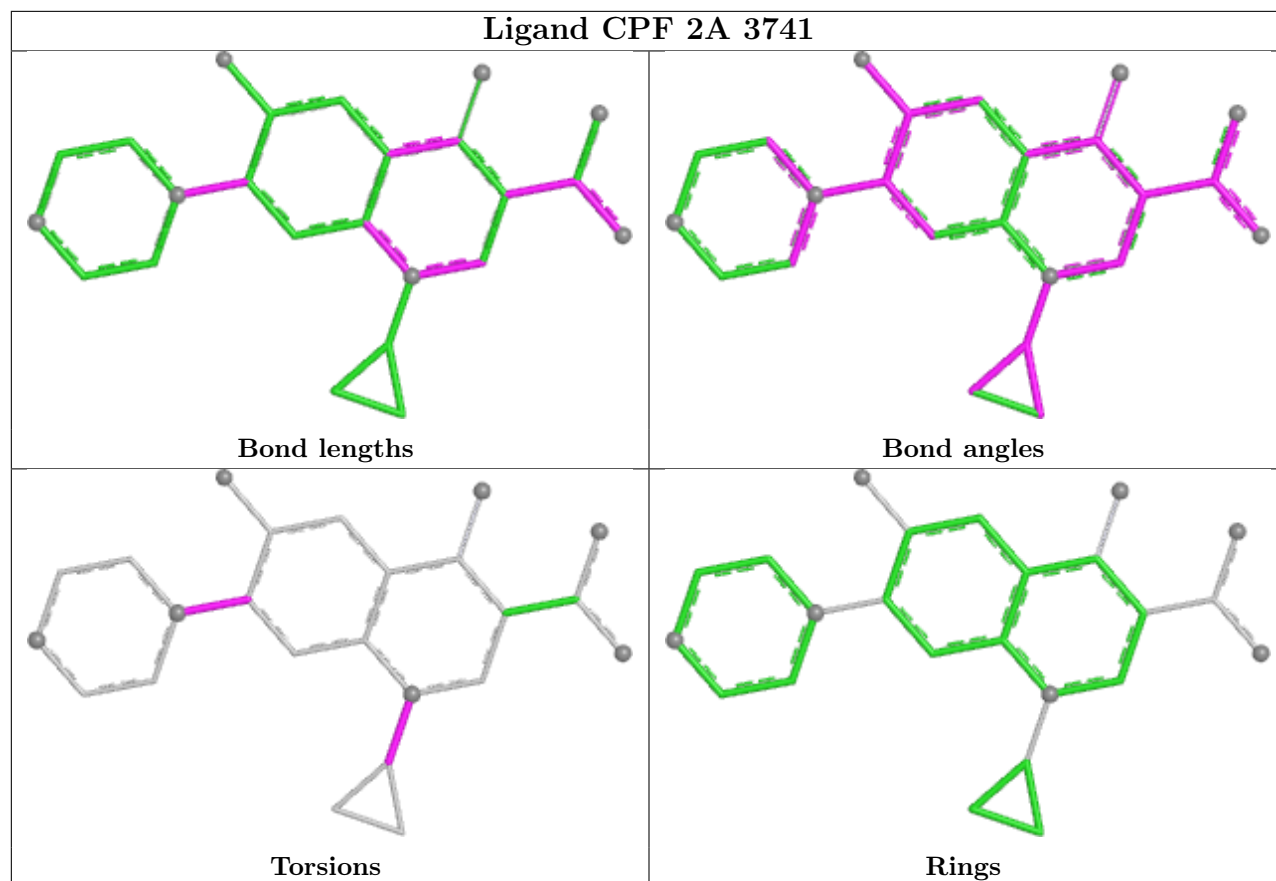
9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	18	104	MPD	1	0
57	1B	230	ARG	1	0
56	1a	1878	MPD	4	0
55	1A	4056	CPF	1	0
55	2A	3741	CPF	3	0
57	1F	320	ARG	2	0
56	1A	4058	MPD	1	0
56	1O	202	MPD	1	0
56	2A	3743	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%)	-0.39	154 (5%) 31 26	24, 40, 97, 109	0
1	2A	2856/2915 (97%)	0.06	181 (6%) 26 20	31, 57, 100, 110	0
2	1B	120/121 (99%)	-0.17	2 (1%) 69 64	38, 56, 70, 88	0
2	2B	120/121 (99%)	0.81	6 (5%) 34 28	62, 82, 89, 98	0
3	1D	275/276 (99%)	-0.11	4 (1%) 72 68	25, 39, 55, 76	0
3	2D	275/276 (99%)	0.16	2 (0%) 84 82	32, 50, 63, 78	0
4	1E	204/206 (99%)	-0.07	3 (1%) 72 68	23, 42, 64, 78	0
4	2E	204/206 (99%)	0.18	3 (1%) 72 68	36, 57, 73, 81	0
5	1F	203/210 (96%)	-0.01	2 (0%) 79 76	22, 45, 71, 89	0
5	2F	203/210 (96%)	0.38	1 (0%) 87 85	35, 64, 79, 89	0
6	1G	181/182 (99%)	0.69	13 (7%) 21 17	53, 70, 82, 91	0
6	2G	181/182 (99%)	1.55	45 (24%) 2 1	77, 87, 94, 98	0
7	1H	174/180 (96%)	0.33	7 (4%) 42 37	41, 56, 69, 74	0
7	2H	173/180 (96%)	1.42	32 (18%) 3 3	72, 84, 90, 95	0
8	1I	147/148 (99%)	0.85	10 (6%) 23 19	45, 71, 83, 86	0
8	2I	146/148 (98%)	0.86	5 (3%) 48 42	53, 75, 86, 91	0
9	1N	140/140 (100%)	-0.13	1 (0%) 84 82	30, 43, 64, 79	0
9	2N	140/140 (100%)	0.48	3 (2%) 63 58	48, 64, 78, 86	0
10	1O	122/122 (100%)	-0.11	0 100 100	31, 43, 62, 68	0
10	2O	122/122 (100%)	0.12	0 100 100	46, 55, 68, 75	0
11	1P	149/150 (99%)	-0.00	1 (0%) 84 82	24, 48, 68, 81	0
11	2P	149/150 (99%)	0.52	2 (1%) 75 71	39, 66, 83, 88	0
12	1Q	141/141 (100%)	-0.16	0 100 100	31, 43, 57, 71	0
12	2Q	141/141 (100%)	0.69	6 (4%) 40 34	47, 65, 76, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.15	0 100 100	29, 41, 55, 63	0
13	2R	118/118 (100%)	0.19	0 100 100	40, 54, 64, 70	0
14	1S	110/112 (98%)	0.27	1 (0%) 81 78	43, 55, 67, 72	0
14	2S	110/112 (98%)	1.29	21 (19%) 3 2	67, 76, 82, 89	0
15	1T	131/146 (89%)	0.09	5 (3%) 44 38	38, 47, 70, 81	0
15	2T	131/146 (89%)	0.37	2 (1%) 72 68	47, 59, 76, 86	0
16	1U	116/118 (98%)	-0.29	0 100 100	28, 35, 49, 65	0
16	2U	116/118 (98%)	0.36	0 100 100	42, 59, 72, 80	0
17	1V	101/101 (100%)	-0.17	0 100 100	27, 46, 63, 71	0
17	2V	101/101 (100%)	0.71	3 (2%) 52 47	41, 69, 77, 84	0
18	1W	112/113 (99%)	-0.18	2 (1%) 67 63	28, 36, 54, 84	0
18	2W	112/113 (99%)	0.13	2 (1%) 67 63	41, 50, 66, 91	0
19	1X	95/96 (98%)	-0.00	2 (2%) 63 58	31, 42, 66, 77	0
19	2X	95/96 (98%)	0.53	6 (6%) 26 20	45, 60, 77, 86	0
20	1Y	107/110 (97%)	0.18	1 (0%) 81 78	37, 51, 68, 78	0
20	2Y	107/110 (97%)	0.93	6 (5%) 30 24	59, 70, 79, 90	0
21	1Z	203/206 (98%)	0.42	4 (1%) 65 60	44, 62, 75, 86	0
21	2Z	201/206 (97%)	1.14	17 (8%) 16 13	68, 79, 85, 92	0
22	10	77/85 (90%)	0.08	1 (1%) 75 71	32, 41, 60, 65	0
22	20	77/85 (90%)	0.80	6 (7%) 19 15	50, 65, 74, 77	0
23	11	97/98 (98%)	0.14	1 (1%) 79 76	32, 45, 69, 75	0
23	21	97/98 (98%)	0.55	5 (5%) 33 27	41, 55, 76, 80	0
24	12	70/72 (97%)	0.18	1 (1%) 73 69	40, 51, 62, 83	0
24	22	70/72 (97%)	0.65	1 (1%) 73 69	61, 70, 77, 79	0
25	13	59/60 (98%)	-0.09	0 100 100	31, 42, 66, 72	0
25	23	59/60 (98%)	0.47	3 (5%) 33 28	51, 62, 80, 84	0
26	14	69/71 (97%)	1.32	20 (28%) 1 1	64, 83, 95, 98	0
26	24	69/71 (97%)	1.93	25 (36%) 1 0	85, 92, 99, 103	0
27	15	59/60 (98%)	-0.15	1 (1%) 69 64	26, 40, 63, 74	0
27	25	59/60 (98%)	0.10	0 100 100	35, 52, 69, 79	0
28	16	53/54 (98%)	-0.21	0 100 100	38, 46, 60, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.52	0 100 100	53, 62, 71, 74	0
29	17	48/49 (97%)	-0.11	4 (8%) 17 13	25, 32, 61, 66	0
29	27	48/49 (97%)	0.14	5 (10%) 11 9	34, 41, 69, 77	0
30	18	64/65 (98%)	-0.23	1 (1%) 70 66	29, 37, 46, 54	0
30	28	64/65 (98%)	0.43	2 (3%) 51 45	48, 56, 63, 72	0
31	19	37/37 (100%)	0.05	1 (2%) 56 50	35, 45, 60, 63	0
31	29	37/37 (100%)	1.18	3 (8%) 18 14	61, 70, 79, 81	0
32	1a	1488/1521 (97%)	0.45	66 (4%) 39 33	39, 73, 96, 110	0
32	2a	1492/1521 (98%)	0.71	115 (7%) 19 15	47, 77, 98, 109	0
33	1b	231/256 (90%)	1.39	53 (22%) 2 2	69, 81, 90, 96	0
33	2b	231/256 (90%)	1.62	68 (29%) 1 1	74, 85, 93, 98	0
34	1c	206/239 (86%)	1.06	21 (10%) 12 9	65, 76, 87, 89	0
34	2c	206/239 (86%)	1.79	68 (33%) 1 1	78, 86, 91, 96	0
35	1d	208/209 (99%)	1.04	21 (10%) 12 9	59, 74, 82, 89	0
35	2d	208/209 (99%)	1.13	24 (11%) 9 7	62, 72, 81, 84	0
36	1e	148/162 (91%)	0.63	4 (2%) 56 50	49, 68, 77, 90	0
36	2e	148/162 (91%)	0.96	8 (5%) 31 26	57, 73, 82, 93	0
37	1f	100/101 (99%)	0.47	2 (2%) 65 60	51, 68, 78, 82	0
37	2f	100/101 (99%)	0.59	0 100 100	56, 69, 78, 84	0
38	1g	155/156 (99%)	0.67	5 (3%) 50 44	68, 75, 83, 90	0
38	2g	155/156 (99%)	1.31	27 (17%) 4 3	76, 84, 89, 92	0
39	1h	137/138 (99%)	0.75	6 (4%) 39 33	58, 70, 78, 80	0
39	2h	137/138 (99%)	0.89	6 (4%) 39 33	62, 74, 81, 83	0
40	1i	127/128 (99%)	1.65	36 (28%) 1 1	66, 81, 87, 89	0
40	2i	126/128 (98%)	2.53	85 (67%) 0 0	77, 88, 93, 94	0
41	1j	97/105 (92%)	1.60	28 (28%) 1 1	65, 81, 90, 94	0
41	2j	96/105 (91%)	2.63	70 (72%) 0 0	79, 89, 93, 97	0
42	1k	114/129 (88%)	0.48	4 (3%) 47 41	46, 66, 76, 81	0
42	2k	114/129 (88%)	0.97	10 (8%) 15 12	60, 73, 82, 86	0
43	1l	121/132 (91%)	0.61	5 (4%) 41 36	51, 62, 73, 79	0
43	2l	121/132 (91%)	0.70	6 (4%) 34 28	56, 67, 76, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	1.36	19 (16%) 4 3	68, 79, 84, 90	0
44	2m	114/126 (90%)	1.73	36 (31%) 1 1	80, 88, 93, 95	0
45	1n	60/61 (98%)	1.23	5 (8%) 17 13	67, 76, 83, 86	0
45	2n	60/61 (98%)	2.59	38 (63%) 0 0	80, 87, 93, 97	0
46	1o	88/89 (98%)	0.61	3 (3%) 48 42	47, 69, 80, 82	0
46	2o	88/89 (98%)	0.88	7 (7%) 18 14	58, 73, 81, 86	0
47	1p	82/88 (93%)	1.69	21 (25%) 1 1	62, 74, 83, 88	0
47	2p	82/88 (93%)	1.10	5 (6%) 27 22	62, 70, 80, 83	0
48	1q	99/105 (94%)	1.00	5 (5%) 33 28	57, 71, 80, 84	0
48	2q	99/105 (94%)	0.81	3 (3%) 52 47	55, 72, 79, 82	0
49	1r	68/88 (77%)	0.51	2 (2%) 53 48	58, 67, 80, 86	0
49	2r	68/88 (77%)	0.70	2 (2%) 53 48	62, 71, 82, 84	0
50	1s	83/93 (89%)	1.11	10 (12%) 9 7	71, 81, 87, 90	0
50	2s	83/93 (89%)	2.12	44 (53%) 0 0	79, 91, 95, 96	0
51	1t	96/106 (90%)	1.31	20 (20%) 2 2	64, 75, 86, 90	0
51	2t	98/106 (92%)	0.96	7 (7%) 22 17	60, 73, 84, 87	0
52	1u	23/27 (85%)	1.50	6 (26%) 1 1	72, 77, 81, 81	0
52	2u	23/27 (85%)	2.95	19 (82%) 0 0	80, 86, 89, 90	0
53	1y	97/113 (85%)	0.79	6 (6%) 26 21	59, 69, 78, 84	0
53	2y	96/113 (84%)	1.82	33 (34%) 1 1	73, 83, 88, 91	0
All	All	20766/21468 (96%)	0.45	1664 (8%) 18 14	22, 65, 92, 110	0

The worst 5 of 1664 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1076	C	8.4
45	2n	2	ALA	7.8
41	2j	37	PRO	7.2
7	1H	2	SER	7.1
1	1A	1087	G	6.9

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MU	2A	1915	21/22	0.84	0.11	80,89,96,109	0
1	PSU	2A	1917	20/21	0.86	0.10	78,83,98,100	0
32	2MG	2a	1207	24/25	0.86	0.13	89,94,98,101	0
43	0TD	2l	92	10/11	0.86	0.16	65,71,73,93	0
32	M2G	2a	966	25/26	0.87	0.16	65,72,87,92	0
1	PSU	2A	1911	20/21	0.88	0.09	69,77,90,92	0
1	5MU	1A	1915	21/22	0.88	0.12	73,81,86,90	0
43	0TD	1l	92	10/11	0.89	0.13	56,60,66,80	0
32	5MC	2a	967	21/22	0.89	0.14	71,78,88,88	0
1	PSU	1A	1917	20/21	0.90	0.10	70,75,86,86	0
32	2MG	1a	1207	24/25	0.90	0.12	72,78,83,86	0
1	PSU	1A	1911	20/21	0.92	0.09	63,70,72,72	0
32	PSU	2a	516	20/21	0.93	0.09	79,81,87,87	0
32	5MC	2a	1404	21/22	0.93	0.10	58,64,70,70	0
32	5MC	2a	1407	21/22	0.93	0.11	62,68,74,77	0
32	G7M	2a	527	24/25	0.93	0.12	68,73,75,77	0
1	OMC	2A	1920	21/22	0.94	0.09	63,73,78,82	0
32	5MC	1a	967	21/22	0.94	0.11	66,72,80,82	0
32	UR3	2a	1498	21/22	0.94	0.10	58,65,71,74	0
32	MA6	2a	1518	24/25	0.94	0.12	57,67,73,75	0
32	4OC	2a	1402	22/23	0.94	0.11	61,69,73,74	0
32	M2G	1a	966	25/26	0.95	0.11	60,66,73,78	0
32	5MC	2a	1400	21/22	0.95	0.13	72,76,80,83	0
32	PSU	1a	516	20/21	0.95	0.08	63,68,74,75	0
32	MA6	2a	1519	24/25	0.95	0.12	61,67,71,74	0
32	G7M	1a	527	24/25	0.95	0.11	49,58,62,67	0
32	5MC	1a	1404	21/22	0.96	0.09	51,54,60,64	0
32	5MC	1a	1407	21/22	0.96	0.10	48,56,61,63	0
1	5MC	2A	1942	21/22	0.96	0.08	46,56,60,61	0
32	UR3	1a	1498	21/22	0.96	0.09	48,54,60,70	0
32	MA6	1a	1519	24/25	0.96	0.10	44,52,58,60	0
1	OMC	1A	1920	21/22	0.96	0.10	53,58,63,66	0
32	5MC	1a	1400	21/22	0.96	0.10	53,60,64,67	0
32	4OC	1a	1402	22/23	0.96	0.09	48,57,60,64	0
1	OMG	2A	2251	24/25	0.97	0.09	37,41,44,48	0
1	2MA	2A	2503	23/24	0.97	0.08	30,38,42,44	0
1	OMU	2A	2552	21/22	0.97	0.08	36,42,46,50	0
32	MA6	1a	1518	24/25	0.97	0.10	46,52,57,59	0
1	5MC	1A	1962	21/22	0.97	0.07	29,37,43,45	0
1	2MA	1A	2503	23/24	0.97	0.08	20,28,31,31	0
1	5MC	1A	1942	21/22	0.97	0.08	34,38,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MC	2A	1962	21/22	0.97	0.09	44,50,54,63	0
1	OMU	1A	2552	21/22	0.98	0.06	27,33,35,38	0
1	PSU	1A	2605	20/21	0.98	0.07	26,30,36,37	0
1	OMG	1A	2251	24/25	0.98	0.06	26,30,33,35	0
1	5MU	2A	1939	21/22	0.98	0.07	36,41,45,46	0
1	PSU	2A	2605	20/21	0.98	0.07	35,41,44,44	0
1	5MU	1A	1939	21/22	0.98	0.07	26,32,36,37	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	3986	1/1	0.48	0.27	43,43,43,43	0
54	MG	2a	3041	1/1	0.59	0.24	86,86,86,86	0
54	MG	1a	1743	1/1	0.60	0.21	87,87,87,87	0
54	MG	1a	1836	1/1	0.60	0.20	84,84,84,84	0
54	MG	2A	3380	1/1	0.60	0.23	59,59,59,59	0
54	MG	1A	3872	1/1	0.60	0.20	75,75,75,75	0
54	MG	1A	3213	1/1	0.62	0.26	73,73,73,73	0
54	MG	2A	3208	1/1	0.63	0.28	77,77,77,77	0
54	MG	2A	3034	1/1	0.65	0.29	87,87,87,87	0
54	MG	1A	3581	1/1	0.65	0.20	53,53,53,53	0
54	MG	2A	3343	1/1	0.65	0.25	85,85,85,85	0
54	MG	1a	1676	1/1	0.65	0.20	85,85,85,85	0
54	MG	2G	202	1/1	0.65	0.23	80,80,80,80	0
54	MG	1a	1874	1/1	0.65	0.39	84,84,84,84	0
54	MG	2A	3116	1/1	0.66	0.21	82,82,82,82	0
54	MG	1G	202	1/1	0.67	0.20	71,71,71,71	0
54	MG	1a	1855	1/1	0.67	0.25	86,86,86,86	0
54	MG	2A	3461	1/1	0.67	0.25	72,72,72,72	0
54	MG	1a	1796	1/1	0.67	0.21	86,86,86,86	0
54	MG	2A	3235	1/1	0.67	0.24	83,83,83,83	0
54	MG	2A	3604	1/1	0.68	0.19	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	3835	1/1	0.68	0.17	63,63,63,63	0
54	MG	2A	3579	1/1	0.68	0.18	62,62,62,62	0
54	MG	2a	3097	1/1	0.68	0.36	86,86,86,86	0
54	MG	2a	3174	1/1	0.68	0.20	86,86,86,86	0
54	MG	2A	3421	1/1	0.69	0.16	69,69,69,69	0
54	MG	1A	3781	1/1	0.69	0.18	33,33,33,33	0
54	MG	14	101	1/1	0.69	0.14	81,81,81,81	0
54	MG	1A	3812	1/1	0.69	0.17	78,78,78,78	0
54	MG	2A	3736	1/1	0.69	0.24	86,86,86,86	0
54	MG	1A	3261	1/1	0.69	0.30	86,86,86,86	0
54	MG	1A	3641	1/1	0.69	0.41	48,48,48,48	0
54	MG	1A	3983	1/1	0.69	0.18	81,81,81,81	0
54	MG	1A	3699	1/1	0.69	0.22	73,73,73,73	0
54	MG	1a	1795	1/1	0.70	0.16	84,84,84,84	0
54	MG	1A	3849	1/1	0.70	0.18	71,71,71,71	0
54	MG	2A	3610	1/1	0.70	0.17	82,82,82,82	0
54	MG	1a	1865	1/1	0.70	0.20	76,76,76,76	0
56	MPD	1O	202	8/8	0.70	0.24	67,75,81,81	0
54	MG	1A	3756	1/1	0.71	0.23	67,67,67,67	0
54	MG	1A	3891	1/1	0.71	0.23	60,60,60,60	0
54	MG	1a	1818	1/1	0.71	0.24	86,86,86,86	0
54	MG	1a	1754	1/1	0.71	0.20	90,90,90,90	0
54	MG	2a	3194	1/1	0.71	0.20	86,86,86,86	0
54	MG	1a	1837	1/1	0.71	0.22	89,89,89,89	0
54	MG	1A	3796	1/1	0.72	0.31	74,74,74,74	0
54	MG	2A	3364	1/1	0.72	0.21	84,84,84,84	0
54	MG	1A	3924	1/1	0.72	0.20	37,37,37,37	0
54	MG	1a	1671	1/1	0.72	0.17	73,73,73,73	0
54	MG	1a	1765	1/1	0.72	0.20	81,81,81,81	0
54	MG	2a	3062	1/1	0.73	0.21	85,85,85,85	0
54	MG	2a	3092	1/1	0.73	0.15	80,80,80,80	0
54	MG	1a	1794	1/1	0.73	0.44	92,92,92,92	0
54	MG	2A	3420	1/1	0.73	0.28	76,76,76,76	0
54	MG	2a	3002	1/1	0.73	0.19	81,81,81,81	0
54	MG	2j	201	1/1	0.73	0.13	82,82,82,82	0
54	MG	2A	3525	1/1	0.73	0.16	63,63,63,63	0
54	MG	1g	202	1/1	0.74	0.14	73,73,73,73	0
54	MG	2B	201	1/1	0.74	0.15	85,85,85,85	0
54	MG	1A	3686	1/1	0.74	0.15	77,77,77,77	0
54	MG	2O	202	1/1	0.74	0.19	80,80,80,80	0
54	MG	1A	3930	1/1	0.74	0.21	63,63,63,63	0
54	MG	2a	3016	1/1	0.74	0.18	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3441	1/1	0.74	0.19	67,67,67,67	0
54	MG	1A	4034	1/1	0.74	0.28	59,59,59,59	0
54	MG	2A	3507	1/1	0.74	0.20	42,42,42,42	0
54	MG	1a	1675	1/1	0.74	0.31	84,84,84,84	0
54	MG	2A	3558	1/1	0.74	0.17	45,45,45,45	0
54	MG	2A	3266	1/1	0.74	0.35	74,74,74,74	0
54	MG	1A	4040	1/1	0.74	0.20	63,63,63,63	0
54	MG	1a	1684	1/1	0.74	0.36	78,78,78,78	0
54	MG	1a	1857	1/1	0.75	0.25	81,81,81,81	0
54	MG	1A	3703	1/1	0.75	0.24	59,59,59,59	0
54	MG	2A	3729	1/1	0.75	0.33	82,82,82,82	0
54	MG	1A	4037	1/1	0.75	0.27	71,71,71,71	0
54	MG	2A	3409	1/1	0.75	0.40	84,84,84,84	0
54	MG	1A	3860	1/1	0.75	0.18	85,85,85,85	0
54	MG	1a	1808	1/1	0.75	0.17	92,92,92,92	0
54	MG	1A	3964	1/1	0.75	0.25	66,66,66,66	0
54	MG	2A	3460	1/1	0.75	0.22	64,64,64,64	0
54	MG	2A	3193	1/1	0.75	0.20	68,68,68,68	0
54	MG	2A	3474	1/1	0.75	0.19	58,58,58,58	0
54	MG	1A	3362	1/1	0.75	0.18	70,70,70,70	0
54	MG	1a	1761	1/1	0.75	0.20	70,70,70,70	0
54	MG	2A	3540	1/1	0.75	0.17	85,85,85,85	0
54	MG	1A	3520	1/1	0.75	0.14	61,61,61,61	0
54	MG	2A	3561	1/1	0.75	0.24	54,54,54,54	0
54	MG	2A	3300	1/1	0.75	0.21	71,71,71,71	0
56	MPD	2B	219	8/8	0.75	0.30	66,74,79,84	0
54	MG	1A	3531	1/1	0.76	0.23	68,68,68,68	0
54	MG	1A	3996	1/1	0.76	0.43	62,62,62,62	0
54	MG	1a	1860	1/1	0.76	0.17	79,79,79,79	0
54	MG	15	105	1/1	0.76	0.17	56,56,56,56	0
54	MG	15	107	1/1	0.76	0.19	77,77,77,77	0
54	MG	2A	3433	1/1	0.76	0.20	62,62,62,62	0
54	MG	1A	3565	1/1	0.76	0.26	63,63,63,63	0
54	MG	1A	3511	1/1	0.76	0.22	54,54,54,54	0
54	MG	2a	3040	1/1	0.76	0.37	78,78,78,78	0
54	MG	1a	1800	1/1	0.76	0.23	71,71,71,71	0
54	MG	2a	3052	1/1	0.76	0.32	87,87,87,87	0
54	MG	2A	3185	1/1	0.76	0.31	86,86,86,86	0
54	MG	1a	1802	1/1	0.76	0.25	90,90,90,90	0
54	MG	1A	3483	1/1	0.76	0.14	31,31,31,31	0
54	MG	1B	220	1/1	0.76	0.18	50,50,50,50	0
54	MG	1a	1826	1/1	0.76	0.20	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3272	1/1	0.76	0.26	76,76,76,76	0
54	MG	1a	1690	1/1	0.76	0.30	73,73,73,73	0
54	MG	1E	306	1/1	0.76	0.30	70,70,70,70	0
54	MG	2A	3299	1/1	0.77	0.26	70,70,70,70	0
54	MG	2G	201	1/1	0.77	0.14	84,84,84,84	0
54	MG	1a	1828	1/1	0.77	0.21	84,84,84,84	0
54	MG	2A	3493	1/1	0.77	0.21	73,73,73,73	0
54	MG	1A	3984	1/1	0.77	0.20	65,65,65,65	0
54	MG	2A	3509	1/1	0.77	0.23	65,65,65,65	0
54	MG	2a	3035	1/1	0.77	0.30	72,72,72,72	0
54	MG	2A	3053	1/1	0.77	0.28	77,77,77,77	0
54	MG	1B	217	1/1	0.77	0.17	67,67,67,67	0
54	MG	1A	3437	1/1	0.77	0.20	59,59,59,59	0
54	MG	1A	3677	1/1	0.77	0.21	67,67,67,67	0
54	MG	1A	3683	1/1	0.77	0.16	68,68,68,68	0
54	MG	2A	3584	1/1	0.77	0.23	69,69,69,69	0
54	MG	2a	3156	1/1	0.77	0.21	73,73,73,73	0
54	MG	2a	3173	1/1	0.77	0.21	83,83,83,83	0
54	MG	2A	3426	1/1	0.77	0.23	59,59,59,59	0
54	MG	1a	1783	1/1	0.77	0.18	80,80,80,80	0
54	MG	2f	202	1/1	0.77	0.13	69,69,69,69	0
54	MG	2A	3698	1/1	0.77	0.26	62,62,62,62	0
54	MG	1a	1866	1/1	0.77	0.18	80,80,80,80	0
54	MG	1A	3892	1/1	0.77	0.18	59,59,59,59	0
54	MG	2A	3276	1/1	0.78	0.20	87,87,87,87	0
54	MG	2B	214	1/1	0.78	0.15	70,70,70,70	0
54	MG	1a	1820	1/1	0.78	0.19	68,68,68,68	0
54	MG	2A	3489	1/1	0.78	0.20	72,72,72,72	0
54	MG	1a	1825	1/1	0.78	0.18	51,51,51,51	0
54	MG	1a	1777	1/1	0.78	0.18	82,82,82,82	0
54	MG	2A	3345	1/1	0.78	0.16	80,80,80,80	0
54	MG	2a	3019	1/1	0.78	0.18	78,78,78,78	0
54	MG	2A	3515	1/1	0.78	0.26	75,75,75,75	0
54	MG	1A	3878	1/1	0.78	0.22	40,40,40,40	0
54	MG	1A	3624	1/1	0.78	0.20	34,34,34,34	0
54	MG	2a	3049	1/1	0.78	0.26	84,84,84,84	0
54	MG	2A	3153	1/1	0.78	0.14	71,71,71,71	0
54	MG	2A	3410	1/1	0.78	0.23	71,71,71,71	0
54	MG	2a	3074	1/1	0.78	0.24	70,70,70,70	0
54	MG	2a	3077	1/1	0.78	0.21	75,75,75,75	0
54	MG	1a	1715	1/1	0.78	0.22	86,86,86,86	0
54	MG	1A	4017	1/1	0.78	0.24	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3149	1/1	0.78	0.21	71,71,71,71	0
54	MG	2A	3598	1/1	0.78	0.24	62,62,62,62	0
54	MG	1A	3505	1/1	0.78	0.15	63,63,63,63	0
54	MG	1A	3357	1/1	0.78	0.14	49,49,49,49	0
54	MG	2A	3614	1/1	0.78	0.13	71,71,71,71	0
54	MG	1T	204	1/1	0.78	0.11	81,81,81,81	0
54	MG	2A	3707	1/1	0.78	0.36	56,56,56,56	0
54	MG	2A	3442	1/1	0.78	0.13	69,69,69,69	0
54	MG	1a	1771	1/1	0.78	0.18	77,77,77,77	0
57	ARG	1F	320	12/12	0.78	0.20	58,76,81,84	0
54	MG	2A	3400	1/1	0.79	0.17	83,83,83,83	0
54	MG	1a	1641	1/1	0.79	0.25	81,81,81,81	0
54	MG	1a	1833	1/1	0.79	0.27	72,72,72,72	0
54	MG	2a	3038	1/1	0.79	0.18	89,89,89,89	0
54	MG	1A	3910	1/1	0.79	0.15	27,27,27,27	0
54	MG	1A	3611	1/1	0.79	0.16	72,72,72,72	0
54	MG	1A	3441	1/1	0.79	0.22	71,71,71,71	0
54	MG	1A	3284	1/1	0.79	0.21	77,77,77,77	0
54	MG	1A	3859	1/1	0.79	0.17	34,34,34,34	0
54	MG	2A	3270	1/1	0.79	0.30	83,83,83,83	0
54	MG	2A	3657	1/1	0.79	0.17	45,45,45,45	0
54	MG	2a	3079	1/1	0.79	0.56	85,85,85,85	0
54	MG	2A	3693	1/1	0.79	0.27	60,60,60,60	0
54	MG	1a	1863	1/1	0.79	0.16	78,78,78,78	0
54	MG	1A	3704	1/1	0.79	0.22	53,53,53,53	0
54	MG	1A	3738	1/1	0.79	0.12	54,54,54,54	0
54	MG	2a	3160	1/1	0.79	0.47	82,82,82,82	0
54	MG	1A	3646	1/1	0.79	0.15	78,78,78,78	0
54	MG	1A	3497	1/1	0.79	0.18	48,48,48,48	0
54	MG	1A	3591	1/1	0.79	0.19	53,53,53,53	0
54	MG	2A	3052	1/1	0.79	0.28	72,72,72,72	0
54	MG	2A	3368	1/1	0.79	0.23	79,79,79,79	0
54	MG	2A	3524	1/1	0.79	0.16	85,85,85,85	0
54	MG	2I	101	1/1	0.79	0.33	84,84,84,84	0
54	MG	19	102	1/1	0.79	0.17	79,79,79,79	0
54	MG	2A	3557	1/1	0.80	0.20	43,43,43,43	0
54	MG	2A	3190	1/1	0.80	0.43	75,75,75,75	0
54	MG	1a	1780	1/1	0.80	0.21	85,85,85,85	0
54	MG	2A	3565	1/1	0.80	0.20	72,72,72,72	0
54	MG	1a	1655	1/1	0.80	0.12	76,76,76,76	0
54	MG	1A	3870	1/1	0.80	0.14	46,46,46,46	0
54	MG	1A	3305	1/1	0.80	0.16	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3600	1/1	0.80	0.15	44,44,44,44	0
54	MG	1A	3456	1/1	0.80	0.19	64,64,64,64	0
54	MG	2a	3050	1/1	0.80	0.28	69,69,69,69	0
54	MG	2A	3606	1/1	0.80	0.20	62,62,62,62	0
54	MG	1D	309	1/1	0.80	0.40	57,57,57,57	0
54	MG	2A	3611	1/1	0.80	0.20	37,37,37,37	0
54	MG	2A	3273	1/1	0.80	0.21	61,61,61,61	0
54	MG	2A	3618	1/1	0.80	0.09	88,88,88,88	0
54	MG	1A	3888	1/1	0.80	0.12	38,38,38,38	0
54	MG	1A	3480	1/1	0.80	0.13	25,25,25,25	0
54	MG	1A	3379	1/1	0.80	0.18	74,74,74,74	0
54	MG	1a	1746	1/1	0.80	0.17	80,80,80,80	0
54	MG	2A	3501	1/1	0.80	0.12	85,85,85,85	0
54	MG	1A	3909	1/1	0.80	0.12	19,19,19,19	0
54	MG	1A	4026	1/1	0.80	0.17	56,56,56,56	0
54	MG	2B	202	1/1	0.80	0.13	82,82,82,82	0
54	MG	2B	213	1/1	0.80	0.19	78,78,78,78	0
54	MG	2A	3093	1/1	0.80	0.18	76,76,76,76	0
54	MG	1A	4033	1/1	0.80	0.22	75,75,75,75	0
54	MG	1A	3188	1/1	0.80	0.17	68,68,68,68	0
54	MG	1A	3790	1/1	0.80	0.24	61,61,61,61	0
54	MG	1a	1867	1/1	0.81	0.27	73,73,73,73	0
54	MG	1a	1694	1/1	0.81	0.17	69,69,69,69	0
54	MG	1d	305	1/1	0.81	0.12	94,94,94,94	0
54	MG	1A	3537	1/1	0.81	0.15	51,51,51,51	0
54	MG	1a	1726	1/1	0.81	0.12	82,82,82,82	0
54	MG	2A	3366	1/1	0.81	0.14	43,43,43,43	0
54	MG	1a	1813	1/1	0.81	0.19	69,69,69,69	0
54	MG	2A	3379	1/1	0.81	0.20	58,58,58,58	0
54	MG	1a	1735	1/1	0.81	0.22	70,70,70,70	0
54	MG	2A	3072	1/1	0.81	0.23	70,70,70,70	0
54	MG	2A	3089	1/1	0.81	0.22	70,70,70,70	0
54	MG	2A	3090	1/1	0.81	0.16	72,72,72,72	0
54	MG	1A	3235	1/1	0.81	0.17	79,79,79,79	0
54	MG	1A	3364	1/1	0.81	0.12	48,48,48,48	0
54	MG	1A	3585	1/1	0.81	0.25	45,45,45,45	0
54	MG	1a	1611	1/1	0.81	0.27	69,69,69,69	0
54	MG	1A	3516	1/1	0.81	0.14	29,29,29,29	0
54	MG	1A	3367	1/1	0.81	0.13	26,26,26,26	0
54	MG	2A	3443	1/1	0.81	0.27	61,61,61,61	0
54	MG	2A	3677	1/1	0.81	0.24	74,74,74,74	0
54	MG	1A	3840	1/1	0.81	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	1A	3450	1/1	0.81	0.19	74,74,74,74	0
54	MG	2A	3253	1/1	0.81	0.21	72,72,72,72	0
54	MG	2A	3486	1/1	0.81	0.23	70,70,70,70	0
54	MG	1a	1781	1/1	0.81	0.14	90,90,90,90	0
54	MG	1A	4024	1/1	0.81	0.16	65,65,65,65	0
54	MG	2A	3499	1/1	0.81	0.12	78,78,78,78	0
54	MG	2n	101	1/1	0.81	0.32	81,81,81,81	0
54	MG	1A	3534	1/1	0.81	0.15	55,55,55,55	0
54	MG	1a	1689	1/1	0.81	0.26	70,70,70,70	0
54	MG	10	106	1/1	0.81	0.11	60,60,60,60	0
54	MG	2E	304	1/1	0.82	0.17	41,41,41,41	0
54	MG	1A	3320	1/1	0.82	0.29	77,77,77,77	0
54	MG	2A	3538	1/1	0.82	0.12	58,58,58,58	0
54	MG	1a	1696	1/1	0.82	0.23	66,66,66,66	0
54	MG	1A	3471	1/1	0.82	0.16	58,58,58,58	0
54	MG	1A	4044	1/1	0.82	0.39	46,46,46,46	0
54	MG	1B	205	1/1	0.82	0.10	59,59,59,59	0
54	MG	1A	3642	1/1	0.82	0.17	67,67,67,67	0
54	MG	2a	3031	1/1	0.82	0.11	80,80,80,80	0
54	MG	2A	3416	1/1	0.82	0.18	58,58,58,58	0
54	MG	1A	3555	1/1	0.82	0.12	44,44,44,44	0
54	MG	2A	3250	1/1	0.82	0.27	73,73,73,73	0
54	MG	1a	1749	1/1	0.82	0.11	61,61,61,61	0
54	MG	1A	3671	1/1	0.82	0.14	65,65,65,65	0
54	MG	1D	318	1/1	0.82	0.19	59,59,59,59	0
54	MG	2A	3608	1/1	0.82	0.26	84,84,84,84	0
54	MG	1a	1764	1/1	0.82	0.14	82,82,82,82	0
54	MG	2a	3064	1/1	0.82	0.35	78,78,78,78	0
54	MG	2A	3036	1/1	0.82	0.26	78,78,78,78	0
54	MG	2A	3046	1/1	0.82	0.14	65,65,65,65	0
54	MG	2A	3297	1/1	0.82	0.13	49,49,49,49	0
54	MG	1A	3489	1/1	0.82	0.11	26,26,26,26	0
54	MG	2A	3675	1/1	0.82	0.12	60,60,60,60	0
54	MG	2a	3119	1/1	0.82	0.18	86,86,86,86	0
54	MG	2A	3477	1/1	0.82	0.14	75,75,75,75	0
54	MG	2A	3684	1/1	0.82	0.15	51,51,51,51	0
54	MG	1A	3940	1/1	0.82	0.18	54,54,54,54	0
54	MG	2A	3301	1/1	0.82	0.14	60,60,60,60	0
54	MG	2A	3333	1/1	0.82	0.24	62,62,62,62	0
54	MG	2A	3339	1/1	0.82	0.13	37,37,37,37	0
54	MG	2a	3195	1/1	0.82	0.18	81,81,81,81	0
54	MG	1Q	204	1/1	0.82	0.18	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	3962	1/1	0.82	0.15	53,53,53,53	0
54	MG	2A	3354	1/1	0.82	0.23	78,78,78,78	0
54	MG	1A	3749	1/1	0.82	0.17	68,68,68,68	0
54	MG	1a	1850	1/1	0.82	0.15	66,66,66,66	0
54	MG	2D	308	1/1	0.82	0.20	77,77,77,77	0
54	MG	1A	3389	1/1	0.83	0.12	33,33,33,33	0
54	MG	1A	4000	1/1	0.83	0.20	84,84,84,84	0
54	MG	1A	3785	1/1	0.83	0.13	41,41,41,41	0
54	MG	1A	3688	1/1	0.83	0.26	70,70,70,70	0
54	MG	1A	3435	1/1	0.83	0.13	39,39,39,39	0
54	MG	1A	3900	1/1	0.83	0.13	59,59,59,59	0
54	MG	1A	3543	1/1	0.83	0.17	65,65,65,65	0
54	MG	1a	1774	1/1	0.83	0.18	78,78,78,78	0
54	MG	1A	3833	1/1	0.83	0.24	63,63,63,63	0
54	MG	1A	3667	1/1	0.83	0.14	31,31,31,31	0
54	MG	1a	1657	1/1	0.83	0.41	77,77,77,77	0
54	MG	1a	1871	1/1	0.83	0.18	78,78,78,78	0
54	MG	1a	1669	1/1	0.83	0.32	66,66,66,66	0
54	MG	1A	3722	1/1	0.83	0.12	40,40,40,40	0
54	MG	1A	4047	1/1	0.83	0.14	55,55,55,55	0
54	MG	2A	3316	1/1	0.83	0.14	53,53,53,53	0
54	MG	2A	3328	1/1	0.83	0.13	50,50,50,50	0
54	MG	1i	201	1/1	0.83	0.20	77,77,77,77	0
54	MG	2A	3012	1/1	0.83	0.20	68,68,68,68	0
54	MG	2a	3039	1/1	0.83	0.25	70,70,70,70	0
54	MG	1A	4051	1/1	0.83	0.27	49,49,49,49	0
54	MG	1a	1799	1/1	0.83	0.15	67,67,67,67	0
54	MG	2A	3350	1/1	0.83	0.22	55,55,55,55	0
54	MG	1A	4057	1/1	0.83	0.16	44,44,44,44	0
54	MG	2A	3570	1/1	0.83	0.13	56,56,56,56	0
54	MG	2a	3054	1/1	0.83	0.26	83,83,83,83	0
54	MG	1a	1801	1/1	0.83	0.19	71,71,71,71	0
54	MG	1A	3735	1/1	0.83	0.13	63,63,63,63	0
54	MG	1A	3593	1/1	0.83	0.18	66,66,66,66	0
54	MG	2A	3086	1/1	0.83	0.31	80,80,80,80	0
54	MG	1A	3216	1/1	0.83	0.29	50,50,50,50	0
54	MG	2A	3384	1/1	0.83	0.16	60,60,60,60	0
54	MG	1A	3975	1/1	0.83	0.18	56,56,56,56	0
54	MG	2A	3405	1/1	0.83	0.13	49,49,49,49	0
54	MG	2a	3142	1/1	0.83	0.17	66,66,66,66	0
54	MG	1A	3282	1/1	0.83	0.08	84,84,84,84	0
54	MG	2A	3109	1/1	0.83	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3615	1/1	0.83	0.20	71,71,71,71	0
54	MG	1A	3778	1/1	0.83	0.13	28,28,28,28	0
54	MG	2A	3619	1/1	0.83	0.34	53,53,53,53	0
54	MG	1A	3874	1/1	0.83	0.13	53,53,53,53	0
54	MG	2A	3162	1/1	0.83	0.17	68,68,68,68	0
54	MG	2A	3182	1/1	0.83	0.20	60,60,60,60	0
54	MG	2A	3681	1/1	0.83	0.12	78,78,78,78	0
54	MG	2A	3683	1/1	0.83	0.16	78,78,78,78	0
54	MG	2A	3429	1/1	0.83	0.22	43,43,43,43	0
54	MG	1A	3988	1/1	0.83	0.09	75,75,75,75	0
54	MG	2A	3440	1/1	0.83	0.14	68,68,68,68	0
54	MG	1A	4008	1/1	0.84	0.16	49,49,49,49	0
54	MG	1A	3782	1/1	0.84	0.15	45,45,45,45	0
54	MG	2A	3503	1/1	0.84	0.18	73,73,73,73	0
54	MG	2A	3042	1/1	0.84	0.31	81,81,81,81	0
54	MG	10	105	1/1	0.84	0.14	57,57,57,57	0
54	MG	1a	1741	1/1	0.84	0.25	68,68,68,68	0
54	MG	2A	3517	1/1	0.84	0.18	70,70,70,70	0
54	MG	2G	203	1/1	0.84	0.17	78,78,78,78	0
54	MG	2A	3521	1/1	0.84	0.16	74,74,74,74	0
54	MG	1a	1821	1/1	0.84	0.14	78,78,78,78	0
54	MG	2A	3061	1/1	0.84	0.27	61,61,61,61	0
54	MG	1A	3647	1/1	0.84	0.29	68,68,68,68	0
54	MG	1A	3662	1/1	0.84	0.12	45,45,45,45	0
54	MG	1a	1827	1/1	0.84	0.18	86,86,86,86	0
54	MG	1A	3182	1/1	0.84	0.19	76,76,76,76	0
54	MG	1A	3803	1/1	0.84	0.22	63,63,63,63	0
54	MG	2A	3098	1/1	0.84	0.26	67,67,67,67	0
54	MG	1A	3719	1/1	0.84	0.13	74,74,74,74	0
54	MG	2A	3574	1/1	0.84	0.14	60,60,60,60	0
54	MG	2A	3577	1/1	0.84	0.19	59,59,59,59	0
54	MG	1A	3821	1/1	0.84	0.18	77,77,77,77	0
54	MG	2A	3391	1/1	0.84	0.29	75,75,75,75	0
54	MG	1a	1637	1/1	0.84	0.24	72,72,72,72	0
54	MG	1A	3670	1/1	0.84	0.29	37,37,37,37	0
54	MG	2A	3406	1/1	0.84	0.15	66,66,66,66	0
54	MG	1A	3478	1/1	0.84	0.14	32,32,32,32	0
54	MG	1a	1859	1/1	0.84	0.19	78,78,78,78	0
54	MG	1A	3673	1/1	0.84	0.12	65,65,65,65	0
54	MG	1a	1664	1/1	0.84	0.15	83,83,83,83	0
54	MG	2A	3202	1/1	0.84	0.24	74,74,74,74	0
54	MG	1A	3739	1/1	0.84	0.16	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3134	1/1	0.84	0.17	69,69,69,69	0
54	MG	2A	3216	1/1	0.84	0.13	67,67,67,67	0
54	MG	1A	3271	1/1	0.84	0.11	48,48,48,48	0
54	MG	2a	3154	1/1	0.84	0.12	67,67,67,67	0
54	MG	1B	210	1/1	0.84	0.38	84,84,84,84	0
54	MG	1A	3753	1/1	0.84	0.12	27,27,27,27	0
54	MG	1A	3404	1/1	0.84	0.15	30,30,30,30	0
54	MG	1a	1876	1/1	0.84	0.24	74,74,74,74	0
54	MG	2a	3181	1/1	0.84	0.20	78,78,78,78	0
54	MG	2A	3457	1/1	0.84	0.10	84,84,84,84	0
54	MG	1A	3760	1/1	0.84	0.17	63,63,63,63	0
54	MG	1A	3645	1/1	0.84	0.28	49,49,49,49	0
54	MG	2A	3275	1/1	0.84	0.15	59,59,59,59	0
54	MG	1A	3374	1/1	0.84	0.12	67,67,67,67	0
54	MG	1l	202	1/1	0.84	0.18	83,83,83,83	0
54	MG	1A	3882	1/1	0.84	0.11	40,40,40,40	0
54	MG	2A	3024	1/1	0.84	0.20	67,67,67,67	0
54	MG	1a	1699	1/1	0.85	0.13	64,64,64,64	0
54	MG	1a	1712	1/1	0.85	0.14	64,64,64,64	0
54	MG	1P	206	1/1	0.85	0.12	48,48,48,48	0
54	MG	1A	3082	1/1	0.85	0.15	57,57,57,57	0
54	MG	1A	3764	1/1	0.85	0.19	59,59,59,59	0
54	MG	2A	3688	1/1	0.85	0.11	75,75,75,75	0
54	MG	1A	3131	1/1	0.85	0.14	59,59,59,59	0
54	MG	1A	3947	1/1	0.85	0.15	52,52,52,52	0
54	MG	2A	3148	1/1	0.85	0.25	66,66,66,66	0
54	MG	1A	3959	1/1	0.85	0.12	59,59,59,59	0
54	MG	2A	3161	1/1	0.85	0.22	84,84,84,84	0
54	MG	2A	3737	1/1	0.85	0.30	72,72,72,72	0
54	MG	1A	3536	1/1	0.85	0.16	44,44,44,44	0
54	MG	1A	3416	1/1	0.85	0.16	68,68,68,68	0
54	MG	2B	204	1/1	0.85	0.11	75,75,75,75	0
54	MG	2B	207	1/1	0.85	0.16	81,81,81,81	0
54	MG	1a	1755	1/1	0.85	0.22	74,74,74,74	0
54	MG	1A	3967	1/1	0.85	0.18	75,75,75,75	0
54	MG	2B	217	1/1	0.85	0.11	83,83,83,83	0
54	MG	1A	3297	1/1	0.85	0.11	53,53,53,53	0
54	MG	2A	3444	1/1	0.85	0.17	66,66,66,66	0
54	MG	2A	3451	1/1	0.85	0.17	70,70,70,70	0
54	MG	2A	3196	1/1	0.85	0.15	63,63,63,63	0
54	MG	1A	3979	1/1	0.85	0.11	50,50,50,50	0
54	MG	1a	1861	1/1	0.85	0.16	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3210	1/1	0.85	0.15	62,62,62,62	0
54	MG	1a	1766	1/1	0.85	0.25	84,84,84,84	0
54	MG	2A	3227	1/1	0.85	0.14	65,65,65,65	0
54	MG	2A	3229	1/1	0.85	0.21	67,67,67,67	0
54	MG	1a	1638	1/1	0.85	0.41	80,80,80,80	0
54	MG	1A	3202	1/1	0.85	0.18	66,66,66,66	0
54	MG	2a	3037	1/1	0.85	0.21	74,74,74,74	0
54	MG	1a	1775	1/1	0.85	0.12	86,86,86,86	0
54	MG	1a	1870	1/1	0.85	0.29	72,72,72,72	0
54	MG	1a	1654	1/1	0.85	0.14	80,80,80,80	0
54	MG	1A	3370	1/1	0.85	0.11	47,47,47,47	0
54	MG	1A	3157	1/1	0.85	0.35	73,73,73,73	0
54	MG	1A	3376	1/1	0.85	0.10	43,43,43,43	0
54	MG	2a	3051	1/1	0.85	0.30	77,77,77,77	0
54	MG	1a	1787	1/1	0.85	0.15	72,72,72,72	0
54	MG	2A	3277	1/1	0.85	0.14	34,34,34,34	0
54	MG	2a	3056	1/1	0.85	0.23	76,76,76,76	0
54	MG	2a	3058	1/1	0.85	0.23	77,77,77,77	0
54	MG	1h	201	1/1	0.85	0.27	59,59,59,59	0
54	MG	1B	224	1/1	0.85	0.20	72,72,72,72	0
54	MG	1B	226	1/1	0.85	0.11	73,73,73,73	0
54	MG	1n	101	1/1	0.85	0.46	78,78,78,78	0
54	MG	2A	3313	1/1	0.85	0.23	63,63,63,63	0
54	MG	1t	201	1/1	0.85	0.13	74,74,74,74	0
54	MG	2a	3093	1/1	0.85	0.19	76,76,76,76	0
54	MG	1A	3587	1/1	0.85	0.18	64,64,64,64	0
54	MG	2A	3023	1/1	0.85	0.19	69,69,69,69	0
54	MG	1D	315	1/1	0.85	0.17	73,73,73,73	0
54	MG	2A	3028	1/1	0.85	0.15	61,61,61,61	0
54	MG	1A	3519	1/1	0.85	0.12	27,27,27,27	0
54	MG	1E	303	1/1	0.85	0.13	29,29,29,29	0
54	MG	1A	3332	1/1	0.85	0.14	29,29,29,29	0
54	MG	2A	3356	1/1	0.85	0.14	72,72,72,72	0
54	MG	2A	3361	1/1	0.85	0.22	63,63,63,63	0
54	MG	2A	3363	1/1	0.85	0.20	71,71,71,71	0
54	MG	1a	1805	1/1	0.85	0.12	70,70,70,70	0
54	MG	1a	1691	1/1	0.85	0.15	59,59,59,59	0
54	MG	1a	1810	1/1	0.85	0.19	76,76,76,76	0
54	MG	2A	3054	1/1	0.85	0.32	76,76,76,76	0
54	MG	2A	3056	1/1	0.85	0.30	59,59,59,59	0
54	MG	2A	3383	1/1	0.85	0.17	52,52,52,52	0
54	MG	1F	312	1/1	0.85	0.15	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MPD	1a	1878	8/8	0.85	0.15	55,70,73,73	0
56	MPD	2A	3743	8/8	0.85	0.28	46,57,62,63	0
56	MPD	2A	3744	8/8	0.85	0.25	63,68,74,74	0
54	MG	2A	3623	1/1	0.85	0.21	62,62,62,62	0
54	MG	1A	3522	1/1	0.85	0.13	58,58,58,58	0
54	MG	1a	1811	1/1	0.86	0.11	71,71,71,71	0
54	MG	2A	3385	1/1	0.86	0.20	65,65,65,65	0
54	MG	2A	3682	1/1	0.86	0.10	74,74,74,74	0
54	MG	1A	3281	1/1	0.86	0.09	77,77,77,77	0
54	MG	2A	3091	1/1	0.86	0.27	68,68,68,68	0
54	MG	1A	3452	1/1	0.86	0.12	53,53,53,53	0
54	MG	1A	3605	1/1	0.86	0.10	42,42,42,42	0
54	MG	2A	3695	1/1	0.86	0.12	53,53,53,53	0
54	MG	1A	3823	1/1	0.86	0.20	42,42,42,42	0
54	MG	2A	3706	1/1	0.86	0.17	65,65,65,65	0
54	MG	1A	3702	1/1	0.86	0.20	43,43,43,43	0
54	MG	2A	3724	1/1	0.86	0.26	71,71,71,71	0
54	MG	1A	3340	1/1	0.86	0.11	65,65,65,65	0
54	MG	1A	3837	1/1	0.86	0.13	44,44,44,44	0
54	MG	2A	3160	1/1	0.86	0.20	75,75,75,75	0
54	MG	2A	3742	1/1	0.86	0.14	50,50,50,50	0
54	MG	1A	3380	1/1	0.86	0.13	63,63,63,63	0
54	MG	1a	1829	1/1	0.86	0.14	83,83,83,83	0
54	MG	1A	3627	1/1	0.86	0.17	39,39,39,39	0
54	MG	1A	3628	1/1	0.86	0.12	65,65,65,65	0
54	MG	2B	208	1/1	0.86	0.26	66,66,66,66	0
54	MG	2B	209	1/1	0.86	0.19	70,70,70,70	0
54	MG	1E	309	1/1	0.86	0.22	58,58,58,58	0
54	MG	1a	1730	1/1	0.86	0.27	75,75,75,75	0
54	MG	2B	215	1/1	0.86	0.09	75,75,75,75	0
54	MG	1A	3987	1/1	0.86	0.14	53,53,53,53	0
54	MG	1a	1740	1/1	0.86	0.14	65,65,65,65	0
54	MG	2A	3450	1/1	0.86	0.13	70,70,70,70	0
54	MG	2A	3207	1/1	0.86	0.17	74,74,74,74	0
54	MG	2A	3453	1/1	0.86	0.12	74,74,74,74	0
54	MG	1G	201	1/1	0.86	0.11	77,77,77,77	0
54	MG	1A	3636	1/1	0.86	0.18	68,68,68,68	0
54	MG	20	103	1/1	0.86	0.19	72,72,72,72	0
54	MG	1A	3993	1/1	0.86	0.28	52,52,52,52	0
54	MG	1A	3036	1/1	0.86	0.30	62,62,62,62	0
54	MG	2a	3003	1/1	0.86	0.15	70,70,70,70	0
54	MG	1a	1752	1/1	0.86	0.19	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3230	1/1	0.86	0.33	68,68,68,68	0
54	MG	2a	3026	1/1	0.86	0.20	78,78,78,78	0
54	MG	2A	3234	1/1	0.86	0.18	75,75,75,75	0
54	MG	1A	3027	1/1	0.86	0.16	65,65,65,65	0
54	MG	2A	3249	1/1	0.86	0.27	68,68,68,68	0
54	MG	1Z	301	1/1	0.86	0.18	69,69,69,69	0
54	MG	1a	1868	1/1	0.86	0.21	65,65,65,65	0
54	MG	2A	3261	1/1	0.86	0.18	62,62,62,62	0
54	MG	1a	1759	1/1	0.86	0.13	76,76,76,76	0
54	MG	1A	4004	1/1	0.86	0.16	86,86,86,86	0
54	MG	1a	1763	1/1	0.86	0.15	68,68,68,68	0
54	MG	1A	3034	1/1	0.86	0.12	63,63,63,63	0
54	MG	1A	3486	1/1	0.86	0.10	32,32,32,32	0
54	MG	1A	3550	1/1	0.86	0.11	47,47,47,47	0
54	MG	1A	3886	1/1	0.86	0.10	31,31,31,31	0
54	MG	2A	3290	1/1	0.86	0.12	62,62,62,62	0
54	MG	2A	3554	1/1	0.86	0.11	77,77,77,77	0
54	MG	18	101	1/1	0.86	0.21	77,77,77,77	0
54	MG	2a	3072	1/1	0.86	0.16	82,82,82,82	0
54	MG	1A	3654	1/1	0.86	0.14	69,69,69,69	0
54	MG	1A	3554	1/1	0.86	0.24	44,44,44,44	0
54	MG	1a	1778	1/1	0.86	0.20	76,76,76,76	0
54	MG	2A	3567	1/1	0.86	0.15	54,54,54,54	0
54	MG	1a	1630	1/1	0.86	0.23	68,68,68,68	0
54	MG	1a	1632	1/1	0.86	0.08	42,42,42,42	0
54	MG	1a	1635	1/1	0.86	0.37	65,65,65,65	0
54	MG	1A	3768	1/1	0.86	0.20	55,55,55,55	0
54	MG	2A	3031	1/1	0.86	0.19	77,77,77,77	0
54	MG	2a	3145	1/1	0.86	0.11	82,82,82,82	0
54	MG	2A	3595	1/1	0.86	0.12	65,65,65,65	0
54	MG	1a	1791	1/1	0.86	0.18	75,75,75,75	0
54	MG	1A	3426	1/1	0.86	0.15	40,40,40,40	0
54	MG	1A	3434	1/1	0.86	0.20	65,65,65,65	0
54	MG	2a	3164	1/1	0.86	0.11	69,69,69,69	0
54	MG	2A	3043	1/1	0.86	0.15	56,56,56,56	0
54	MG	1A	3576	1/1	0.86	0.18	52,52,52,52	0
54	MG	1A	3189	1/1	0.86	0.13	68,68,68,68	0
54	MG	2a	3186	1/1	0.86	0.23	78,78,78,78	0
54	MG	1A	4053	1/1	0.86	0.13	53,53,53,53	0
54	MG	1a	1659	1/1	0.86	0.23	64,64,64,64	0
54	MG	1A	3142	1/1	0.86	0.14	58,58,58,58	0
54	MG	2A	3059	1/1	0.86	0.17	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3377	1/1	0.86	0.13	58,58,58,58	0
54	MG	2o	101	1/1	0.86	0.16	69,69,69,69	0
54	MG	2A	3622	1/1	0.86	0.14	66,66,66,66	0
54	MG	1B	203	1/1	0.86	0.26	69,69,69,69	0
54	MG	2A	3624	1/1	0.86	0.17	76,76,76,76	0
54	MG	1A	3331	1/1	0.86	0.10	30,30,30,30	0
54	MG	2A	3660	1/1	0.86	0.09	31,31,31,31	0
54	MG	1B	206	1/1	0.86	0.19	64,64,64,64	0
54	MG	1A	3754	1/1	0.87	0.20	48,48,48,48	0
54	MG	1A	3973	1/1	0.87	0.12	44,44,44,44	0
54	MG	2A	3470	1/1	0.87	0.14	84,84,84,84	0
54	MG	1a	1674	1/1	0.87	0.20	76,76,76,76	0
54	MG	1A	3144	1/1	0.87	0.14	69,69,69,69	0
54	MG	1A	3584	1/1	0.87	0.19	53,53,53,53	0
54	MG	1A	3763	1/1	0.87	0.19	65,65,65,65	0
54	MG	1D	314	1/1	0.87	0.11	60,60,60,60	0
54	MG	1A	3124	1/1	0.87	0.14	39,39,39,39	0
54	MG	1A	3873	1/1	0.87	0.10	47,47,47,47	0
54	MG	2A	3502	1/1	0.87	0.14	69,69,69,69	0
54	MG	1A	3548	1/1	0.87	0.10	38,38,38,38	0
54	MG	2A	3298	1/1	0.87	0.16	64,64,64,64	0
54	MG	1A	3875	1/1	0.87	0.13	69,69,69,69	0
54	MG	1A	3989	1/1	0.87	0.14	53,53,53,53	0
54	MG	1A	3694	1/1	0.87	0.09	71,71,71,71	0
54	MG	2A	3520	1/1	0.87	0.14	62,62,62,62	0
54	MG	1a	1713	1/1	0.87	0.10	94,94,94,94	0
54	MG	2A	3057	1/1	0.87	0.20	58,58,58,58	0
54	MG	1A	3428	1/1	0.87	0.18	47,47,47,47	0
54	MG	1a	1822	1/1	0.87	0.13	71,71,71,71	0
54	MG	2a	3004	1/1	0.87	0.21	73,73,73,73	0
54	MG	1a	1722	1/1	0.87	0.17	61,61,61,61	0
54	MG	2A	3546	1/1	0.87	0.09	74,74,74,74	0
54	MG	2A	3342	1/1	0.87	0.13	40,40,40,40	0
54	MG	2a	3027	1/1	0.87	0.31	74,74,74,74	0
54	MG	2A	3083	1/1	0.87	0.15	48,48,48,48	0
54	MG	1A	3884	1/1	0.87	0.14	65,65,65,65	0
54	MG	1A	3308	1/1	0.87	0.36	49,49,49,49	0
54	MG	1a	1731	1/1	0.87	0.17	59,59,59,59	0
54	MG	1a	1734	1/1	0.87	0.28	69,69,69,69	0
54	MG	1A	3650	1/1	0.87	0.11	53,53,53,53	0
54	MG	1A	4012	1/1	0.87	0.21	69,69,69,69	0
54	MG	2a	3043	1/1	0.87	0.28	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	2a	3045	1/1	0.87	0.22	84,84,84,84	0
54	MG	2A	3576	1/1	0.87	0.10	66,66,66,66	0
54	MG	2A	3100	1/1	0.87	0.28	63,63,63,63	0
54	MG	1A	4015	1/1	0.87	0.25	48,48,48,48	0
54	MG	1A	3468	1/1	0.87	0.14	60,60,60,60	0
54	MG	2A	3593	1/1	0.87	0.10	72,72,72,72	0
54	MG	2A	3137	1/1	0.87	0.15	51,51,51,51	0
54	MG	1a	1853	1/1	0.87	0.12	66,66,66,66	0
54	MG	1A	3792	1/1	0.87	0.13	35,35,35,35	0
54	MG	2A	3381	1/1	0.87	0.14	47,47,47,47	0
54	MG	10	107	1/1	0.87	0.14	73,73,73,73	0
54	MG	1A	3716	1/1	0.87	0.18	29,29,29,29	0
54	MG	2a	3075	1/1	0.87	0.17	70,70,70,70	0
54	MG	1A	4030	1/1	0.87	0.18	75,75,75,75	0
54	MG	1A	3606	1/1	0.87	0.18	50,50,50,50	0
54	MG	15	108	1/1	0.87	0.31	42,42,42,42	0
54	MG	2A	3189	1/1	0.87	0.25	66,66,66,66	0
54	MG	1A	3665	1/1	0.87	0.07	22,22,22,22	0
54	MG	2a	3110	1/1	0.87	0.23	77,77,77,77	0
54	MG	2a	3112	1/1	0.87	0.15	55,55,55,55	0
54	MG	1A	3561	1/1	0.87	0.12	54,54,54,54	0
54	MG	1A	3925	1/1	0.87	0.13	54,54,54,54	0
54	MG	2A	3414	1/1	0.87	0.15	91,91,91,91	0
54	MG	2a	3143	1/1	0.87	0.12	55,55,55,55	0
54	MG	2A	3198	1/1	0.87	0.29	77,77,77,77	0
54	MG	2A	3654	1/1	0.87	0.10	85,85,85,85	0
54	MG	2A	3417	1/1	0.87	0.19	68,68,68,68	0
54	MG	1a	1616	1/1	0.87	0.15	73,73,73,73	0
54	MG	2A	3663	1/1	0.87	0.16	85,85,85,85	0
54	MG	1A	3354	1/1	0.87	0.16	60,60,60,60	0
54	MG	1A	4045	1/1	0.87	0.16	64,64,64,64	0
54	MG	1A	3935	1/1	0.87	0.14	53,53,53,53	0
54	MG	2a	3179	1/1	0.87	0.18	69,69,69,69	0
54	MG	2A	3213	1/1	0.87	0.26	64,64,64,64	0
54	MG	2A	3434	1/1	0.87	0.11	63,63,63,63	0
54	MG	2a	3191	1/1	0.87	0.12	88,88,88,88	0
54	MG	2A	3438	1/1	0.87	0.12	54,54,54,54	0
54	MG	1A	3567	1/1	0.87	0.16	64,64,64,64	0
54	MG	1b	301	1/1	0.87	0.15	80,80,80,80	0
54	MG	1A	3834	1/1	0.87	0.15	59,59,59,59	0
54	MG	1A	3950	1/1	0.87	0.17	51,51,51,51	0
54	MG	2A	3701	1/1	0.87	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2p	101	1/1	0.87	0.44	67,67,67,67	0
54	MG	2t	201	1/1	0.87	0.15	54,54,54,54	0
54	MG	1B	202	1/1	0.87	0.14	74,74,74,74	0
54	MG	2A	3449	1/1	0.87	0.21	58,58,58,58	0
54	MG	1A	3952	1/1	0.87	0.07	68,68,68,68	0
54	MG	1A	3746	1/1	0.87	0.21	57,57,57,57	0
54	MG	1A	3164	1/1	0.87	0.18	51,51,51,51	0
54	MG	1A	3676	1/1	0.87	0.11	44,44,44,44	0
54	MG	1A	3916	1/1	0.88	0.11	39,39,39,39	0
54	MG	1A	4023	1/1	0.88	0.09	28,28,28,28	0
54	MG	1a	1804	1/1	0.88	0.10	71,71,71,71	0
54	MG	1A	3918	1/1	0.88	0.16	51,51,51,51	0
54	MG	1A	3484	1/1	0.88	0.10	30,30,30,30	0
54	MG	1A	3092	1/1	0.88	0.12	62,62,62,62	0
54	MG	2B	210	1/1	0.88	0.20	82,82,82,82	0
54	MG	1A	3538	1/1	0.88	0.17	63,63,63,63	0
54	MG	2A	3494	1/1	0.88	0.10	53,53,53,53	0
54	MG	1A	3600	1/1	0.88	0.16	44,44,44,44	0
54	MG	1a	1814	1/1	0.88	0.12	64,64,64,64	0
54	MG	1A	3601	1/1	0.88	0.12	66,66,66,66	0
54	MG	2D	310	1/1	0.88	0.10	31,31,31,31	0
54	MG	1A	4038	1/1	0.88	0.18	60,60,60,60	0
54	MG	2F	303	1/1	0.88	0.17	59,59,59,59	0
54	MG	1A	3487	1/1	0.88	0.14	34,34,34,34	0
54	MG	1A	3839	1/1	0.88	0.12	39,39,39,39	0
54	MG	2A	3308	1/1	0.88	0.16	67,67,67,67	0
54	MG	1A	3208	1/1	0.88	0.26	73,73,73,73	0
54	MG	1A	3462	1/1	0.88	0.17	43,43,43,43	0
54	MG	2A	3319	1/1	0.88	0.12	53,53,53,53	0
54	MG	28	102	1/1	0.88	0.20	60,60,60,60	0
54	MG	1a	1737	1/1	0.88	0.32	79,79,79,79	0
54	MG	1A	3463	1/1	0.88	0.11	27,27,27,27	0
54	MG	1a	1601	1/1	0.88	0.26	78,78,78,78	0
54	MG	2a	3008	1/1	0.88	0.43	75,75,75,75	0
54	MG	1A	3685	1/1	0.88	0.10	70,70,70,70	0
54	MG	1A	3508	1/1	0.88	0.10	47,47,47,47	0
54	MG	2A	3552	1/1	0.88	0.11	80,80,80,80	0
54	MG	2A	3553	1/1	0.88	0.09	75,75,75,75	0
54	MG	2A	3344	1/1	0.88	0.11	40,40,40,40	0
54	MG	2a	3033	1/1	0.88	0.20	65,65,65,65	0
54	MG	1a	1628	1/1	0.88	0.23	77,77,77,77	0
54	MG	2A	3347	1/1	0.88	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	2A	3099	1/1	0.88	0.13	65,65,65,65	0
54	MG	1a	1846	1/1	0.88	0.12	80,80,80,80	0
54	MG	1a	1751	1/1	0.88	0.20	64,64,64,64	0
54	MG	2A	3113	1/1	0.88	0.27	76,76,76,76	0
54	MG	1A	3560	1/1	0.88	0.12	42,42,42,42	0
54	MG	2A	3121	1/1	0.88	0.24	72,72,72,72	0
54	MG	2A	3124	1/1	0.88	0.17	76,76,76,76	0
54	MG	1a	1631	1/1	0.88	0.23	74,74,74,74	0
54	MG	2A	3370	1/1	0.88	0.24	73,73,73,73	0
54	MG	2A	3375	1/1	0.88	0.11	40,40,40,40	0
54	MG	2A	3142	1/1	0.88	0.18	68,68,68,68	0
54	MG	2a	3055	1/1	0.88	0.26	74,74,74,74	0
54	MG	1A	3689	1/1	0.88	0.15	47,47,47,47	0
54	MG	1a	1756	1/1	0.88	0.18	66,66,66,66	0
54	MG	1A	3976	1/1	0.88	0.15	53,53,53,53	0
54	MG	2A	3605	1/1	0.88	0.12	68,68,68,68	0
54	MG	1A	3394	1/1	0.88	0.11	37,37,37,37	0
54	MG	1A	3469	1/1	0.88	0.10	57,57,57,57	0
54	MG	2A	3170	1/1	0.88	0.20	67,67,67,67	0
54	MG	2a	3076	1/1	0.88	0.09	72,72,72,72	0
54	MG	2A	3388	1/1	0.88	0.20	72,72,72,72	0
54	MG	2A	3176	1/1	0.88	0.16	65,65,65,65	0
54	MG	1A	3784	1/1	0.88	0.12	49,49,49,49	0
54	MG	1a	1644	1/1	0.88	0.29	61,61,61,61	0
54	MG	2A	3186	1/1	0.88	0.25	54,54,54,54	0
54	MG	2a	3107	1/1	0.88	0.13	75,75,75,75	0
54	MG	1a	1645	1/1	0.88	0.29	74,74,74,74	0
54	MG	1a	1770	1/1	0.88	0.14	68,68,68,68	0
54	MG	1a	1653	1/1	0.88	0.21	59,59,59,59	0
54	MG	2a	3125	1/1	0.88	0.16	82,82,82,82	0
54	MG	2A	3628	1/1	0.88	0.16	90,90,90,90	0
54	MG	2a	3137	1/1	0.88	0.14	68,68,68,68	0
54	MG	2A	3195	1/1	0.88	0.23	67,67,67,67	0
54	MG	1a	1772	1/1	0.88	0.29	71,71,71,71	0
54	MG	2A	3658	1/1	0.88	0.11	42,42,42,42	0
54	MG	1B	218	1/1	0.88	0.10	59,59,59,59	0
54	MG	2a	3151	1/1	0.88	0.22	68,68,68,68	0
54	MG	1A	3265	1/1	0.88	0.17	62,62,62,62	0
54	MG	2A	3205	1/1	0.88	0.14	63,63,63,63	0
54	MG	2a	3157	1/1	0.88	0.14	93,93,93,93	0
54	MG	1a	1656	1/1	0.88	0.19	50,50,50,50	0
54	MG	2A	3680	1/1	0.88	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3430	1/1	0.88	0.12	60,60,60,60	0
54	MG	1A	3409	1/1	0.88	0.21	59,59,59,59	0
54	MG	2a	3176	1/1	0.88	0.23	63,63,63,63	0
54	MG	1A	3580	1/1	0.88	0.10	24,24,24,24	0
54	MG	2A	3437	1/1	0.88	0.12	69,69,69,69	0
54	MG	2a	3182	1/1	0.88	0.12	66,66,66,66	0
54	MG	1A	3411	1/1	0.88	0.23	73,73,73,73	0
54	MG	1h	202	1/1	0.88	0.14	64,64,64,64	0
54	MG	2a	3193	1/1	0.88	0.26	76,76,76,76	0
54	MG	2A	3218	1/1	0.88	0.29	72,72,72,72	0
54	MG	1A	3799	1/1	0.88	0.20	70,70,70,70	0
54	MG	1A	3481	1/1	0.88	0.14	40,40,40,40	0
54	MG	1A	3270	1/1	0.88	0.12	65,65,65,65	0
54	MG	1n	102	1/1	0.88	0.14	67,67,67,67	0
54	MG	2A	3720	1/1	0.88	0.13	57,57,57,57	0
54	MG	2A	3723	1/1	0.88	0.22	67,67,67,67	0
54	MG	2r	101	1/1	0.88	0.13	68,68,68,68	0
54	MG	1A	3904	1/1	0.88	0.10	69,69,69,69	0
56	MPD	1A	4058	8/8	0.88	0.20	51,55,64,66	0
54	MG	1A	3813	1/1	0.88	0.19	38,38,38,38	0
54	MG	2A	3730	1/1	0.88	0.24	74,74,74,74	0
54	MG	2A	3735	1/1	0.88	0.09	77,77,77,77	0
54	MG	1A	3820	1/1	0.88	0.15	53,53,53,53	0
54	MG	1A	4014	1/1	0.88	0.09	67,67,67,67	0
54	MG	1A	3913	1/1	0.88	0.10	29,29,29,29	0
58	ZN	24	501	1/1	0.88	0.20	157,157,157,157	0
54	MG	1B	228	1/1	0.89	0.09	68,68,68,68	0
54	MG	1A	3562	1/1	0.89	0.19	71,71,71,71	0
54	MG	1D	311	1/1	0.89	0.19	49,49,49,49	0
54	MG	1A	3889	1/1	0.89	0.11	45,45,45,45	0
54	MG	2A	3731	1/1	0.89	0.18	72,72,72,72	0
54	MG	2A	3732	1/1	0.89	0.09	74,74,74,74	0
54	MG	1a	1779	1/1	0.89	0.11	55,55,55,55	0
54	MG	2A	3221	1/1	0.89	0.12	65,65,65,65	0
54	MG	2A	3446	1/1	0.89	0.18	64,64,64,64	0
54	MG	2A	3448	1/1	0.89	0.14	56,56,56,56	0
54	MG	1A	3692	1/1	0.89	0.11	65,65,65,65	0
54	MG	1A	3693	1/1	0.89	0.17	69,69,69,69	0
54	MG	1A	3563	1/1	0.89	0.11	51,51,51,51	0
54	MG	1y	204	1/1	0.89	0.11	86,86,86,86	0
54	MG	2A	3455	1/1	0.89	0.13	42,42,42,42	0
54	MG	2A	3003	1/1	0.89	0.09	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	2A	3242	1/1	0.89	0.16	66,66,66,66	0
54	MG	2A	3010	1/1	0.89	0.16	73,73,73,73	0
54	MG	1a	1784	1/1	0.89	0.14	66,66,66,66	0
54	MG	2A	3471	1/1	0.89	0.10	55,55,55,55	0
54	MG	2A	3252	1/1	0.89	0.15	65,65,65,65	0
54	MG	2D	304	1/1	0.89	0.38	52,52,52,52	0
54	MG	2A	3016	1/1	0.89	0.28	74,74,74,74	0
54	MG	2D	309	1/1	0.89	0.27	42,42,42,42	0
54	MG	2A	3480	1/1	0.89	0.20	61,61,61,61	0
54	MG	2E	301	1/1	0.89	0.15	73,73,73,73	0
54	MG	2A	3482	1/1	0.89	0.09	64,64,64,64	0
54	MG	1A	3250	1/1	0.89	0.12	64,64,64,64	0
54	MG	2A	3488	1/1	0.89	0.09	73,73,73,73	0
54	MG	1a	1789	1/1	0.89	0.15	66,66,66,66	0
54	MG	1E	307	1/1	0.89	0.12	34,34,34,34	0
54	MG	1A	3907	1/1	0.89	0.09	53,53,53,53	0
54	MG	2R	203	1/1	0.89	0.22	60,60,60,60	0
54	MG	2W	203	1/1	0.89	0.15	64,64,64,64	0
54	MG	1A	3801	1/1	0.89	0.10	49,49,49,49	0
54	MG	1a	1677	1/1	0.89	0.14	63,63,63,63	0
54	MG	1F	315	1/1	0.89	0.13	47,47,47,47	0
54	MG	1a	1687	1/1	0.89	0.14	59,59,59,59	0
54	MG	2A	3286	1/1	0.89	0.17	52,52,52,52	0
54	MG	2A	3508	1/1	0.89	0.13	67,67,67,67	0
54	MG	1A	3369	1/1	0.89	0.17	65,65,65,65	0
54	MG	2a	3009	1/1	0.89	0.17	70,70,70,70	0
54	MG	2A	3294	1/1	0.89	0.09	43,43,43,43	0
54	MG	1A	3074	1/1	0.89	0.20	53,53,53,53	0
54	MG	2a	3021	1/1	0.89	0.20	71,71,71,71	0
54	MG	2a	3023	1/1	0.89	0.15	62,62,62,62	0
54	MG	2a	3025	1/1	0.89	0.23	70,70,70,70	0
54	MG	1N	203	1/1	0.89	0.12	63,63,63,63	0
54	MG	1N	205	1/1	0.89	0.15	60,60,60,60	0
54	MG	1A	3578	1/1	0.89	0.15	72,72,72,72	0
54	MG	1a	1809	1/1	0.89	0.10	72,72,72,72	0
54	MG	2A	3528	1/1	0.89	0.11	42,42,42,42	0
54	MG	2A	3535	1/1	0.89	0.09	67,67,67,67	0
54	MG	2A	3304	1/1	0.89	0.12	77,77,77,77	0
54	MG	1A	3299	1/1	0.89	0.21	67,67,67,67	0
54	MG	2A	3543	1/1	0.89	0.18	56,56,56,56	0
54	MG	1a	1706	1/1	0.89	0.19	60,60,60,60	0
54	MG	2A	3067	1/1	0.89	0.21	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	1709	1/1	0.89	0.15	56,56,56,56	0
54	MG	2A	3321	1/1	0.89	0.12	48,48,48,48	0
54	MG	1a	1711	1/1	0.89	0.14	74,74,74,74	0
54	MG	2A	3330	1/1	0.89	0.10	35,35,35,35	0
54	MG	2A	3560	1/1	0.89	0.11	44,44,44,44	0
54	MG	1A	3278	1/1	0.89	0.43	56,56,56,56	0
54	MG	1A	4028	1/1	0.89	0.12	51,51,51,51	0
54	MG	10	102	1/1	0.89	0.25	56,56,56,56	0
54	MG	1a	1720	1/1	0.89	0.19	70,70,70,70	0
54	MG	1A	3485	1/1	0.89	0.10	46,46,46,46	0
54	MG	1A	3829	1/1	0.89	0.17	45,45,45,45	0
54	MG	2a	3069	1/1	0.89	0.25	68,68,68,68	0
54	MG	2A	3346	1/1	0.89	0.14	42,42,42,42	0
54	MG	2a	3073	1/1	0.89	0.15	75,75,75,75	0
54	MG	1A	3421	1/1	0.89	0.12	29,29,29,29	0
54	MG	11	104	1/1	0.89	0.12	55,55,55,55	0
54	MG	1A	3424	1/1	0.89	0.12	69,69,69,69	0
54	MG	1A	3946	1/1	0.89	0.09	31,31,31,31	0
54	MG	1A	3181	1/1	0.89	0.17	58,58,58,58	0
54	MG	2a	3084	1/1	0.89	0.10	41,41,41,41	0
54	MG	2A	3118	1/1	0.89	0.29	45,45,45,45	0
54	MG	1A	3664	1/1	0.89	0.12	64,64,64,64	0
54	MG	2a	3096	1/1	0.89	0.13	65,65,65,65	0
54	MG	1A	3465	1/1	0.89	0.17	73,73,73,73	0
54	MG	2a	3102	1/1	0.89	0.28	66,66,66,66	0
54	MG	2a	3103	1/1	0.89	0.18	70,70,70,70	0
54	MG	2A	3125	1/1	0.89	0.24	66,66,66,66	0
54	MG	2a	3109	1/1	0.89	0.18	78,78,78,78	0
54	MG	2A	3132	1/1	0.89	0.10	54,54,54,54	0
54	MG	1A	3595	1/1	0.89	0.15	60,60,60,60	0
54	MG	2a	3113	1/1	0.89	0.14	69,69,69,69	0
54	MG	2A	3376	1/1	0.89	0.11	37,37,37,37	0
54	MG	2A	3613	1/1	0.89	0.13	61,61,61,61	0
54	MG	2a	3126	1/1	0.89	0.15	75,75,75,75	0
54	MG	1A	4049	1/1	0.89	0.12	62,62,62,62	0
54	MG	2A	3378	1/1	0.89	0.14	74,74,74,74	0
54	MG	1a	1605	1/1	0.89	0.20	67,67,67,67	0
54	MG	2A	3152	1/1	0.89	0.13	52,52,52,52	0
54	MG	2A	3621	1/1	0.89	0.22	64,64,64,64	0
54	MG	1A	3427	1/1	0.89	0.14	59,59,59,59	0
54	MG	1a	1858	1/1	0.89	0.11	61,61,61,61	0
54	MG	1A	3269	1/1	0.89	0.13	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	3155	1/1	0.89	0.17	54,54,54,54	0
54	MG	2A	3625	1/1	0.89	0.12	74,74,74,74	0
54	MG	1A	3603	1/1	0.89	0.10	45,45,45,45	0
54	MG	2A	3642	1/1	0.89	0.12	80,80,80,80	0
54	MG	2a	3161	1/1	0.89	0.18	64,64,64,64	0
54	MG	1A	3509	1/1	0.89	0.10	32,32,32,32	0
54	MG	2A	3656	1/1	0.89	0.16	33,33,33,33	0
54	MG	2A	3174	1/1	0.89	0.14	70,70,70,70	0
54	MG	1A	3325	1/1	0.89	0.08	39,39,39,39	0
54	MG	2A	3178	1/1	0.89	0.10	61,61,61,61	0
54	MG	2a	3180	1/1	0.89	0.10	76,76,76,76	0
54	MG	1A	3767	1/1	0.89	0.15	67,67,67,67	0
54	MG	2A	3670	1/1	0.89	0.10	71,71,71,71	0
54	MG	2a	3185	1/1	0.89	0.15	77,77,77,77	0
54	MG	2A	3672	1/1	0.89	0.10	48,48,48,48	0
54	MG	2a	3189	1/1	0.89	0.13	60,60,60,60	0
54	MG	1A	3679	1/1	0.89	0.11	70,70,70,70	0
54	MG	2a	3192	1/1	0.89	0.15	82,82,82,82	0
54	MG	1A	3610	1/1	0.89	0.37	41,41,41,41	0
54	MG	2A	3411	1/1	0.89	0.24	49,49,49,49	0
54	MG	2A	3412	1/1	0.89	0.11	50,50,50,50	0
54	MG	2A	3188	1/1	0.89	0.17	54,54,54,54	0
54	MG	1A	3476	1/1	0.89	0.12	51,51,51,51	0
54	MG	1A	3985	1/1	0.89	0.08	54,54,54,54	0
54	MG	1A	3616	1/1	0.89	0.22	38,38,38,38	0
54	MG	1a	1767	1/1	0.89	0.16	79,79,79,79	0
54	MG	1A	3783	1/1	0.89	0.14	43,43,43,43	0
54	MG	1a	1652	1/1	0.89	0.24	60,60,60,60	0
54	MG	2A	3700	1/1	0.89	0.14	61,61,61,61	0
54	MG	1d	303	1/1	0.89	0.24	74,74,74,74	0
54	MG	2A	3702	1/1	0.89	0.10	60,60,60,60	0
54	MG	2A	3705	1/1	0.89	0.13	51,51,51,51	0
54	MG	2A	3203	1/1	0.89	0.18	56,56,56,56	0
54	MG	1A	3622	1/1	0.89	0.20	69,69,69,69	0
54	MG	2A	3715	1/1	0.89	0.13	67,67,67,67	0
54	MG	1f	201	1/1	0.89	0.23	71,71,71,71	0
54	MG	2A	3462	1/1	0.90	0.11	56,56,56,56	0
54	MG	2A	3464	1/1	0.90	0.11	70,70,70,70	0
54	MG	1P	203	1/1	0.90	0.15	39,39,39,39	0
54	MG	1A	3353	1/1	0.90	0.12	47,47,47,47	0
54	MG	2A	3220	1/1	0.90	0.10	61,61,61,61	0
54	MG	1a	1877	1/1	0.90	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3479	1/1	0.90	0.12	42,42,42,42	0
54	MG	1A	3991	1/1	0.90	0.08	50,50,50,50	0
54	MG	1A	3853	1/1	0.90	0.12	50,50,50,50	0
54	MG	1A	3994	1/1	0.90	0.15	49,49,49,49	0
54	MG	1A	3995	1/1	0.90	0.21	46,46,46,46	0
54	MG	1g	201	1/1	0.90	0.23	67,67,67,67	0
54	MG	1a	1742	1/1	0.90	0.14	80,80,80,80	0
54	MG	2A	3245	1/1	0.90	0.21	62,62,62,62	0
54	MG	2A	3495	1/1	0.90	0.26	70,70,70,70	0
54	MG	1A	3575	1/1	0.90	0.14	47,47,47,47	0
54	MG	1A	3997	1/1	0.90	0.21	43,43,43,43	0
54	MG	1A	3010	1/1	0.90	0.14	58,58,58,58	0
54	MG	2N	201	1/1	0.90	0.09	77,77,77,77	0
54	MG	1A	4002	1/1	0.90	0.13	56,56,56,56	0
54	MG	13	103	1/1	0.90	0.10	69,69,69,69	0
54	MG	1A	4003	1/1	0.90	0.15	62,62,62,62	0
54	MG	2A	3269	1/1	0.90	0.30	66,66,66,66	0
54	MG	15	104	1/1	0.90	0.22	31,31,31,31	0
54	MG	25	101	1/1	0.90	0.22	70,70,70,70	0
54	MG	1y	203	1/1	0.90	0.24	80,80,80,80	0
54	MG	2A	3519	1/1	0.90	0.10	72,72,72,72	0
54	MG	1A	3262	1/1	0.90	0.18	51,51,51,51	0
54	MG	2A	3001	1/1	0.90	0.24	70,70,70,70	0
54	MG	2A	3002	1/1	0.90	0.15	50,50,50,50	0
54	MG	1A	3748	1/1	0.90	0.30	67,67,67,67	0
54	MG	1A	3579	1/1	0.90	0.10	62,62,62,62	0
54	MG	17	106	1/1	0.90	0.21	59,59,59,59	0
54	MG	1A	3649	1/1	0.90	0.20	40,40,40,40	0
54	MG	2a	3022	1/1	0.90	0.17	77,77,77,77	0
54	MG	1A	3196	1/1	0.90	0.32	67,67,67,67	0
54	MG	1A	3755	1/1	0.90	0.12	62,62,62,62	0
54	MG	2A	3545	1/1	0.90	0.18	77,77,77,77	0
54	MG	1A	3518	1/1	0.90	0.11	60,60,60,60	0
54	MG	1A	3757	1/1	0.90	0.14	46,46,46,46	0
54	MG	2A	3032	1/1	0.90	0.14	58,58,58,58	0
54	MG	2a	3034	1/1	0.90	0.18	73,73,73,73	0
54	MG	1A	3656	1/1	0.90	0.13	55,55,55,55	0
54	MG	1a	1618	1/1	0.90	0.11	65,65,65,65	0
54	MG	2A	3311	1/1	0.90	0.16	56,56,56,56	0
54	MG	1a	1620	1/1	0.90	0.11	64,64,64,64	0
54	MG	1A	3467	1/1	0.90	0.09	49,49,49,49	0
54	MG	2A	3564	1/1	0.90	0.10	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	1776	1/1	0.90	0.21	71,71,71,71	0
54	MG	1A	3414	1/1	0.90	0.25	59,59,59,59	0
54	MG	1A	3765	1/1	0.90	0.15	47,47,47,47	0
54	MG	2A	3329	1/1	0.90	0.11	51,51,51,51	0
54	MG	1A	3586	1/1	0.90	0.25	58,58,58,58	0
54	MG	2A	3332	1/1	0.90	0.18	67,67,67,67	0
54	MG	1a	1634	1/1	0.90	0.26	75,75,75,75	0
54	MG	1A	3300	1/1	0.90	0.20	68,68,68,68	0
54	MG	1A	3163	1/1	0.90	0.11	44,44,44,44	0
54	MG	1A	3133	1/1	0.90	0.40	51,51,51,51	0
54	MG	2a	3060	1/1	0.90	0.10	67,67,67,67	0
54	MG	1a	1640	1/1	0.90	0.14	83,83,83,83	0
54	MG	2a	3063	1/1	0.90	0.10	68,68,68,68	0
54	MG	1A	4043	1/1	0.90	0.10	62,62,62,62	0
54	MG	2A	3602	1/1	0.90	0.10	48,48,48,48	0
54	MG	2a	3071	1/1	0.90	0.28	69,69,69,69	0
54	MG	2A	3081	1/1	0.90	0.16	48,48,48,48	0
54	MG	1A	3908	1/1	0.90	0.23	40,40,40,40	0
54	MG	1A	3594	1/1	0.90	0.18	75,75,75,75	0
54	MG	1a	1650	1/1	0.90	0.21	69,69,69,69	0
54	MG	1A	3310	1/1	0.90	0.18	64,64,64,64	0
54	MG	1A	3598	1/1	0.90	0.13	68,68,68,68	0
54	MG	2A	3092	1/1	0.90	0.19	65,65,65,65	0
54	MG	1A	3678	1/1	0.90	0.19	42,42,42,42	0
54	MG	2a	3085	1/1	0.90	0.21	68,68,68,68	0
54	MG	2A	3094	1/1	0.90	0.09	55,55,55,55	0
54	MG	1A	3139	1/1	0.90	0.29	67,67,67,67	0
54	MG	2a	3095	1/1	0.90	0.09	58,58,58,58	0
54	MG	1A	3071	1/1	0.90	0.23	49,49,49,49	0
54	MG	1A	3429	1/1	0.90	0.09	29,29,29,29	0
54	MG	2A	3106	1/1	0.90	0.12	54,54,54,54	0
54	MG	2A	3107	1/1	0.90	0.18	58,58,58,58	0
54	MG	2a	3105	1/1	0.90	0.14	72,72,72,72	0
54	MG	1A	3378	1/1	0.90	0.11	46,46,46,46	0
54	MG	1a	1660	1/1	0.90	0.13	71,71,71,71	0
54	MG	1A	3187	1/1	0.90	0.12	59,59,59,59	0
54	MG	2A	3630	1/1	0.90	0.12	61,61,61,61	0
54	MG	2A	3640	1/1	0.90	0.14	74,74,74,74	0
54	MG	2a	3117	1/1	0.90	0.14	71,71,71,71	0
54	MG	1a	1665	1/1	0.90	0.27	77,77,77,77	0
54	MG	2A	3649	1/1	0.90	0.09	76,76,76,76	0
54	MG	2A	3652	1/1	0.90	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1667	1/1	0.90	0.17	64,64,64,64	0
54	MG	1A	3014	1/1	0.90	0.31	65,65,65,65	0
54	MG	1A	3804	1/1	0.90	0.09	57,57,57,57	0
54	MG	1A	3386	1/1	0.90	0.15	67,67,67,67	0
54	MG	2a	3144	1/1	0.90	0.21	47,47,47,47	0
54	MG	2A	3134	1/1	0.90	0.17	70,70,70,70	0
54	MG	2A	3392	1/1	0.90	0.32	62,62,62,62	0
54	MG	1A	3558	1/1	0.90	0.16	64,64,64,64	0
54	MG	2a	3153	1/1	0.90	0.09	78,78,78,78	0
54	MG	1A	3283	1/1	0.90	0.11	49,49,49,49	0
54	MG	2A	3674	1/1	0.90	0.09	72,72,72,72	0
54	MG	2A	3146	1/1	0.90	0.17	56,56,56,56	0
54	MG	1A	3451	1/1	0.90	0.12	57,57,57,57	0
54	MG	1a	1680	1/1	0.90	0.37	75,75,75,75	0
54	MG	1A	3960	1/1	0.90	0.08	65,65,65,65	0
54	MG	1A	3501	1/1	0.90	0.08	67,67,67,67	0
54	MG	1A	3504	1/1	0.90	0.13	61,61,61,61	0
54	MG	1A	3965	1/1	0.90	0.12	59,59,59,59	0
54	MG	1A	3831	1/1	0.90	0.08	26,26,26,26	0
54	MG	2a	3177	1/1	0.90	0.23	72,72,72,72	0
54	MG	1a	1835	1/1	0.90	0.08	64,64,64,64	0
54	MG	2A	3694	1/1	0.90	0.13	69,69,69,69	0
54	MG	1A	3968	1/1	0.90	0.25	51,51,51,51	0
54	MG	2A	3696	1/1	0.90	0.13	63,63,63,63	0
54	MG	1A	3969	1/1	0.90	0.16	60,60,60,60	0
54	MG	2A	3180	1/1	0.90	0.21	69,69,69,69	0
54	MG	1a	1698	1/1	0.90	0.13	60,60,60,60	0
54	MG	1a	1847	1/1	0.90	0.21	73,73,73,73	0
54	MG	1A	3832	1/1	0.90	0.11	52,52,52,52	0
54	MG	1a	1702	1/1	0.90	0.16	56,56,56,56	0
54	MG	1a	1703	1/1	0.90	0.09	39,39,39,39	0
54	MG	1a	1705	1/1	0.90	0.11	78,78,78,78	0
54	MG	2d	301	1/1	0.90	0.18	67,67,67,67	0
54	MG	2e	201	1/1	0.90	0.16	65,65,65,65	0
54	MG	2A	3716	1/1	0.90	0.12	40,40,40,40	0
54	MG	2A	3192	1/1	0.90	0.25	65,65,65,65	0
54	MG	1A	3630	1/1	0.90	0.11	27,27,27,27	0
54	MG	1A	3709	1/1	0.90	0.15	66,66,66,66	0
54	MG	1A	3710	1/1	0.90	0.10	52,52,52,52	0
54	MG	1A	3390	1/1	0.90	0.12	28,28,28,28	0
54	MG	1A	3838	1/1	0.90	0.09	60,60,60,60	0
54	MG	1A	3638	1/1	0.90	0.23	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3204	1/1	0.90	0.16	68,68,68,68	0
54	MG	1A	3639	1/1	0.90	0.11	46,46,46,46	0
54	MG	1A	3845	1/1	0.90	0.30	60,60,60,60	0
54	MG	1A	3848	1/1	0.90	0.17	53,53,53,53	0
54	MG	1a	1727	1/1	0.90	0.20	46,46,46,46	0
54	MG	1O	201	1/1	0.90	0.12	59,59,59,59	0
54	MG	2A	3215	1/1	0.90	0.14	63,63,63,63	0
54	MG	1A	3459	1/1	0.91	0.10	52,52,52,52	0
54	MG	1a	1869	1/1	0.91	0.15	66,66,66,66	0
54	MG	1A	3766	1/1	0.91	0.07	31,31,31,31	0
54	MG	1A	3326	1/1	0.91	0.17	44,44,44,44	0
54	MG	1a	1872	1/1	0.91	0.14	65,65,65,65	0
54	MG	1a	1873	1/1	0.91	0.21	61,61,61,61	0
54	MG	2A	3206	1/1	0.91	0.30	55,55,55,55	0
54	MG	2B	206	1/1	0.91	0.18	69,69,69,69	0
54	MG	1A	3244	1/1	0.91	0.37	45,45,45,45	0
54	MG	1a	1875	1/1	0.91	0.12	87,87,87,87	0
54	MG	1A	3772	1/1	0.91	0.09	34,34,34,34	0
54	MG	2A	3211	1/1	0.91	0.23	64,64,64,64	0
54	MG	2A	3465	1/1	0.91	0.10	60,60,60,60	0
54	MG	1A	3061	1/1	0.91	0.13	55,55,55,55	0
54	MG	1a	1733	1/1	0.91	0.20	62,62,62,62	0
54	MG	2A	3472	1/1	0.91	0.17	62,62,62,62	0
54	MG	1A	3392	1/1	0.91	0.10	37,37,37,37	0
54	MG	1I	105	1/1	0.91	0.10	44,44,44,44	0
54	MG	1A	4005	1/1	0.91	0.25	38,38,38,38	0
54	MG	1A	3260	1/1	0.91	0.13	62,62,62,62	0
54	MG	2A	3225	1/1	0.91	0.22	49,49,49,49	0
54	MG	2A	3483	1/1	0.91	0.08	61,61,61,61	0
54	MG	1A	3541	1/1	0.91	0.19	63,63,63,63	0
54	MG	2A	3487	1/1	0.91	0.12	52,52,52,52	0
54	MG	1A	3398	1/1	0.91	0.11	34,34,34,34	0
54	MG	1A	3893	1/1	0.91	0.13	60,60,60,60	0
54	MG	1A	4016	1/1	0.91	0.10	63,63,63,63	0
54	MG	1A	3895	1/1	0.91	0.21	39,39,39,39	0
54	MG	2Q	202	1/1	0.91	0.11	66,66,66,66	0
54	MG	1A	4020	1/1	0.91	0.15	61,61,61,61	0
54	MG	2T	201	1/1	0.91	0.25	68,68,68,68	0
54	MG	2A	3498	1/1	0.91	0.10	73,73,73,73	0
54	MG	2Y	201	1/1	0.91	0.18	60,60,60,60	0
54	MG	2O	102	1/1	0.91	0.08	71,71,71,71	0
54	MG	2A	3244	1/1	0.91	0.09	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	4022	1/1	0.91	0.14	54,54,54,54	0
54	MG	1A	3896	1/1	0.91	0.13	49,49,49,49	0
54	MG	1y	201	1/1	0.91	0.09	76,76,76,76	0
54	MG	1a	1602	1/1	0.91	0.16	78,78,78,78	0
54	MG	1A	3343	1/1	0.91	0.09	43,43,43,43	0
54	MG	1A	3346	1/1	0.91	0.10	40,40,40,40	0
54	MG	2A	3513	1/1	0.91	0.12	56,56,56,56	0
54	MG	1a	1760	1/1	0.91	0.24	68,68,68,68	0
54	MG	2A	3268	1/1	0.91	0.22	58,58,58,58	0
54	MG	1a	1614	1/1	0.91	0.19	68,68,68,68	0
54	MG	1a	1615	1/1	0.91	0.11	57,57,57,57	0
54	MG	1A	3551	1/1	0.91	0.17	46,46,46,46	0
54	MG	2A	3522	1/1	0.91	0.18	64,64,64,64	0
54	MG	1A	3793	1/1	0.91	0.12	64,64,64,64	0
54	MG	2A	3017	1/1	0.91	0.12	61,61,61,61	0
54	MG	2A	3526	1/1	0.91	0.10	58,58,58,58	0
54	MG	2a	3030	1/1	0.91	0.15	73,73,73,73	0
54	MG	2A	3019	1/1	0.91	0.29	51,51,51,51	0
54	MG	1A	3795	1/1	0.91	0.14	70,70,70,70	0
54	MG	2A	3278	1/1	0.91	0.21	60,60,60,60	0
54	MG	1a	1621	1/1	0.91	0.14	58,58,58,58	0
54	MG	2a	3036	1/1	0.91	0.23	58,58,58,58	0
54	MG	2A	3287	1/1	0.91	0.18	65,65,65,65	0
54	MG	1A	3199	1/1	0.91	0.14	48,48,48,48	0
54	MG	1A	4036	1/1	0.91	0.09	65,65,65,65	0
54	MG	2A	3547	1/1	0.91	0.09	38,38,38,38	0
54	MG	1A	3288	1/1	0.91	0.14	46,46,46,46	0
54	MG	2a	3042	1/1	0.91	0.29	74,74,74,74	0
54	MG	1A	3625	1/1	0.91	0.10	30,30,30,30	0
54	MG	2A	3035	1/1	0.91	0.26	68,68,68,68	0
54	MG	1A	3093	1/1	0.91	0.13	64,64,64,64	0
54	MG	1A	3700	1/1	0.91	0.10	49,49,49,49	0
54	MG	1A	3359	1/1	0.91	0.12	41,41,41,41	0
54	MG	2A	3045	1/1	0.91	0.15	67,67,67,67	0
54	MG	1A	3423	1/1	0.91	0.09	32,32,32,32	0
54	MG	1A	3264	1/1	0.91	0.27	30,30,30,30	0
54	MG	1A	3938	1/1	0.91	0.08	59,59,59,59	0
54	MG	1a	1642	1/1	0.91	0.25	68,68,68,68	0
54	MG	1A	3637	1/1	0.91	0.08	46,46,46,46	0
54	MG	2a	3061	1/1	0.91	0.14	68,68,68,68	0
54	MG	2A	3327	1/1	0.91	0.10	42,42,42,42	0
54	MG	1A	4052	1/1	0.91	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1785	1/1	0.91	0.12	79,79,79,79	0
54	MG	1A	3941	1/1	0.91	0.09	50,50,50,50	0
54	MG	2A	3589	1/1	0.91	0.09	66,66,66,66	0
54	MG	2A	3064	1/1	0.91	0.08	55,55,55,55	0
54	MG	1a	1788	1/1	0.91	0.11	73,73,73,73	0
54	MG	2A	3071	1/1	0.91	0.14	50,50,50,50	0
54	MG	1A	3943	1/1	0.91	0.12	65,65,65,65	0
54	MG	1a	1790	1/1	0.91	0.27	74,74,74,74	0
54	MG	1A	3822	1/1	0.91	0.11	31,31,31,31	0
54	MG	2a	3078	1/1	0.91	0.25	70,70,70,70	0
54	MG	1A	3425	1/1	0.91	0.12	32,32,32,32	0
54	MG	2a	3083	1/1	0.91	0.13	82,82,82,82	0
54	MG	1A	3949	1/1	0.91	0.09	60,60,60,60	0
54	MG	1A	3828	1/1	0.91	0.09	18,18,18,18	0
54	MG	2a	3086	1/1	0.91	0.15	62,62,62,62	0
54	MG	2a	3090	1/1	0.91	0.13	58,58,58,58	0
54	MG	1A	3715	1/1	0.91	0.14	28,28,28,28	0
54	MG	2A	3351	1/1	0.91	0.29	61,61,61,61	0
54	MG	1B	214	1/1	0.91	0.08	49,49,49,49	0
54	MG	1A	3956	1/1	0.91	0.12	67,67,67,67	0
54	MG	1a	1662	1/1	0.91	0.23	67,67,67,67	0
54	MG	2a	3098	1/1	0.91	0.11	85,85,85,85	0
54	MG	2a	3099	1/1	0.91	0.12	74,74,74,74	0
54	MG	2A	3616	1/1	0.91	0.09	58,58,58,58	0
54	MG	1A	3119	1/1	0.91	0.30	54,54,54,54	0
54	MG	1A	3718	1/1	0.91	0.18	53,53,53,53	0
54	MG	2A	3620	1/1	0.91	0.14	58,58,58,58	0
54	MG	1B	221	1/1	0.91	0.20	66,66,66,66	0
54	MG	2A	3367	1/1	0.91	0.09	66,66,66,66	0
54	MG	1a	1668	1/1	0.91	0.18	60,60,60,60	0
54	MG	1A	3961	1/1	0.91	0.12	69,69,69,69	0
54	MG	1A	3366	1/1	0.91	0.09	54,54,54,54	0
54	MG	2A	3111	1/1	0.91	0.14	51,51,51,51	0
54	MG	2A	3629	1/1	0.91	0.12	73,73,73,73	0
54	MG	1A	3963	1/1	0.91	0.10	66,66,66,66	0
54	MG	2a	3127	1/1	0.91	0.23	74,74,74,74	0
54	MG	2a	3131	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3574	1/1	0.91	0.12	65,65,65,65	0
54	MG	1A	3643	1/1	0.91	0.23	38,38,38,38	0
54	MG	2a	3139	1/1	0.91	0.10	73,73,73,73	0
54	MG	2A	3647	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3266	1/1	0.91	0.36	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1679	1/1	0.91	0.28	72,72,72,72	0
54	MG	1A	3368	1/1	0.91	0.11	24,24,24,24	0
54	MG	2a	3148	1/1	0.91	0.12	67,67,67,67	0
54	MG	2A	3126	1/1	0.91	0.19	67,67,67,67	0
54	MG	1a	1823	1/1	0.91	0.10	65,65,65,65	0
54	MG	1D	316	1/1	0.91	0.15	53,53,53,53	0
54	MG	1A	3011	1/1	0.91	0.16	66,66,66,66	0
54	MG	2A	3138	1/1	0.91	0.33	62,62,62,62	0
54	MG	2A	3666	1/1	0.91	0.08	62,62,62,62	0
54	MG	1A	3309	1/1	0.91	0.34	41,41,41,41	0
54	MG	2a	3158	1/1	0.91	0.09	68,68,68,68	0
54	MG	2A	3402	1/1	0.91	0.09	45,45,45,45	0
54	MG	2A	3403	1/1	0.91	0.11	39,39,39,39	0
54	MG	1A	3214	1/1	0.91	0.13	58,58,58,58	0
54	MG	2A	3676	1/1	0.91	0.08	55,55,55,55	0
54	MG	2A	3147	1/1	0.91	0.33	79,79,79,79	0
54	MG	1A	3653	1/1	0.91	0.09	54,54,54,54	0
54	MG	1A	3317	1/1	0.91	0.32	54,54,54,54	0
54	MG	1a	1834	1/1	0.91	0.10	51,51,51,51	0
54	MG	2A	3158	1/1	0.91	0.20	44,44,44,44	0
54	MG	1a	1695	1/1	0.91	0.23	65,65,65,65	0
54	MG	2A	3686	1/1	0.91	0.13	67,67,67,67	0
54	MG	1A	3851	1/1	0.91	0.10	54,54,54,54	0
54	MG	1a	1697	1/1	0.91	0.29	68,68,68,68	0
54	MG	1F	314	1/1	0.91	0.31	43,43,43,43	0
54	MG	1A	3319	1/1	0.91	0.14	60,60,60,60	0
54	MG	2A	3422	1/1	0.91	0.15	61,61,61,61	0
54	MG	1a	1700	1/1	0.91	0.21	64,64,64,64	0
54	MG	1A	3515	1/1	0.91	0.12	28,28,28,28	0
54	MG	1A	3172	1/1	0.91	0.14	67,67,67,67	0
54	MG	2A	3432	1/1	0.91	0.23	78,78,78,78	0
54	MG	1A	3863	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3864	1/1	0.91	0.09	51,51,51,51	0
54	MG	2A	3436	1/1	0.91	0.07	49,49,49,49	0
54	MG	2A	3709	1/1	0.91	0.20	74,74,74,74	0
54	MG	2A	3711	1/1	0.91	0.08	74,74,74,74	0
54	MG	1A	3867	1/1	0.91	0.18	45,45,45,45	0
54	MG	1a	1710	1/1	0.91	0.13	67,67,67,67	0
54	MG	1A	3193	1/1	0.91	0.11	64,64,64,64	0
54	MG	2A	3722	1/1	0.91	0.15	48,48,48,48	0
54	MG	1A	3383	1/1	0.91	0.11	54,54,54,54	0
54	MG	2A	3191	1/1	0.91	0.26	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3727	1/1	0.91	0.18	62,62,62,62	0
54	MG	1A	3458	1/1	0.91	0.12	55,55,55,55	0
54	MG	1T	201	1/1	0.91	0.12	52,52,52,52	0
54	MG	1a	1717	1/1	0.91	0.12	70,70,70,70	0
54	MG	2A	3447	1/1	0.91	0.10	44,44,44,44	0
54	MG	2A	3038	1/1	0.92	0.16	67,67,67,67	0
54	MG	1A	3255	1/1	0.92	0.17	47,47,47,47	0
54	MG	1A	3635	1/1	0.92	0.11	31,31,31,31	0
54	MG	1A	3566	1/1	0.92	0.08	61,61,61,61	0
54	MG	1A	3510	1/1	0.92	0.10	73,73,73,73	0
54	MG	1a	1792	1/1	0.92	0.12	66,66,66,66	0
54	MG	2A	3281	1/1	0.92	0.11	24,24,24,24	0
54	MG	2A	3285	1/1	0.92	0.12	54,54,54,54	0
54	MG	1A	3460	1/1	0.92	0.11	63,63,63,63	0
54	MG	2E	305	1/1	0.92	0.09	57,57,57,57	0
54	MG	2E	307	1/1	0.92	0.19	67,67,67,67	0
54	MG	1A	3512	1/1	0.92	0.11	60,60,60,60	0
54	MG	1A	3150	1/1	0.92	0.48	45,45,45,45	0
54	MG	1A	3713	1/1	0.92	0.11	54,54,54,54	0
54	MG	1F	316	1/1	0.92	0.12	57,57,57,57	0
54	MG	1a	1678	1/1	0.92	0.08	65,65,65,65	0
54	MG	2O	201	1/1	0.92	0.14	65,65,65,65	0
54	MG	1A	3210	1/1	0.92	0.10	55,55,55,55	0
54	MG	1A	3905	1/1	0.92	0.10	75,75,75,75	0
54	MG	1a	1682	1/1	0.92	0.20	59,59,59,59	0
54	MG	2A	3302	1/1	0.92	0.13	55,55,55,55	0
54	MG	2T	203	1/1	0.92	0.09	63,63,63,63	0
54	MG	2V	203	1/1	0.92	0.13	69,69,69,69	0
54	MG	2W	202	1/1	0.92	0.13	52,52,52,52	0
54	MG	1a	1807	1/1	0.92	0.19	60,60,60,60	0
54	MG	2A	3307	1/1	0.92	0.11	45,45,45,45	0
54	MG	1a	1683	1/1	0.92	0.18	78,78,78,78	0
54	MG	1A	3811	1/1	0.92	0.32	47,47,47,47	0
54	MG	2A	3533	1/1	0.92	0.13	57,57,57,57	0
54	MG	2A	3085	1/1	0.92	0.21	75,75,75,75	0
54	MG	1a	1686	1/1	0.92	0.13	66,66,66,66	0
54	MG	1A	3464	1/1	0.92	0.09	46,46,46,46	0
54	MG	2A	3320	1/1	0.92	0.14	69,69,69,69	0
54	MG	1A	3330	1/1	0.92	0.10	65,65,65,65	0
54	MG	1A	4006	1/1	0.92	0.12	18,18,18,18	0
54	MG	1a	1817	1/1	0.92	0.15	76,76,76,76	0
54	MG	2a	3010	1/1	0.92	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3548	1/1	0.92	0.12	72,72,72,72	0
54	MG	1A	4007	1/1	0.92	0.12	42,42,42,42	0
54	MG	2a	3020	1/1	0.92	0.18	63,63,63,63	0
54	MG	1A	3817	1/1	0.92	0.10	41,41,41,41	0
54	MG	1R	202	1/1	0.92	0.19	50,50,50,50	0
54	MG	1A	3098	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3102	1/1	0.92	0.10	36,36,36,36	0
54	MG	1V	206	1/1	0.92	0.14	59,59,59,59	0
54	MG	1W	201	1/1	0.92	0.14	50,50,50,50	0
54	MG	1A	3725	1/1	0.92	0.07	36,36,36,36	0
54	MG	2A	3110	1/1	0.92	0.23	56,56,56,56	0
54	MG	1A	3728	1/1	0.92	0.12	39,39,39,39	0
54	MG	1A	3648	1/1	0.92	0.13	57,57,57,57	0
54	MG	1A	3063	1/1	0.92	0.12	42,42,42,42	0
54	MG	1A	3932	1/1	0.92	0.14	61,61,61,61	0
54	MG	2A	3352	1/1	0.92	0.18	65,65,65,65	0
54	MG	1a	1708	1/1	0.92	0.14	72,72,72,72	0
54	MG	2A	3582	1/1	0.92	0.10	60,60,60,60	0
54	MG	1A	3532	1/1	0.92	0.18	55,55,55,55	0
54	MG	1A	3936	1/1	0.92	0.12	47,47,47,47	0
54	MG	2A	3590	1/1	0.92	0.09	41,41,41,41	0
54	MG	2A	3591	1/1	0.92	0.12	49,49,49,49	0
54	MG	1a	1844	1/1	0.92	0.09	65,65,65,65	0
54	MG	2a	3048	1/1	0.92	0.14	74,74,74,74	0
54	MG	13	102	1/1	0.92	0.12	46,46,46,46	0
54	MG	2A	3597	1/1	0.92	0.10	41,41,41,41	0
54	MG	2A	3365	1/1	0.92	0.14	65,65,65,65	0
54	MG	1A	3740	1/1	0.92	0.10	31,31,31,31	0
54	MG	1a	1849	1/1	0.92	0.34	72,72,72,72	0
54	MG	1A	3741	1/1	0.92	0.08	51,51,51,51	0
54	MG	1a	1851	1/1	0.92	0.18	72,72,72,72	0
54	MG	2a	3057	1/1	0.92	0.08	88,88,88,88	0
54	MG	2A	3372	1/1	0.92	0.17	71,71,71,71	0
54	MG	2a	3059	1/1	0.92	0.23	75,75,75,75	0
54	MG	1A	3342	1/1	0.92	0.09	48,48,48,48	0
54	MG	1A	3121	1/1	0.92	0.13	49,49,49,49	0
54	MG	1a	1856	1/1	0.92	0.12	63,63,63,63	0
54	MG	2A	3151	1/1	0.92	0.20	67,67,67,67	0
54	MG	1a	1719	1/1	0.92	0.10	75,75,75,75	0
54	MG	2a	3065	1/1	0.92	0.17	64,64,64,64	0
54	MG	15	106	1/1	0.92	0.10	50,50,50,50	0
54	MG	1A	3945	1/1	0.92	0.07	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	3344	1/1	0.92	0.09	32,32,32,32	0
54	MG	1A	3303	1/1	0.92	0.15	42,42,42,42	0
54	MG	1A	3236	1/1	0.92	0.24	64,64,64,64	0
54	MG	2A	3166	1/1	0.92	0.10	61,61,61,61	0
54	MG	2A	3167	1/1	0.92	0.14	53,53,53,53	0
54	MG	1A	3237	1/1	0.92	0.28	58,58,58,58	0
54	MG	2A	3397	1/1	0.92	0.11	57,57,57,57	0
54	MG	2A	3172	1/1	0.92	0.15	65,65,65,65	0
54	MG	2A	3401	1/1	0.92	0.10	50,50,50,50	0
54	MG	1a	1732	1/1	0.92	0.08	56,56,56,56	0
54	MG	2A	3175	1/1	0.92	0.26	75,75,75,75	0
54	MG	2A	3636	1/1	0.92	0.07	58,58,58,58	0
54	MG	2A	3637	1/1	0.92	0.07	64,64,64,64	0
54	MG	2A	3404	1/1	0.92	0.16	70,70,70,70	0
54	MG	1A	3951	1/1	0.92	0.10	68,68,68,68	0
54	MG	2A	3643	1/1	0.92	0.08	56,56,56,56	0
54	MG	2A	3177	1/1	0.92	0.10	71,71,71,71	0
54	MG	1A	3546	1/1	0.92	0.10	35,35,35,35	0
54	MG	1A	3955	1/1	0.92	0.09	31,31,31,31	0
54	MG	2A	3653	1/1	0.92	0.11	57,57,57,57	0
54	MG	1A	3039	1/1	0.92	0.14	57,57,57,57	0
54	MG	1a	1612	1/1	0.92	0.18	84,84,84,84	0
54	MG	1A	4048	1/1	0.92	0.14	54,54,54,54	0
54	MG	1A	3958	1/1	0.92	0.17	54,54,54,54	0
54	MG	1A	3273	1/1	0.92	0.10	39,39,39,39	0
54	MG	1a	1744	1/1	0.92	0.18	63,63,63,63	0
54	MG	2a	3111	1/1	0.92	0.15	66,66,66,66	0
54	MG	1A	3604	1/1	0.92	0.08	43,43,43,43	0
54	MG	2A	3669	1/1	0.92	0.12	60,60,60,60	0
54	MG	2a	3115	1/1	0.92	0.08	69,69,69,69	0
54	MG	1A	3444	1/1	0.92	0.10	50,50,50,50	0
54	MG	1a	1750	1/1	0.92	0.08	60,60,60,60	0
54	MG	2A	3194	1/1	0.92	0.09	47,47,47,47	0
54	MG	1A	3448	1/1	0.92	0.12	49,49,49,49	0
54	MG	1a	1624	1/1	0.92	0.12	59,59,59,59	0
54	MG	1A	3449	1/1	0.92	0.10	63,63,63,63	0
54	MG	2A	3678	1/1	0.92	0.07	62,62,62,62	0
54	MG	2a	3136	1/1	0.92	0.11	75,75,75,75	0
54	MG	2A	3679	1/1	0.92	0.08	48,48,48,48	0
54	MG	2a	3138	1/1	0.92	0.15	70,70,70,70	0
54	MG	1f	202	1/1	0.92	0.12	49,49,49,49	0
54	MG	1A	3557	1/1	0.92	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3314	1/1	0.92	0.20	39,39,39,39	0
54	MG	1A	3771	1/1	0.92	0.11	54,54,54,54	0
54	MG	2A	3439	1/1	0.92	0.18	52,52,52,52	0
54	MG	2a	3146	1/1	0.92	0.14	70,70,70,70	0
54	MG	1B	207	1/1	0.92	0.30	61,61,61,61	0
54	MG	2A	3687	1/1	0.92	0.11	62,62,62,62	0
54	MG	1A	3868	1/1	0.92	0.08	65,65,65,65	0
54	MG	1l	201	1/1	0.92	0.16	65,65,65,65	0
54	MG	1A	3619	1/1	0.92	0.10	44,44,44,44	0
54	MG	1B	215	1/1	0.92	0.18	56,56,56,56	0
54	MG	2A	3445	1/1	0.92	0.11	66,66,66,66	0
54	MG	2A	3212	1/1	0.92	0.14	67,67,67,67	0
54	MG	1B	216	1/1	0.92	0.19	69,69,69,69	0
54	MG	1o	3100	1/1	0.92	0.10	50,50,50,50	0
54	MG	1A	3775	1/1	0.92	0.09	34,34,34,34	0
54	MG	1A	3620	1/1	0.92	0.25	45,45,45,45	0
54	MG	2a	3172	1/1	0.92	0.14	78,78,78,78	0
54	MG	1a	1768	1/1	0.92	0.19	74,74,74,74	0
54	MG	2A	3452	1/1	0.92	0.12	38,38,38,38	0
54	MG	1a	1769	1/1	0.92	0.15	67,67,67,67	0
54	MG	1A	3559	1/1	0.92	0.09	52,52,52,52	0
54	MG	2A	3456	1/1	0.92	0.13	75,75,75,75	0
54	MG	1A	3399	1/1	0.92	0.08	40,40,40,40	0
54	MG	2A	3718	1/1	0.92	0.12	51,51,51,51	0
54	MG	1a	1649	1/1	0.92	0.23	63,63,63,63	0
54	MG	2A	3721	1/1	0.92	0.10	68,68,68,68	0
54	MG	1A	3980	1/1	0.92	0.12	57,57,57,57	0
54	MG	2A	3232	1/1	0.92	0.09	59,59,59,59	0
54	MG	1A	3981	1/1	0.92	0.10	60,60,60,60	0
54	MG	2A	3725	1/1	0.92	0.09	75,75,75,75	0
54	MG	1A	3982	1/1	0.92	0.13	51,51,51,51	0
54	MG	2A	3728	1/1	0.92	0.09	87,87,87,87	0
54	MG	2A	3466	1/1	0.92	0.10	73,73,73,73	0
54	MG	2A	3468	1/1	0.92	0.12	69,69,69,69	0
54	MG	1B	229	1/1	0.92	0.08	62,62,62,62	0
54	MG	2A	3243	1/1	0.92	0.12	44,44,44,44	0
54	MG	1A	3403	1/1	0.92	0.09	23,23,23,23	0
54	MG	1A	3880	1/1	0.92	0.09	57,57,57,57	0
54	MG	1D	312	1/1	0.92	0.30	44,44,44,44	0
54	MG	1D	313	1/1	0.92	0.12	66,66,66,66	0
54	MG	1a	1782	1/1	0.92	0.12	70,70,70,70	0
54	MG	1A	3245	1/1	0.92	0.22	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	3033	1/1	0.92	0.17	53,53,53,53	0
54	MG	2A	3485	1/1	0.92	0.08	42,42,42,42	0
54	MG	1A	3145	1/1	0.92	0.17	56,56,56,56	0
54	MG	1a	1663	1/1	0.92	0.09	69,69,69,69	0
54	MG	1A	3788	1/1	0.92	0.11	66,66,66,66	0
54	MG	2A	3037	1/1	0.92	0.20	52,52,52,52	0
54	MG	2B	211	1/1	0.92	0.12	63,63,63,63	0
58	ZN	14	102	1/1	0.92	0.13	144,144,144,144	0
54	MG	2A	3492	1/1	0.92	0.12	54,54,54,54	0
54	MG	1a	1672	1/1	0.93	0.11	48,48,48,48	0
54	MG	1A	3088	1/1	0.93	0.29	40,40,40,40	0
54	MG	2A	3490	1/1	0.93	0.10	65,65,65,65	0
54	MG	1A	3974	1/1	0.93	0.12	64,64,64,64	0
54	MG	2A	3280	1/1	0.93	0.07	53,53,53,53	0
54	MG	1A	3205	1/1	0.93	0.24	43,43,43,43	0
54	MG	1A	3207	1/1	0.93	0.27	46,46,46,46	0
54	MG	2A	3497	1/1	0.93	0.12	45,45,45,45	0
54	MG	2B	216	1/1	0.93	0.16	69,69,69,69	0
54	MG	1A	3494	1/1	0.93	0.07	67,67,67,67	0
54	MG	2D	303	1/1	0.93	0.33	45,45,45,45	0
54	MG	1A	3495	1/1	0.93	0.09	31,31,31,31	0
54	MG	2A	3289	1/1	0.93	0.19	53,53,53,53	0
54	MG	2A	3074	1/1	0.93	0.12	58,58,58,58	0
54	MG	2A	3079	1/1	0.93	0.13	61,61,61,61	0
54	MG	2A	3504	1/1	0.93	0.10	63,63,63,63	0
54	MG	1E	304	1/1	0.93	0.09	52,52,52,52	0
54	MG	1a	1681	1/1	0.93	0.16	59,59,59,59	0
54	MG	1A	3854	1/1	0.93	0.12	48,48,48,48	0
54	MG	2A	3510	1/1	0.93	0.08	38,38,38,38	0
54	MG	2A	3511	1/1	0.93	0.15	66,66,66,66	0
54	MG	1A	3856	1/1	0.93	0.07	47,47,47,47	0
54	MG	1A	3747	1/1	0.93	0.08	65,65,65,65	0
54	MG	1A	3496	1/1	0.93	0.07	28,28,28,28	0
54	MG	2A	3518	1/1	0.93	0.07	61,61,61,61	0
54	MG	1A	3173	1/1	0.93	0.23	46,46,46,46	0
54	MG	1a	1688	1/1	0.93	0.29	77,77,77,77	0
54	MG	1A	3570	1/1	0.93	0.10	57,57,57,57	0
54	MG	2A	3309	1/1	0.93	0.10	55,55,55,55	0
54	MG	2A	3523	1/1	0.93	0.14	51,51,51,51	0
54	MG	2A	3310	1/1	0.93	0.11	67,67,67,67	0
54	MG	1A	3866	1/1	0.93	0.09	46,46,46,46	0
54	MG	2A	3096	1/1	0.93	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3315	1/1	0.93	0.11	30,30,30,30	0
54	MG	2A	3530	1/1	0.93	0.10	44,44,44,44	0
54	MG	1A	3572	1/1	0.93	0.09	25,25,25,25	0
54	MG	1A	3178	1/1	0.93	0.18	52,52,52,52	0
54	MG	1G	204	1/1	0.93	0.14	60,60,60,60	0
54	MG	2A	3539	1/1	0.93	0.06	56,56,56,56	0
54	MG	2a	3001	1/1	0.93	0.09	49,49,49,49	0
54	MG	1A	3990	1/1	0.93	0.16	61,61,61,61	0
54	MG	2A	3542	1/1	0.93	0.16	69,69,69,69	0
54	MG	1A	3371	1/1	0.93	0.08	34,34,34,34	0
54	MG	1a	1831	1/1	0.93	0.14	66,66,66,66	0
54	MG	1A	3438	1/1	0.93	0.13	61,61,61,61	0
54	MG	1A	3758	1/1	0.93	0.10	52,52,52,52	0
54	MG	2a	3014	1/1	0.93	0.16	63,63,63,63	0
54	MG	2A	3112	1/1	0.93	0.15	58,58,58,58	0
54	MG	2A	3551	1/1	0.93	0.11	53,53,53,53	0
54	MG	1A	3651	1/1	0.93	0.11	43,43,43,43	0
54	MG	1Q	202	1/1	0.93	0.07	36,36,36,36	0
54	MG	2A	3341	1/1	0.93	0.15	53,53,53,53	0
54	MG	2A	3556	1/1	0.93	0.10	65,65,65,65	0
54	MG	1Q	203	1/1	0.93	0.12	56,56,56,56	0
54	MG	1a	1838	1/1	0.93	0.13	74,74,74,74	0
54	MG	2A	3123	1/1	0.93	0.23	42,42,42,42	0
54	MG	2a	3028	1/1	0.93	0.29	67,67,67,67	0
54	MG	1a	1842	1/1	0.93	0.09	67,67,67,67	0
54	MG	1A	3577	1/1	0.93	0.12	46,46,46,46	0
54	MG	2a	3032	1/1	0.93	0.08	92,92,92,92	0
54	MG	1A	3507	1/1	0.93	0.10	46,46,46,46	0
54	MG	2A	3349	1/1	0.93	0.09	34,34,34,34	0
54	MG	2A	3569	1/1	0.93	0.11	71,71,71,71	0
54	MG	1A	3440	1/1	0.93	0.11	72,72,72,72	0
54	MG	1a	1848	1/1	0.93	0.15	66,66,66,66	0
54	MG	1A	4001	1/1	0.93	0.14	81,81,81,81	0
54	MG	1V	201	1/1	0.93	0.24	38,38,38,38	0
54	MG	1A	3267	1/1	0.93	0.29	55,55,55,55	0
54	MG	2A	3580	1/1	0.93	0.09	54,54,54,54	0
54	MG	2A	3360	1/1	0.93	0.17	50,50,50,50	0
54	MG	1A	3101	1/1	0.93	0.20	43,43,43,43	0
54	MG	2A	3362	1/1	0.93	0.12	62,62,62,62	0
54	MG	2a	3046	1/1	0.93	0.12	61,61,61,61	0
54	MG	1A	3147	1/1	0.93	0.16	45,45,45,45	0
54	MG	1A	3770	1/1	0.93	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	3150	1/1	0.93	0.13	68,68,68,68	0
54	MG	1A	3186	1/1	0.93	0.10	60,60,60,60	0
54	MG	1A	3890	1/1	0.93	0.08	50,50,50,50	0
54	MG	1A	3328	1/1	0.93	0.13	65,65,65,65	0
54	MG	2A	3599	1/1	0.93	0.06	56,56,56,56	0
54	MG	2A	3154	1/1	0.93	0.16	59,59,59,59	0
54	MG	2A	3371	1/1	0.93	0.08	74,74,74,74	0
54	MG	1l	101	1/1	0.93	0.13	45,45,45,45	0
54	MG	1a	1724	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	4009	1/1	0.93	0.16	64,64,64,64	0
54	MG	1A	4011	1/1	0.93	0.11	53,53,53,53	0
54	MG	2A	3163	1/1	0.93	0.10	63,63,63,63	0
54	MG	1a	1729	1/1	0.93	0.11	69,69,69,69	0
54	MG	2A	3612	1/1	0.93	0.14	57,57,57,57	0
54	MG	1A	3329	1/1	0.93	0.13	31,31,31,31	0
54	MG	1A	3517	1/1	0.93	0.08	44,44,44,44	0
54	MG	2a	3070	1/1	0.93	0.14	54,54,54,54	0
54	MG	1A	3675	1/1	0.93	0.17	55,55,55,55	0
54	MG	1A	3232	1/1	0.93	0.13	41,41,41,41	0
54	MG	1A	3387	1/1	0.93	0.13	41,41,41,41	0
54	MG	2A	3387	1/1	0.93	0.17	72,72,72,72	0
54	MG	1A	3070	1/1	0.93	0.08	44,44,44,44	0
54	MG	1A	3112	1/1	0.93	0.32	42,42,42,42	0
54	MG	1A	3681	1/1	0.93	0.12	56,56,56,56	0
54	MG	2A	3393	1/1	0.93	0.07	34,34,34,34	0
54	MG	2A	3394	1/1	0.93	0.19	64,64,64,64	0
54	MG	2A	3396	1/1	0.93	0.09	37,37,37,37	0
54	MG	1A	3682	1/1	0.93	0.12	56,56,56,56	0
54	MG	2A	3399	1/1	0.93	0.11	39,39,39,39	0
54	MG	1A	3791	1/1	0.93	0.17	65,65,65,65	0
54	MG	2a	3088	1/1	0.93	0.23	49,49,49,49	0
54	MG	2A	3631	1/1	0.93	0.10	71,71,71,71	0
54	MG	2A	3632	1/1	0.93	0.11	86,86,86,86	0
54	MG	2A	3633	1/1	0.93	0.14	61,61,61,61	0
54	MG	2a	3094	1/1	0.93	0.09	62,62,62,62	0
54	MG	2A	3635	1/1	0.93	0.09	59,59,59,59	0
54	MG	1A	3599	1/1	0.93	0.07	47,47,47,47	0
54	MG	1A	3335	1/1	0.93	0.08	32,32,32,32	0
54	MG	2A	3187	1/1	0.93	0.14	58,58,58,58	0
54	MG	1a	1745	1/1	0.93	0.08	57,57,57,57	0
54	MG	1A	4031	1/1	0.93	0.07	66,66,66,66	0
54	MG	2A	3645	1/1	0.93	0.07	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1603	1/1	0.93	0.13	72,72,72,72	0
54	MG	2A	3407	1/1	0.93	0.20	70,70,70,70	0
54	MG	2A	3408	1/1	0.93	0.11	56,56,56,56	0
54	MG	1A	3914	1/1	0.93	0.07	38,38,38,38	0
54	MG	1A	3794	1/1	0.93	0.10	39,39,39,39	0
54	MG	1A	4035	1/1	0.93	0.11	62,62,62,62	0
54	MG	1A	3158	1/1	0.93	0.16	64,64,64,64	0
54	MG	1A	3243	1/1	0.93	0.11	46,46,46,46	0
54	MG	2A	3415	1/1	0.93	0.10	47,47,47,47	0
54	MG	1A	3798	1/1	0.93	0.13	65,65,65,65	0
54	MG	2a	3120	1/1	0.93	0.07	55,55,55,55	0
54	MG	2a	3122	1/1	0.93	0.11	78,78,78,78	0
54	MG	2a	3123	1/1	0.93	0.07	64,64,64,64	0
54	MG	1A	3161	1/1	0.93	0.10	43,43,43,43	0
54	MG	2A	3200	1/1	0.93	0.13	42,42,42,42	0
54	MG	1A	4042	1/1	0.93	0.11	67,67,67,67	0
54	MG	1A	3195	1/1	0.93	0.10	52,52,52,52	0
54	MG	1A	3934	1/1	0.93	0.08	63,63,63,63	0
54	MG	1A	3466	1/1	0.93	0.09	57,57,57,57	0
54	MG	1A	3608	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3805	1/1	0.93	0.09	44,44,44,44	0
54	MG	1y	202	1/1	0.93	0.09	71,71,71,71	0
54	MG	2a	3141	1/1	0.93	0.09	64,64,64,64	0
54	MG	2A	3209	1/1	0.93	0.10	58,58,58,58	0
54	MG	1A	3806	1/1	0.93	0.26	42,42,42,42	0
54	MG	1A	3808	1/1	0.93	0.10	62,62,62,62	0
54	MG	1A	3810	1/1	0.93	0.10	64,64,64,64	0
54	MG	1A	3539	1/1	0.93	0.09	64,64,64,64	0
54	MG	2a	3147	1/1	0.93	0.12	64,64,64,64	0
54	MG	1A	4054	1/1	0.93	0.13	64,64,64,64	0
54	MG	1a	1639	1/1	0.93	0.14	68,68,68,68	0
54	MG	1A	3540	1/1	0.93	0.10	57,57,57,57	0
54	MG	1A	3701	1/1	0.93	0.30	41,41,41,41	0
54	MG	2A	3692	1/1	0.93	0.07	44,44,44,44	0
54	MG	1A	3615	1/1	0.93	0.19	38,38,38,38	0
54	MG	2A	3018	1/1	0.93	0.40	54,54,54,54	0
54	MG	1A	3289	1/1	0.93	0.18	58,58,58,58	0
54	MG	2A	3228	1/1	0.93	0.17	71,71,71,71	0
54	MG	1A	3408	1/1	0.93	0.19	57,57,57,57	0
54	MG	1A	3347	1/1	0.93	0.10	55,55,55,55	0
54	MG	1B	209	1/1	0.93	0.09	62,62,62,62	0
54	MG	1A	3953	1/1	0.93	0.07	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3290	1/1	0.93	0.13	56,56,56,56	0
54	MG	2A	3237	1/1	0.93	0.14	48,48,48,48	0
54	MG	2A	3241	1/1	0.93	0.19	54,54,54,54	0
54	MG	1A	3826	1/1	0.93	0.18	35,35,35,35	0
54	MG	2A	3710	1/1	0.93	0.09	63,63,63,63	0
54	MG	1A	3064	1/1	0.93	0.27	43,43,43,43	0
54	MG	2A	3712	1/1	0.93	0.12	61,61,61,61	0
54	MG	2A	3458	1/1	0.93	0.17	64,64,64,64	0
54	MG	2a	3183	1/1	0.93	0.11	70,70,70,70	0
54	MG	1A	3355	1/1	0.93	0.07	38,38,38,38	0
54	MG	1A	3251	1/1	0.93	0.28	76,76,76,76	0
54	MG	1A	3254	1/1	0.93	0.09	76,76,76,76	0
54	MG	2A	3463	1/1	0.93	0.11	56,56,56,56	0
54	MG	1A	3360	1/1	0.93	0.07	26,26,26,26	0
54	MG	1A	3720	1/1	0.93	0.25	43,43,43,43	0
54	MG	1A	3632	1/1	0.93	0.11	50,50,50,50	0
54	MG	2A	3467	1/1	0.93	0.11	34,34,34,34	0
54	MG	2A	3255	1/1	0.93	0.15	51,51,51,51	0
54	MG	2A	3259	1/1	0.93	0.10	49,49,49,49	0
54	MG	2A	3260	1/1	0.93	0.10	31,31,31,31	0
54	MG	2A	3044	1/1	0.93	0.20	65,65,65,65	0
54	MG	2A	3473	1/1	0.93	0.20	66,66,66,66	0
54	MG	2A	3264	1/1	0.93	0.24	73,73,73,73	0
54	MG	2A	3734	1/1	0.93	0.11	51,51,51,51	0
54	MG	1A	3724	1/1	0.93	0.12	54,54,54,54	0
54	MG	1A	3634	1/1	0.93	0.09	35,35,35,35	0
54	MG	1D	303	1/1	0.93	0.10	41,41,41,41	0
54	MG	2A	3738	1/1	0.93	0.12	81,81,81,81	0
54	MG	2A	3740	1/1	0.93	0.14	69,69,69,69	0
54	MG	1A	3197	1/1	0.93	0.10	56,56,56,56	0
54	MG	1A	3120	1/1	0.93	0.20	52,52,52,52	0
54	MG	2A	3055	1/1	0.93	0.12	43,43,43,43	0
54	MG	2B	203	1/1	0.93	0.22	70,70,70,70	0
54	MG	2A	3274	1/1	0.93	0.07	43,43,43,43	0
54	MG	1A	3970	1/1	0.93	0.10	70,70,70,70	0
54	MG	1A	3253	1/1	0.94	0.09	46,46,46,46	0
54	MG	1H	201	1/1	0.94	0.16	66,66,66,66	0
54	MG	1H	203	1/1	0.94	0.11	66,66,66,66	0
54	MG	1A	3589	1/1	0.94	0.17	69,69,69,69	0
54	MG	1A	3492	1/1	0.94	0.08	24,24,24,24	0
54	MG	1A	3047	1/1	0.94	0.32	48,48,48,48	0
54	MG	2A	3197	1/1	0.94	0.11	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	3402	1/1	0.94	0.12	29,29,29,29	0
54	MG	1A	3836	1/1	0.94	0.07	53,53,53,53	0
54	MG	1A	3048	1/1	0.94	0.24	47,47,47,47	0
54	MG	1A	3327	1/1	0.94	0.10	56,56,56,56	0
54	MG	1a	1714	1/1	0.94	0.14	73,73,73,73	0
54	MG	1A	3406	1/1	0.94	0.08	28,28,28,28	0
54	MG	1A	3711	1/1	0.94	0.07	39,39,39,39	0
54	MG	1d	301	1/1	0.94	0.26	75,75,75,75	0
54	MG	1R	204	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	3712	1/1	0.94	0.10	66,66,66,66	0
54	MG	1A	3846	1/1	0.94	0.09	55,55,55,55	0
54	MG	2A	3739	1/1	0.94	0.15	60,60,60,60	0
54	MG	2A	3459	1/1	0.94	0.09	73,73,73,73	0
54	MG	1T	205	1/1	0.94	0.10	62,62,62,62	0
54	MG	1U	201	1/1	0.94	0.15	41,41,41,41	0
54	MG	1A	3503	1/1	0.94	0.10	43,43,43,43	0
54	MG	1a	1728	1/1	0.94	0.11	56,56,56,56	0
54	MG	1V	204	1/1	0.94	0.14	54,54,54,54	0
54	MG	1V	205	1/1	0.94	0.12	63,63,63,63	0
54	MG	1A	3258	1/1	0.94	0.18	38,38,38,38	0
54	MG	1A	3602	1/1	0.94	0.09	53,53,53,53	0
54	MG	1m	201	1/1	0.94	0.07	79,79,79,79	0
54	MG	2A	3469	1/1	0.94	0.08	64,64,64,64	0
54	MG	2A	3226	1/1	0.94	0.24	57,57,57,57	0
54	MG	1A	3259	1/1	0.94	0.15	45,45,45,45	0
54	MG	1A	3506	1/1	0.94	0.10	53,53,53,53	0
54	MG	1n	103	1/1	0.94	0.20	73,73,73,73	0
54	MG	1A	3123	1/1	0.94	0.05	35,35,35,35	0
54	MG	2A	3476	1/1	0.94	0.10	61,61,61,61	0
54	MG	1A	3857	1/1	0.94	0.07	62,62,62,62	0
54	MG	2A	3478	1/1	0.94	0.14	34,34,34,34	0
54	MG	2D	306	1/1	0.94	0.15	47,47,47,47	0
54	MG	1A	3075	1/1	0.94	0.21	45,45,45,45	0
54	MG	1A	3607	1/1	0.94	0.08	49,49,49,49	0
54	MG	1A	3190	1/1	0.94	0.28	72,72,72,72	0
54	MG	2D	311	1/1	0.94	0.10	65,65,65,65	0
54	MG	2D	312	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3420	1/1	0.94	0.10	29,29,29,29	0
54	MG	2E	302	1/1	0.94	0.23	52,52,52,52	0
54	MG	1A	3731	1/1	0.94	0.08	36,36,36,36	0
54	MG	1A	3076	1/1	0.94	0.19	44,44,44,44	0
54	MG	13	104	1/1	0.94	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3008	1/1	0.94	0.10	53,53,53,53	0
54	MG	2A	3247	1/1	0.94	0.07	60,60,60,60	0
54	MG	2A	3009	1/1	0.94	0.15	56,56,56,56	0
54	MG	1a	1748	1/1	0.94	0.14	67,67,67,67	0
54	MG	1A	3613	1/1	0.94	0.22	40,40,40,40	0
54	MG	1A	3869	1/1	0.94	0.09	39,39,39,39	0
54	MG	2A	3254	1/1	0.94	0.18	46,46,46,46	0
54	MG	2A	3496	1/1	0.94	0.10	72,72,72,72	0
54	MG	2R	202	1/1	0.94	0.12	46,46,46,46	0
54	MG	1A	3422	1/1	0.94	0.11	62,62,62,62	0
54	MG	2A	3256	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3871	1/1	0.94	0.09	46,46,46,46	0
54	MG	2A	3500	1/1	0.94	0.10	61,61,61,61	0
54	MG	1a	1753	1/1	0.94	0.14	59,59,59,59	0
54	MG	2A	3022	1/1	0.94	0.18	51,51,51,51	0
54	MG	2A	3262	1/1	0.94	0.34	52,52,52,52	0
54	MG	1A	3513	1/1	0.94	0.07	23,23,23,23	0
54	MG	2A	3505	1/1	0.94	0.11	64,64,64,64	0
54	MG	1A	3617	1/1	0.94	0.12	48,48,48,48	0
54	MG	2A	3026	1/1	0.94	0.09	58,58,58,58	0
54	MG	27	101	1/1	0.94	0.28	45,45,45,45	0
54	MG	17	103	1/1	0.94	0.29	41,41,41,41	0
54	MG	1a	1757	1/1	0.94	0.19	56,56,56,56	0
54	MG	1a	1758	1/1	0.94	0.18	66,66,66,66	0
54	MG	2A	3512	1/1	0.94	0.21	45,45,45,45	0
54	MG	1A	3745	1/1	0.94	0.10	42,42,42,42	0
54	MG	2a	3005	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3618	1/1	0.94	0.16	36,36,36,36	0
54	MG	18	102	1/1	0.94	0.12	45,45,45,45	0
54	MG	1a	1762	1/1	0.94	0.06	57,57,57,57	0
54	MG	2a	3012	1/1	0.94	0.14	68,68,68,68	0
54	MG	18	103	1/1	0.94	0.21	42,42,42,42	0
54	MG	1A	3876	1/1	0.94	0.07	29,29,29,29	0
54	MG	2a	3018	1/1	0.94	0.09	57,57,57,57	0
54	MG	2A	3279	1/1	0.94	0.07	32,32,32,32	0
54	MG	2A	3039	1/1	0.94	0.16	57,57,57,57	0
54	MG	2A	3041	1/1	0.94	0.06	34,34,34,34	0
54	MG	2A	3283	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3284	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	4019	1/1	0.94	0.15	39,39,39,39	0
54	MG	1A	3337	1/1	0.94	0.10	18,18,18,18	0
54	MG	2A	3529	1/1	0.94	0.08	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	3194	1/1	0.94	0.09	54,54,54,54	0
54	MG	2A	3531	1/1	0.94	0.11	32,32,32,32	0
54	MG	2A	3532	1/1	0.94	0.07	54,54,54,54	0
54	MG	1a	1604	1/1	0.94	0.24	76,76,76,76	0
54	MG	1A	3079	1/1	0.94	0.31	45,45,45,45	0
54	MG	2A	3536	1/1	0.94	0.07	65,65,65,65	0
54	MG	2A	3291	1/1	0.94	0.09	50,50,50,50	0
54	MG	2A	3293	1/1	0.94	0.06	39,39,39,39	0
54	MG	2A	3047	1/1	0.94	0.08	59,59,59,59	0
54	MG	2A	3048	1/1	0.94	0.13	55,55,55,55	0
54	MG	2A	3050	1/1	0.94	0.09	42,42,42,42	0
54	MG	2A	3544	1/1	0.94	0.14	60,60,60,60	0
54	MG	1a	1607	1/1	0.94	0.09	67,67,67,67	0
54	MG	1a	1608	1/1	0.94	0.09	67,67,67,67	0
54	MG	1A	3883	1/1	0.94	0.08	28,28,28,28	0
54	MG	1a	1773	1/1	0.94	0.12	74,74,74,74	0
54	MG	2A	3550	1/1	0.94	0.12	55,55,55,55	0
54	MG	1A	4025	1/1	0.94	0.10	55,55,55,55	0
54	MG	2A	3305	1/1	0.94	0.12	69,69,69,69	0
54	MG	2A	3306	1/1	0.94	0.21	60,60,60,60	0
54	MG	1A	3052	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	3054	1/1	0.94	0.16	58,58,58,58	0
54	MG	2a	3053	1/1	0.94	0.17	64,64,64,64	0
54	MG	1A	3058	1/1	0.94	0.10	45,45,45,45	0
54	MG	2A	3062	1/1	0.94	0.12	61,61,61,61	0
54	MG	2A	3559	1/1	0.94	0.10	62,62,62,62	0
54	MG	2A	3063	1/1	0.94	0.09	48,48,48,48	0
54	MG	1a	1617	1/1	0.94	0.12	67,67,67,67	0
54	MG	2A	3314	1/1	0.94	0.07	49,49,49,49	0
54	MG	2A	3065	1/1	0.94	0.11	51,51,51,51	0
54	MG	1A	3059	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3568	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3318	1/1	0.94	0.09	40,40,40,40	0
54	MG	1A	3523	1/1	0.94	0.07	24,24,24,24	0
54	MG	1A	3631	1/1	0.94	0.10	59,59,59,59	0
54	MG	2a	3067	1/1	0.94	0.19	66,66,66,66	0
54	MG	2a	3068	1/1	0.94	0.15	72,72,72,72	0
54	MG	2A	3575	1/1	0.94	0.07	55,55,55,55	0
54	MG	1a	1623	1/1	0.94	0.20	58,58,58,58	0
54	MG	2A	3322	1/1	0.94	0.09	55,55,55,55	0
54	MG	2A	3578	1/1	0.94	0.06	50,50,50,50	0
54	MG	2A	3326	1/1	0.94	0.18	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3075	1/1	0.94	0.12	58,58,58,58	0
54	MG	2A	3076	1/1	0.94	0.10	54,54,54,54	0
54	MG	1A	3430	1/1	0.94	0.09	29,29,29,29	0
54	MG	2A	3080	1/1	0.94	0.17	68,68,68,68	0
54	MG	1A	3432	1/1	0.94	0.07	18,18,18,18	0
54	MG	1A	3433	1/1	0.94	0.08	40,40,40,40	0
54	MG	2A	3336	1/1	0.94	0.08	49,49,49,49	0
54	MG	2A	3337	1/1	0.94	0.21	67,67,67,67	0
54	MG	2A	3596	1/1	0.94	0.08	49,49,49,49	0
54	MG	1A	3351	1/1	0.94	0.09	52,52,52,52	0
54	MG	2A	3340	1/1	0.94	0.18	79,79,79,79	0
54	MG	1A	3095	1/1	0.94	0.11	51,51,51,51	0
54	MG	2a	3091	1/1	0.94	0.25	69,69,69,69	0
54	MG	2A	3087	1/1	0.94	0.11	49,49,49,49	0
54	MG	1A	3277	1/1	0.94	0.33	36,36,36,36	0
54	MG	1A	3148	1/1	0.94	0.10	51,51,51,51	0
54	MG	1A	3096	1/1	0.94	0.24	49,49,49,49	0
54	MG	1A	3035	1/1	0.94	0.12	53,53,53,53	0
54	MG	1A	3443	1/1	0.94	0.17	62,62,62,62	0
54	MG	1A	3544	1/1	0.94	0.06	24,24,24,24	0
54	MG	1A	3911	1/1	0.94	0.06	39,39,39,39	0
54	MG	2a	3100	1/1	0.94	0.12	60,60,60,60	0
54	MG	2A	3097	1/1	0.94	0.19	54,54,54,54	0
54	MG	1A	3777	1/1	0.94	0.07	38,38,38,38	0
54	MG	1A	3030	1/1	0.94	0.05	35,35,35,35	0
54	MG	1A	3022	1/1	0.94	0.08	45,45,45,45	0
54	MG	2a	3108	1/1	0.94	0.16	71,71,71,71	0
54	MG	1A	3549	1/1	0.94	0.12	51,51,51,51	0
54	MG	1A	3103	1/1	0.94	0.10	45,45,45,45	0
54	MG	2A	3108	1/1	0.94	0.06	57,57,57,57	0
54	MG	1A	3365	1/1	0.94	0.07	24,24,24,24	0
54	MG	1a	1806	1/1	0.94	0.10	74,74,74,74	0
54	MG	2a	3114	1/1	0.94	0.10	79,79,79,79	0
54	MG	1A	3221	1/1	0.94	0.23	41,41,41,41	0
54	MG	1B	204	1/1	0.94	0.08	52,52,52,52	0
54	MG	1A	3787	1/1	0.94	0.11	50,50,50,50	0
54	MG	2A	3115	1/1	0.94	0.15	56,56,56,56	0
54	MG	2A	3627	1/1	0.94	0.08	71,71,71,71	0
54	MG	1A	3230	1/1	0.94	0.34	47,47,47,47	0
54	MG	1A	3294	1/1	0.94	0.16	57,57,57,57	0
54	MG	1A	3105	1/1	0.94	0.10	70,70,70,70	0
54	MG	1A	3937	1/1	0.94	0.12	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	1815	1/1	0.94	0.15	67,67,67,67	0
54	MG	1a	1816	1/1	0.94	0.16	65,65,65,65	0
54	MG	1A	3657	1/1	0.94	0.20	56,56,56,56	0
54	MG	2A	3127	1/1	0.94	0.11	65,65,65,65	0
54	MG	1A	3170	1/1	0.94	0.20	54,54,54,54	0
54	MG	1A	3109	1/1	0.94	0.20	38,38,38,38	0
54	MG	2A	3136	1/1	0.94	0.15	62,62,62,62	0
54	MG	1A	3372	1/1	0.94	0.08	34,34,34,34	0
54	MG	2A	3644	1/1	0.94	0.09	62,62,62,62	0
54	MG	1A	3944	1/1	0.94	0.07	64,64,64,64	0
54	MG	2A	3386	1/1	0.94	0.10	40,40,40,40	0
54	MG	2A	3648	1/1	0.94	0.08	65,65,65,65	0
54	MG	1A	3066	1/1	0.94	0.19	39,39,39,39	0
54	MG	1A	3669	1/1	0.94	0.13	65,65,65,65	0
54	MG	2A	3389	1/1	0.94	0.11	40,40,40,40	0
54	MG	2A	3390	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3655	1/1	0.94	0.09	49,49,49,49	0
54	MG	1a	1670	1/1	0.94	0.10	69,69,69,69	0
54	MG	1B	222	1/1	0.94	0.09	58,58,58,58	0
54	MG	2A	3149	1/1	0.94	0.09	40,40,40,40	0
54	MG	1A	3238	1/1	0.94	0.31	42,42,42,42	0
54	MG	2A	3661	1/1	0.94	0.08	80,80,80,80	0
54	MG	1a	1673	1/1	0.94	0.17	63,63,63,63	0
54	MG	2A	3664	1/1	0.94	0.07	62,62,62,62	0
54	MG	1A	3800	1/1	0.94	0.07	82,82,82,82	0
54	MG	2a	3165	1/1	0.94	0.12	79,79,79,79	0
54	MG	2a	3166	1/1	0.94	0.15	68,68,68,68	0
54	MG	2a	3169	1/1	0.94	0.09	73,73,73,73	0
54	MG	1A	3564	1/1	0.94	0.08	44,44,44,44	0
54	MG	1A	3672	1/1	0.94	0.08	50,50,50,50	0
54	MG	2A	3155	1/1	0.94	0.12	67,67,67,67	0
54	MG	1A	3377	1/1	0.94	0.07	32,32,32,32	0
54	MG	2A	3159	1/1	0.94	0.15	71,71,71,71	0
54	MG	2a	3178	1/1	0.94	0.11	58,58,58,58	0
54	MG	1A	3113	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3179	1/1	0.94	0.16	40,40,40,40	0
54	MG	1A	3118	1/1	0.94	0.11	41,41,41,41	0
54	MG	1A	3809	1/1	0.94	0.11	61,61,61,61	0
54	MG	1A	3381	1/1	0.94	0.10	41,41,41,41	0
54	MG	1A	3312	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3168	1/1	0.94	0.08	51,51,51,51	0
54	MG	2a	3187	1/1	0.94	0.19	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	3188	1/1	0.94	0.20	65,65,65,65	0
54	MG	1A	3475	1/1	0.94	0.12	51,51,51,51	0
54	MG	2A	3171	1/1	0.94	0.08	51,51,51,51	0
54	MG	2A	3413	1/1	0.94	0.26	59,59,59,59	0
54	MG	1A	3384	1/1	0.94	0.14	53,53,53,53	0
54	MG	2A	3173	1/1	0.94	0.11	62,62,62,62	0
54	MG	1A	3815	1/1	0.94	0.11	42,42,42,42	0
54	MG	1A	3313	1/1	0.94	0.17	52,52,52,52	0
54	MG	2A	3418	1/1	0.94	0.06	31,31,31,31	0
54	MG	2f	201	1/1	0.94	0.10	56,56,56,56	0
54	MG	1A	3249	1/1	0.94	0.18	56,56,56,56	0
54	MG	1A	3316	1/1	0.94	0.22	53,53,53,53	0
54	MG	1A	3045	1/1	0.94	0.24	56,56,56,56	0
54	MG	2A	3425	1/1	0.94	0.13	70,70,70,70	0
54	MG	2A	3179	1/1	0.94	0.11	52,52,52,52	0
54	MG	2A	3428	1/1	0.94	0.14	62,62,62,62	0
54	MG	1a	1693	1/1	0.94	0.22	68,68,68,68	0
55	CPF	1A	4056	24/24	0.94	0.13	34,46,55,61	0
55	CPF	2A	3741	24/24	0.94	0.12	39,44,56,58	0
54	MG	1A	3391	1/1	0.94	0.07	30,30,30,30	0
54	MG	2A	3184	1/1	0.94	0.17	66,66,66,66	0
54	MG	1A	3825	1/1	0.94	0.34	45,45,45,45	0
54	MG	1A	3318	1/1	0.94	0.08	30,30,30,30	0
54	MG	1A	3827	1/1	0.94	0.12	59,59,59,59	0
54	MG	1F	317	1/1	0.94	0.11	43,43,43,43	0
54	MG	1A	3183	1/1	0.94	0.18	34,34,34,34	0
54	MG	1A	3395	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3717	1/1	0.94	0.11	64,64,64,64	0
54	MG	1A	3921	1/1	0.95	0.24	44,44,44,44	0
54	MG	2V	201	1/1	0.95	0.13	60,60,60,60	0
54	MG	1A	3612	1/1	0.95	0.10	62,62,62,62	0
54	MG	1A	4039	1/1	0.95	0.17	63,63,63,63	0
54	MG	1A	3128	1/1	0.95	0.06	44,44,44,44	0
54	MG	2A	3571	1/1	0.95	0.09	53,53,53,53	0
54	MG	20	101	1/1	0.95	0.13	65,65,65,65	0
54	MG	2A	3183	1/1	0.95	0.10	61,61,61,61	0
54	MG	2A	3382	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	4041	1/1	0.95	0.31	45,45,45,45	0
54	MG	23	101	1/1	0.95	0.17	59,59,59,59	0
54	MG	1A	3180	1/1	0.95	0.07	57,57,57,57	0
54	MG	1A	3279	1/1	0.95	0.07	51,51,51,51	0
54	MG	28	101	1/1	0.95	0.10	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	3707	1/1	0.95	0.17	50,50,50,50	0
54	MG	1A	3393	1/1	0.95	0.07	44,44,44,44	0
54	MG	1A	4046	1/1	0.95	0.13	69,69,69,69	0
54	MG	1A	3339	1/1	0.95	0.12	37,37,37,37	0
54	MG	2A	3588	1/1	0.95	0.06	38,38,38,38	0
54	MG	1A	3056	1/1	0.95	0.18	36,36,36,36	0
54	MG	2a	3006	1/1	0.95	0.25	58,58,58,58	0
54	MG	2a	3007	1/1	0.95	0.09	71,71,71,71	0
54	MG	2A	3006	1/1	0.95	0.15	54,54,54,54	0
54	MG	1A	3816	1/1	0.95	0.09	53,53,53,53	0
54	MG	1A	4050	1/1	0.95	0.15	76,76,76,76	0
54	MG	1A	3396	1/1	0.95	0.07	24,24,24,24	0
54	MG	2A	3395	1/1	0.95	0.06	61,61,61,61	0
54	MG	2a	3015	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3818	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3942	1/1	0.95	0.06	48,48,48,48	0
54	MG	1A	3621	1/1	0.95	0.11	34,34,34,34	0
54	MG	2A	3199	1/1	0.95	0.06	53,53,53,53	0
54	MG	1A	4055	1/1	0.95	0.10	57,57,57,57	0
54	MG	2A	3603	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3072	1/1	0.95	0.27	32,32,32,32	0
54	MG	1a	1619	1/1	0.95	0.06	47,47,47,47	0
54	MG	1B	201	1/1	0.95	0.14	54,54,54,54	0
54	MG	2A	3607	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3002	1/1	0.95	0.11	53,53,53,53	0
54	MG	2A	3025	1/1	0.95	0.10	52,52,52,52	0
54	MG	1A	3547	1/1	0.95	0.08	41,41,41,41	0
54	MG	2A	3027	1/1	0.95	0.14	39,39,39,39	0
54	MG	1A	3401	1/1	0.95	0.11	26,26,26,26	0
54	MG	1a	1626	1/1	0.95	0.12	64,64,64,64	0
54	MG	1A	3140	1/1	0.95	0.18	41,41,41,41	0
54	MG	1a	1629	1/1	0.95	0.14	51,51,51,51	0
54	MG	1A	3629	1/1	0.95	0.15	60,60,60,60	0
54	MG	1A	3723	1/1	0.95	0.07	32,32,32,32	0
54	MG	1A	3032	1/1	0.95	0.21	51,51,51,51	0
54	MG	1A	3474	1/1	0.95	0.09	45,45,45,45	0
54	MG	1A	3954	1/1	0.95	0.05	31,31,31,31	0
54	MG	1A	3241	1/1	0.95	0.13	48,48,48,48	0
54	MG	2A	3224	1/1	0.95	0.12	56,56,56,56	0
54	MG	1A	3730	1/1	0.95	0.10	67,67,67,67	0
54	MG	1A	3957	1/1	0.95	0.10	55,55,55,55	0
54	MG	2a	3047	1/1	0.95	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	3023	1/1	0.95	0.11	30,30,30,30	0
54	MG	1B	219	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3477	1/1	0.95	0.14	52,52,52,52	0
54	MG	1A	3736	1/1	0.95	0.09	46,46,46,46	0
54	MG	1A	3291	1/1	0.95	0.15	36,36,36,36	0
54	MG	2A	3233	1/1	0.95	0.10	72,72,72,72	0
54	MG	2A	3634	1/1	0.95	0.07	62,62,62,62	0
54	MG	1a	1646	1/1	0.95	0.23	58,58,58,58	0
54	MG	1a	1647	1/1	0.95	0.15	51,51,51,51	0
54	MG	2A	3236	1/1	0.95	0.19	62,62,62,62	0
54	MG	1A	3077	1/1	0.95	0.21	35,35,35,35	0
54	MG	2A	3238	1/1	0.95	0.07	61,61,61,61	0
54	MG	1A	3410	1/1	0.95	0.10	32,32,32,32	0
54	MG	1B	227	1/1	0.95	0.06	61,61,61,61	0
54	MG	1A	3078	1/1	0.95	0.14	52,52,52,52	0
54	MG	1A	3843	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3640	1/1	0.95	0.23	48,48,48,48	0
54	MG	2A	3058	1/1	0.95	0.08	56,56,56,56	0
54	MG	2a	3066	1/1	0.95	0.09	63,63,63,63	0
54	MG	1A	3412	1/1	0.95	0.07	25,25,25,25	0
54	MG	2A	3060	1/1	0.95	0.14	44,44,44,44	0
54	MG	2A	3251	1/1	0.95	0.19	63,63,63,63	0
54	MG	1A	3356	1/1	0.95	0.07	27,27,27,27	0
54	MG	1A	3246	1/1	0.95	0.30	48,48,48,48	0
54	MG	1a	1803	1/1	0.95	0.07	50,50,50,50	0
54	MG	1A	3972	1/1	0.95	0.06	33,33,33,33	0
54	MG	2A	3659	1/1	0.95	0.07	34,34,34,34	0
54	MG	1A	3644	1/1	0.95	0.13	49,49,49,49	0
54	MG	2A	3258	1/1	0.95	0.35	44,44,44,44	0
54	MG	2A	3066	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	3751	1/1	0.95	0.06	32,32,32,32	0
54	MG	1A	3418	1/1	0.95	0.07	42,42,42,42	0
54	MG	2A	3667	1/1	0.95	0.07	62,62,62,62	0
54	MG	1D	317	1/1	0.95	0.09	52,52,52,52	0
54	MG	2A	3073	1/1	0.95	0.26	49,49,49,49	0
54	MG	1A	3247	1/1	0.95	0.10	42,42,42,42	0
54	MG	2A	3673	1/1	0.95	0.07	41,41,41,41	0
54	MG	2a	3089	1/1	0.95	0.05	60,60,60,60	0
54	MG	1A	3491	1/1	0.95	0.12	28,28,28,28	0
54	MG	1A	3248	1/1	0.95	0.12	45,45,45,45	0
54	MG	2A	3077	1/1	0.95	0.12	61,61,61,61	0
54	MG	2A	3271	1/1	0.95	0.06	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3078	1/1	0.95	0.07	53,53,53,53	0
54	MG	1a	1812	1/1	0.95	0.08	63,63,63,63	0
54	MG	1A	3192	1/1	0.95	0.22	45,45,45,45	0
54	MG	1A	3862	1/1	0.95	0.06	45,45,45,45	0
54	MG	1A	3363	1/1	0.95	0.13	63,63,63,63	0
54	MG	1A	3759	1/1	0.95	0.06	48,48,48,48	0
54	MG	1F	313	1/1	0.95	0.28	48,48,48,48	0
54	MG	2a	3101	1/1	0.95	0.09	66,66,66,66	0
54	MG	1A	3025	1/1	0.95	0.20	41,41,41,41	0
54	MG	2A	3088	1/1	0.95	0.24	57,57,57,57	0
54	MG	1A	3761	1/1	0.95	0.08	51,51,51,51	0
54	MG	2A	3689	1/1	0.95	0.08	59,59,59,59	0
54	MG	2A	3690	1/1	0.95	0.07	56,56,56,56	0
54	MG	1A	3081	1/1	0.95	0.51	47,47,47,47	0
54	MG	1A	3500	1/1	0.95	0.06	24,24,24,24	0
54	MG	1F	318	1/1	0.95	0.08	66,66,66,66	0
54	MG	1F	319	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	3020	1/1	0.95	0.31	41,41,41,41	0
54	MG	1A	3115	1/1	0.95	0.20	35,35,35,35	0
54	MG	1G	203	1/1	0.95	0.11	64,64,64,64	0
54	MG	1A	3660	1/1	0.95	0.23	53,53,53,53	0
54	MG	2A	3292	1/1	0.95	0.07	59,59,59,59	0
54	MG	1A	3992	1/1	0.95	0.06	19,19,19,19	0
54	MG	1A	3160	1/1	0.95	0.13	56,56,56,56	0
54	MG	2A	3295	1/1	0.95	0.10	44,44,44,44	0
54	MG	2A	3101	1/1	0.95	0.12	78,78,78,78	0
54	MG	1A	3769	1/1	0.95	0.06	29,29,29,29	0
54	MG	1A	3084	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3583	1/1	0.95	0.11	37,37,37,37	0
54	MG	2A	3714	1/1	0.95	0.12	65,65,65,65	0
54	MG	2a	3135	1/1	0.95	0.08	69,69,69,69	0
54	MG	1A	3666	1/1	0.95	0.08	48,48,48,48	0
54	MG	1P	205	1/1	0.95	0.08	74,74,74,74	0
54	MG	1A	3201	1/1	0.95	0.21	49,49,49,49	0
54	MG	1A	3087	1/1	0.95	0.17	39,39,39,39	0
54	MG	1a	1845	1/1	0.95	0.19	60,60,60,60	0
54	MG	1A	3204	1/1	0.95	0.19	50,50,50,50	0
54	MG	1A	3779	1/1	0.95	0.11	51,51,51,51	0
54	MG	2A	3117	1/1	0.95	0.09	44,44,44,44	0
54	MG	1Q	205	1/1	0.95	0.12	54,54,54,54	0
54	MG	2A	3120	1/1	0.95	0.18	53,53,53,53	0
54	MG	1A	3053	1/1	0.95	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3122	1/1	0.95	0.36	45,45,45,45	0
54	MG	1A	3887	1/1	0.95	0.06	68,68,68,68	0
54	MG	1a	1701	1/1	0.95	0.11	66,66,66,66	0
54	MG	1R	206	1/1	0.95	0.19	58,58,58,58	0
54	MG	1A	3166	1/1	0.95	0.09	41,41,41,41	0
54	MG	1a	1704	1/1	0.95	0.08	46,46,46,46	0
54	MG	2A	3128	1/1	0.95	0.24	62,62,62,62	0
54	MG	2A	3130	1/1	0.95	0.13	64,64,64,64	0
54	MG	2A	3516	1/1	0.95	0.12	67,67,67,67	0
54	MG	2A	3131	1/1	0.95	0.18	64,64,64,64	0
54	MG	1A	3321	1/1	0.95	0.14	55,55,55,55	0
54	MG	1A	3323	1/1	0.95	0.21	37,37,37,37	0
54	MG	1A	3324	1/1	0.95	0.08	33,33,33,33	0
54	MG	1U	203	1/1	0.95	0.34	40,40,40,40	0
54	MG	2a	3168	1/1	0.95	0.08	71,71,71,71	0
54	MG	1U	205	1/1	0.95	0.33	33,33,33,33	0
54	MG	2a	3170	1/1	0.95	0.11	68,68,68,68	0
54	MG	1U	206	1/1	0.95	0.23	43,43,43,43	0
54	MG	2A	3143	1/1	0.95	0.13	42,42,42,42	0
54	MG	2B	205	1/1	0.95	0.15	53,53,53,53	0
54	MG	2a	3175	1/1	0.95	0.10	75,75,75,75	0
54	MG	2A	3145	1/1	0.95	0.17	52,52,52,52	0
54	MG	1A	3067	1/1	0.95	0.08	53,53,53,53	0
54	MG	1V	203	1/1	0.95	0.14	44,44,44,44	0
54	MG	1A	3596	1/1	0.95	0.08	19,19,19,19	0
54	MG	1A	3894	1/1	0.95	0.12	38,38,38,38	0
54	MG	1A	3209	1/1	0.95	0.31	43,43,43,43	0
54	MG	2B	212	1/1	0.95	0.17	72,72,72,72	0
54	MG	1A	3171	1/1	0.95	0.20	36,36,36,36	0
54	MG	1W	203	1/1	0.95	0.17	35,35,35,35	0
54	MG	1A	3037	1/1	0.95	0.09	53,53,53,53	0
54	MG	1A	3903	1/1	0.95	0.06	42,42,42,42	0
54	MG	1A	3385	1/1	0.95	0.12	58,58,58,58	0
54	MG	2A	3156	1/1	0.95	0.20	46,46,46,46	0
54	MG	1A	3094	1/1	0.95	0.11	38,38,38,38	0
54	MG	2D	305	1/1	0.95	0.39	48,48,48,48	0
54	MG	1A	3521	1/1	0.95	0.06	64,64,64,64	0
54	MG	2D	307	1/1	0.95	0.25	51,51,51,51	0
54	MG	1A	3215	1/1	0.95	0.15	38,38,38,38	0
54	MG	2A	3355	1/1	0.95	0.09	53,53,53,53	0
54	MG	11	103	1/1	0.95	0.09	55,55,55,55	0
54	MG	2A	3359	1/1	0.95	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3388	1/1	0.95	0.07	31,31,31,31	0
54	MG	1A	3525	1/1	0.95	0.10	63,63,63,63	0
54	MG	2A	3164	1/1	0.95	0.12	55,55,55,55	0
54	MG	1A	4027	1/1	0.95	0.10	59,59,59,59	0
54	MG	1A	3527	1/1	0.95	0.10	60,60,60,60	0
54	MG	1A	4029	1/1	0.95	0.09	46,46,46,46	0
54	MG	2F	301	1/1	0.95	0.32	48,48,48,48	0
54	MG	1A	3453	1/1	0.95	0.11	55,55,55,55	0
54	MG	2A	3555	1/1	0.95	0.08	72,72,72,72	0
54	MG	1a	1739	1/1	0.95	0.12	66,66,66,66	0
54	MG	15	101	1/1	0.95	0.13	41,41,41,41	0
54	MG	1A	3696	1/1	0.95	0.08	56,56,56,56	0
54	MG	1A	3915	1/1	0.95	0.15	25,25,25,25	0
54	MG	1A	3126	1/1	0.95	0.13	40,40,40,40	0
54	MG	2A	3374	1/1	0.95	0.07	54,54,54,54	0
57	ARG	1B	230	12/12	0.95	0.10	37,56,63,63	0
54	MG	2A	3563	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3917	1/1	0.95	0.12	29,29,29,29	0
54	MG	1A	3457	1/1	0.95	0.09	64,64,64,64	0
54	MG	2A	3617	1/1	0.96	0.08	68,68,68,68	0
54	MG	1A	3780	1/1	0.96	0.12	48,48,48,48	0
54	MG	2A	3240	1/1	0.96	0.32	43,43,43,43	0
54	MG	1A	3024	1/1	0.96	0.15	26,26,26,26	0
54	MG	2A	3068	1/1	0.96	0.25	41,41,41,41	0
54	MG	1A	3358	1/1	0.96	0.09	34,34,34,34	0
54	MG	1A	3498	1/1	0.96	0.12	58,58,58,58	0
54	MG	1A	3499	1/1	0.96	0.10	51,51,51,51	0
54	MG	2A	3246	1/1	0.96	0.10	60,60,60,60	0
54	MG	1P	202	1/1	0.96	0.18	38,38,38,38	0
54	MG	1A	3674	1/1	0.96	0.17	48,48,48,48	0
54	MG	1A	3786	1/1	0.96	0.08	51,51,51,51	0
54	MG	1A	4013	1/1	0.96	0.08	47,47,47,47	0
54	MG	1A	3111	1/1	0.96	0.17	39,39,39,39	0
54	MG	1A	3086	1/1	0.96	0.06	49,49,49,49	0
54	MG	1A	3502	1/1	0.96	0.07	41,41,41,41	0
54	MG	1A	3361	1/1	0.96	0.09	50,50,50,50	0
54	MG	1A	3015	1/1	0.96	0.06	35,35,35,35	0
54	MG	2A	3084	1/1	0.96	0.08	42,42,42,42	0
54	MG	1a	1824	1/1	0.96	0.08	55,55,55,55	0
54	MG	1R	203	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3906	1/1	0.96	0.07	64,64,64,64	0
54	MG	1a	1685	1/1	0.96	0.15	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	1R	205	1/1	0.96	0.15	45,45,45,45	0
54	MG	1A	3295	1/1	0.96	0.11	41,41,41,41	0
54	MG	1A	3242	1/1	0.96	0.33	43,43,43,43	0
54	MG	1a	1832	1/1	0.96	0.06	75,75,75,75	0
54	MG	1T	203	1/1	0.96	0.15	65,65,65,65	0
54	MG	2A	3651	1/1	0.96	0.07	57,57,57,57	0
54	MG	1A	3017	1/1	0.96	0.18	34,34,34,34	0
54	MG	2A	3095	1/1	0.96	0.12	51,51,51,51	0
54	MG	1A	3191	1/1	0.96	0.19	38,38,38,38	0
54	MG	1A	3797	1/1	0.96	0.07	77,77,77,77	0
54	MG	1A	3152	1/1	0.96	0.22	33,33,33,33	0
54	MG	1A	3431	1/1	0.96	0.08	31,31,31,31	0
54	MG	1A	3304	1/1	0.96	0.22	39,39,39,39	0
54	MG	1a	1843	1/1	0.96	0.07	58,58,58,58	0
54	MG	2A	3102	1/1	0.96	0.11	56,56,56,56	0
54	MG	2A	3104	1/1	0.96	0.09	72,72,72,72	0
54	MG	2A	3105	1/1	0.96	0.18	55,55,55,55	0
54	MG	1A	3154	1/1	0.96	0.32	38,38,38,38	0
54	MG	1A	3306	1/1	0.96	0.14	24,24,24,24	0
54	MG	1A	4032	1/1	0.96	0.07	59,59,59,59	0
54	MG	1A	3155	1/1	0.96	0.18	42,42,42,42	0
54	MG	1A	3920	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3116	1/1	0.96	0.08	39,39,39,39	0
54	MG	1W	202	1/1	0.96	0.11	54,54,54,54	0
54	MG	1A	3922	1/1	0.96	0.07	52,52,52,52	0
54	MG	2A	3114	1/1	0.96	0.10	49,49,49,49	0
54	MG	1A	3117	1/1	0.96	0.11	41,41,41,41	0
54	MG	10	101	1/1	0.96	0.13	47,47,47,47	0
54	MG	1A	3439	1/1	0.96	0.10	56,56,56,56	0
54	MG	1A	3159	1/1	0.96	0.10	38,38,38,38	0
54	MG	2A	3119	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3198	1/1	0.96	0.19	45,45,45,45	0
54	MG	2A	3484	1/1	0.96	0.07	58,58,58,58	0
54	MG	1A	3933	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3038	1/1	0.96	0.16	49,49,49,49	0
54	MG	1A	3029	1/1	0.96	0.11	40,40,40,40	0
54	MG	1A	3446	1/1	0.96	0.07	58,58,58,58	0
54	MG	1A	3524	1/1	0.96	0.14	51,51,51,51	0
54	MG	13	101	1/1	0.96	0.15	36,36,36,36	0
54	MG	1A	3043	1/1	0.96	0.12	17,17,17,17	0
54	MG	1A	3526	1/1	0.96	0.11	27,27,27,27	0
54	MG	1A	3614	1/1	0.96	0.26	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1723	1/1	0.96	0.06	60,60,60,60	0
54	MG	1A	3819	1/1	0.96	0.09	48,48,48,48	0
54	MG	2a	3080	1/1	0.96	0.06	75,75,75,75	0
54	MG	1A	3256	1/1	0.96	0.08	44,44,44,44	0
54	MG	15	102	1/1	0.96	0.18	39,39,39,39	0
54	MG	2A	3699	1/1	0.96	0.06	66,66,66,66	0
54	MG	1A	3528	1/1	0.96	0.07	52,52,52,52	0
54	MG	2a	3087	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3530	1/1	0.96	0.28	31,31,31,31	0
54	MG	1A	3060	1/1	0.96	0.07	62,62,62,62	0
54	MG	2A	3704	1/1	0.96	0.11	60,60,60,60	0
54	MG	1A	3824	1/1	0.96	0.08	41,41,41,41	0
54	MG	2A	3144	1/1	0.96	0.14	54,54,54,54	0
54	MG	1A	3008	1/1	0.96	0.05	45,45,45,45	0
54	MG	2A	3708	1/1	0.96	0.06	74,74,74,74	0
54	MG	1A	3206	1/1	0.96	0.13	47,47,47,47	0
54	MG	2A	3324	1/1	0.96	0.09	35,35,35,35	0
54	MG	17	105	1/1	0.96	0.30	49,49,49,49	0
54	MG	1d	304	1/1	0.96	0.17	65,65,65,65	0
54	MG	2A	3713	1/1	0.96	0.06	69,69,69,69	0
54	MG	1A	3721	1/1	0.96	0.17	40,40,40,40	0
54	MG	1A	3535	1/1	0.96	0.07	56,56,56,56	0
54	MG	1A	3167	1/1	0.96	0.09	51,51,51,51	0
54	MG	2A	3331	1/1	0.96	0.08	37,37,37,37	0
54	MG	1A	3012	1/1	0.96	0.10	44,44,44,44	0
54	MG	2a	3106	1/1	0.96	0.06	66,66,66,66	0
54	MG	19	101	1/1	0.96	0.18	56,56,56,56	0
54	MG	2A	3334	1/1	0.96	0.09	37,37,37,37	0
54	MG	1g	203	1/1	0.96	0.09	66,66,66,66	0
54	MG	1A	3125	1/1	0.96	0.27	46,46,46,46	0
54	MG	1A	3100	1/1	0.96	0.34	38,38,38,38	0
54	MG	1A	3729	1/1	0.96	0.10	52,52,52,52	0
54	MG	2A	3726	1/1	0.96	0.06	61,61,61,61	0
54	MG	1k	201	1/1	0.96	0.10	46,46,46,46	0
54	MG	1B	208	1/1	0.96	0.06	45,45,45,45	0
54	MG	2a	3116	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3211	1/1	0.96	0.21	36,36,36,36	0
54	MG	1A	3005	1/1	0.96	0.10	29,29,29,29	0
54	MG	1a	1606	1/1	0.96	0.19	55,55,55,55	0
54	MG	1B	211	1/1	0.96	0.06	61,61,61,61	0
54	MG	2A	3733	1/1	0.96	0.08	64,64,64,64	0
54	MG	2A	3165	1/1	0.96	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3348	1/1	0.96	0.05	38,38,38,38	0
54	MG	1A	3542	1/1	0.96	0.27	35,35,35,35	0
54	MG	2a	3128	1/1	0.96	0.09	71,71,71,71	0
54	MG	1a	1609	1/1	0.96	0.06	60,60,60,60	0
54	MG	1A	3268	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3737	1/1	0.96	0.21	41,41,41,41	0
54	MG	1a	1613	1/1	0.96	0.11	31,31,31,31	0
54	MG	1A	3080	1/1	0.96	0.33	46,46,46,46	0
54	MG	1A	3633	1/1	0.96	0.08	34,34,34,34	0
54	MG	1A	3065	1/1	0.96	0.22	35,35,35,35	0
54	MG	1A	3136	1/1	0.96	0.06	41,41,41,41	0
54	MG	1A	3272	1/1	0.96	0.32	39,39,39,39	0
54	MG	2A	3005	1/1	0.96	0.10	59,59,59,59	0
54	MG	1A	3397	1/1	0.96	0.10	27,27,27,27	0
54	MG	2A	3007	1/1	0.96	0.06	42,42,42,42	0
54	MG	1A	3217	1/1	0.96	0.17	42,42,42,42	0
54	MG	1B	225	1/1	0.96	0.05	44,44,44,44	0
54	MG	1A	3852	1/1	0.96	0.12	43,43,43,43	0
54	MG	1A	3274	1/1	0.96	0.10	63,63,63,63	0
54	MG	1a	1625	1/1	0.96	0.12	55,55,55,55	0
54	MG	1A	3552	1/1	0.96	0.08	55,55,55,55	0
54	MG	1A	3750	1/1	0.96	0.10	46,46,46,46	0
54	MG	1A	3400	1/1	0.96	0.07	45,45,45,45	0
54	MG	1D	305	1/1	0.96	0.12	46,46,46,46	0
54	MG	1A	3752	1/1	0.96	0.09	39,39,39,39	0
54	MG	2D	301	1/1	0.96	0.20	48,48,48,48	0
54	MG	2a	3159	1/1	0.96	0.11	59,59,59,59	0
54	MG	2D	302	1/1	0.96	0.13	46,46,46,46	0
54	MG	1A	3275	1/1	0.96	0.08	33,33,33,33	0
54	MG	1A	3050	1/1	0.96	0.21	32,32,32,32	0
54	MG	1A	3222	1/1	0.96	0.29	42,42,42,42	0
54	MG	1a	1636	1/1	0.96	0.07	40,40,40,40	0
54	MG	2a	3167	1/1	0.96	0.06	51,51,51,51	0
54	MG	1A	3224	1/1	0.96	0.25	42,42,42,42	0
54	MG	2A	3030	1/1	0.96	0.14	33,33,33,33	0
54	MG	1A	3405	1/1	0.96	0.05	24,24,24,24	0
54	MG	2a	3171	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3345	1/1	0.96	0.11	50,50,50,50	0
54	MG	1A	3407	1/1	0.96	0.07	26,26,26,26	0
54	MG	1A	3482	1/1	0.96	0.05	26,26,26,26	0
54	MG	1A	3280	1/1	0.96	0.26	52,52,52,52	0
54	MG	1a	1643	1/1	0.96	0.19	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3225	1/1	0.96	0.13	59,59,59,59	0
54	MG	1E	305	1/1	0.96	0.11	27,27,27,27	0
54	MG	1A	3226	1/1	0.96	0.20	34,34,34,34	0
54	MG	1a	1786	1/1	0.96	0.17	60,60,60,60	0
54	MG	1A	3352	1/1	0.96	0.09	29,29,29,29	0
54	MG	1A	3568	1/1	0.96	0.06	52,52,52,52	0
54	MG	1F	304	1/1	0.96	0.12	34,34,34,34	0
54	MG	1F	308	1/1	0.96	0.18	31,31,31,31	0
54	MG	1F	310	1/1	0.96	0.20	54,54,54,54	0
54	MG	2A	3585	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3569	1/1	0.96	0.11	51,51,51,51	0
54	MG	1a	1793	1/1	0.96	0.06	74,74,74,74	0
54	MG	2a	3190	1/1	0.96	0.10	62,62,62,62	0
54	MG	2Q	203	1/1	0.96	0.10	61,61,61,61	0
54	MG	2A	3049	1/1	0.96	0.16	47,47,47,47	0
54	MG	2A	3217	1/1	0.96	0.08	51,51,51,51	0
54	MG	1A	3659	1/1	0.96	0.11	68,68,68,68	0
54	MG	2A	3594	1/1	0.96	0.10	58,58,58,58	0
54	MG	2A	3051	1/1	0.96	0.10	62,62,62,62	0
54	MG	1A	3106	1/1	0.96	0.19	34,34,34,34	0
54	MG	2W	201	1/1	0.96	0.27	49,49,49,49	0
54	MG	2A	3222	1/1	0.96	0.07	52,52,52,52	0
54	MG	2A	3223	1/1	0.96	0.27	40,40,40,40	0
54	MG	1A	3571	1/1	0.96	0.19	46,46,46,46	0
54	MG	1a	1797	1/1	0.96	0.10	56,56,56,56	0
54	MG	1a	1798	1/1	0.96	0.07	80,80,80,80	0
54	MG	1A	3663	1/1	0.96	0.07	29,29,29,29	0
54	MG	1A	3998	1/1	0.96	0.09	83,83,83,83	0
54	MG	1a	1661	1/1	0.96	0.12	72,72,72,72	0
54	MG	23	102	1/1	0.96	0.10	48,48,48,48	0
54	MG	1A	3999	1/1	0.96	0.09	62,62,62,62	0
54	MG	2A	3231	1/1	0.96	0.09	41,41,41,41	0
56	MPD	18	104	8/8	0.96	0.12	32,39,43,43	0
54	MG	1A	3413	1/1	0.96	0.06	42,42,42,42	0
54	MG	1A	3107	1/1	0.96	0.24	42,42,42,42	0
54	MG	1A	3285	1/1	0.96	0.10	64,64,64,64	0
54	MG	2A	3419	1/1	0.96	0.15	55,55,55,55	0
54	MG	1a	1666	1/1	0.96	0.10	63,63,63,63	0
54	MG	1A	3417	1/1	0.96	0.09	36,36,36,36	0
54	MG	1A	3184	1/1	0.96	0.18	46,46,46,46	0
54	MG	2A	3423	1/1	0.96	0.23	66,66,66,66	0
54	MG	2A	3139	1/1	0.97	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3140	1/1	0.97	0.17	54,54,54,54	0
54	MG	2a	3024	1/1	0.97	0.19	65,65,65,65	0
54	MG	2A	3296	1/1	0.97	0.10	39,39,39,39	0
54	MG	1N	201	1/1	0.97	0.11	46,46,46,46	0
54	MG	1N	202	1/1	0.97	0.10	42,42,42,42	0
54	MG	1A	3003	1/1	0.97	0.05	27,27,27,27	0
54	MG	2a	3029	1/1	0.97	0.08	40,40,40,40	0
54	MG	1A	3926	1/1	0.97	0.04	66,66,66,66	0
54	MG	1A	3928	1/1	0.97	0.07	56,56,56,56	0
54	MG	1P	201	1/1	0.97	0.25	38,38,38,38	0
54	MG	1A	3929	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3293	1/1	0.97	0.17	49,49,49,49	0
54	MG	2A	3004	1/1	0.97	0.07	45,45,45,45	0
54	MG	1P	204	1/1	0.97	0.17	52,52,52,52	0
54	MG	1A	3588	1/1	0.97	0.10	45,45,45,45	0
54	MG	1A	3743	1/1	0.97	0.10	53,53,53,53	0
54	MG	1Q	201	1/1	0.97	0.12	36,36,36,36	0
54	MG	2A	3665	1/1	0.97	0.09	66,66,66,66	0
54	MG	1A	3185	1/1	0.97	0.12	50,50,50,50	0
54	MG	2A	3312	1/1	0.97	0.14	44,44,44,44	0
54	MG	1A	3590	1/1	0.97	0.10	50,50,50,50	0
54	MG	2a	3044	1/1	0.97	0.21	60,60,60,60	0
54	MG	2A	3011	1/1	0.97	0.07	41,41,41,41	0
54	MG	1a	1658	1/1	0.97	0.08	72,72,72,72	0
54	MG	2A	3014	1/1	0.97	0.08	49,49,49,49	0
54	MG	2A	3317	1/1	0.97	0.10	53,53,53,53	0
54	MG	2A	3015	1/1	0.97	0.19	39,39,39,39	0
54	MG	1A	3830	1/1	0.97	0.08	36,36,36,36	0
54	MG	1A	3348	1/1	0.97	0.07	56,56,56,56	0
54	MG	1A	3592	1/1	0.97	0.11	54,54,54,54	0
54	MG	2A	3491	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3939	1/1	0.97	0.05	61,61,61,61	0
54	MG	2A	3323	1/1	0.97	0.10	36,36,36,36	0
54	MG	2A	3020	1/1	0.97	0.16	49,49,49,49	0
54	MG	2A	3021	1/1	0.97	0.07	43,43,43,43	0
54	MG	1A	3085	1/1	0.97	0.15	44,44,44,44	0
54	MG	1A	3296	1/1	0.97	0.11	33,33,33,33	0
54	MG	1A	3057	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3298	1/1	0.97	0.21	60,60,60,60	0
54	MG	1T	202	1/1	0.97	0.08	65,65,65,65	0
54	MG	1A	3127	1/1	0.97	0.29	40,40,40,40	0
54	MG	1A	3533	1/1	0.97	0.05	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3029	1/1	0.97	0.07	45,45,45,45	0
54	MG	1A	3046	1/1	0.97	0.18	42,42,42,42	0
54	MG	1A	3301	1/1	0.97	0.26	44,44,44,44	0
54	MG	2A	3506	1/1	0.97	0.08	62,62,62,62	0
54	MG	2A	3338	1/1	0.97	0.10	41,41,41,41	0
54	MG	1U	202	1/1	0.97	0.13	33,33,33,33	0
54	MG	1A	3948	1/1	0.97	0.11	62,62,62,62	0
54	MG	2A	3181	1/1	0.97	0.12	58,58,58,58	0
54	MG	1U	204	1/1	0.97	0.25	40,40,40,40	0
54	MG	1A	3841	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3257	1/1	0.97	0.22	39,39,39,39	0
54	MG	2A	3514	1/1	0.97	0.11	62,62,62,62	0
54	MG	1U	207	1/1	0.97	0.24	40,40,40,40	0
54	MG	1A	3844	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3218	1/1	0.97	0.06	43,43,43,43	0
54	MG	2A	3040	1/1	0.97	0.11	44,44,44,44	0
54	MG	2a	3082	1/1	0.97	0.06	80,80,80,80	0
54	MG	1A	3219	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3220	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3019	1/1	0.97	0.21	33,33,33,33	0
54	MG	1A	3132	1/1	0.97	0.07	51,51,51,51	0
54	MG	1A	3419	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3609	1/1	0.97	0.06	40,40,40,40	0
54	MG	1A	3680	1/1	0.97	0.11	57,57,57,57	0
54	MG	1A	3855	1/1	0.97	0.12	50,50,50,50	0
54	MG	2A	3719	1/1	0.97	0.09	66,66,66,66	0
54	MG	1A	3263	1/1	0.97	0.20	38,38,38,38	0
54	MG	10	103	1/1	0.97	0.13	52,52,52,52	0
54	MG	10	104	1/1	0.97	0.09	50,50,50,50	0
54	MG	1A	3311	1/1	0.97	0.17	55,55,55,55	0
54	MG	2A	3201	1/1	0.97	0.20	56,56,56,56	0
54	MG	1a	1692	1/1	0.97	0.11	66,66,66,66	0
54	MG	1a	1819	1/1	0.97	0.07	61,61,61,61	0
54	MG	1A	3223	1/1	0.97	0.16	41,41,41,41	0
54	MG	2A	3537	1/1	0.97	0.06	63,63,63,63	0
54	MG	1A	3016	1/1	0.97	0.26	38,38,38,38	0
54	MG	1A	3488	1/1	0.97	0.09	33,33,33,33	0
54	MG	11	102	1/1	0.97	0.07	59,59,59,59	0
54	MG	2a	3104	1/1	0.97	0.09	81,81,81,81	0
54	MG	2A	3541	1/1	0.97	0.07	64,64,64,64	0
54	MG	1A	3134	1/1	0.97	0.10	38,38,38,38	0
54	MG	2A	3373	1/1	0.97	0.06	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	3490	1/1	0.97	0.06	63,63,63,63	0
54	MG	1A	3776	1/1	0.97	0.05	45,45,45,45	0
54	MG	1A	3315	1/1	0.97	0.09	55,55,55,55	0
54	MG	1A	3971	1/1	0.97	0.12	45,45,45,45	0
54	MG	1A	3049	1/1	0.97	0.22	40,40,40,40	0
54	MG	2A	3214	1/1	0.97	0.07	49,49,49,49	0
54	MG	1a	1830	1/1	0.97	0.11	64,64,64,64	0
54	MG	1A	3493	1/1	0.97	0.07	40,40,40,40	0
54	MG	1A	3695	1/1	0.97	0.12	48,48,48,48	0
54	MG	1A	3228	1/1	0.97	0.28	44,44,44,44	0
54	MG	2A	3219	1/1	0.97	0.07	51,51,51,51	0
54	MG	2A	3069	1/1	0.97	0.10	55,55,55,55	0
54	MG	1A	3697	1/1	0.97	0.05	61,61,61,61	0
54	MG	1a	1707	1/1	0.97	0.08	45,45,45,45	0
54	MG	15	103	1/1	0.97	0.30	43,43,43,43	0
54	MG	1A	3698	1/1	0.97	0.19	50,50,50,50	0
54	MG	1A	3556	1/1	0.97	0.09	64,64,64,64	0
54	MG	1a	1839	1/1	0.97	0.09	55,55,55,55	0
54	MG	1a	1840	1/1	0.97	0.05	64,64,64,64	0
54	MG	2a	3132	1/1	0.97	0.08	52,52,52,52	0
54	MG	1A	3229	1/1	0.97	0.23	40,40,40,40	0
54	MG	2A	3566	1/1	0.97	0.10	59,59,59,59	0
54	MG	1A	3137	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3168	1/1	0.97	0.09	33,33,33,33	0
54	MG	1A	3233	1/1	0.97	0.27	38,38,38,38	0
54	MG	2B	218	1/1	0.97	0.07	55,55,55,55	0
54	MG	2a	3140	1/1	0.97	0.07	72,72,72,72	0
54	MG	2A	3082	1/1	0.97	0.50	49,49,49,49	0
54	MG	2A	3398	1/1	0.97	0.17	66,66,66,66	0
54	MG	17	104	1/1	0.97	0.11	38,38,38,38	0
54	MG	1A	3322	1/1	0.97	0.08	44,44,44,44	0
54	MG	1A	3705	1/1	0.97	0.12	43,43,43,43	0
54	MG	1A	3706	1/1	0.97	0.09	53,53,53,53	0
54	MG	1A	3885	1/1	0.97	0.06	44,44,44,44	0
54	MG	1D	301	1/1	0.97	0.29	44,44,44,44	0
54	MG	2A	3239	1/1	0.97	0.48	46,46,46,46	0
54	MG	2a	3150	1/1	0.97	0.06	78,78,78,78	0
54	MG	1A	3062	1/1	0.97	0.12	44,44,44,44	0
54	MG	2a	3152	1/1	0.97	0.10	57,57,57,57	0
54	MG	1a	1854	1/1	0.97	0.06	62,62,62,62	0
54	MG	1A	3031	1/1	0.97	0.08	22,22,22,22	0
54	MG	1A	3051	1/1	0.97	0.33	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	3382	1/1	0.97	0.06	50,50,50,50	0
54	MG	2E	303	1/1	0.97	0.09	47,47,47,47	0
54	MG	1A	3276	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3097	1/1	0.97	0.19	36,36,36,36	0
54	MG	2E	306	1/1	0.97	0.10	32,32,32,32	0
54	MG	1A	3714	1/1	0.97	0.04	39,39,39,39	0
54	MG	2a	3163	1/1	0.97	0.05	71,71,71,71	0
54	MG	2A	3248	1/1	0.97	0.11	57,57,57,57	0
54	MG	2F	302	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3239	1/1	0.97	0.19	37,37,37,37	0
54	MG	2F	304	1/1	0.97	0.17	46,46,46,46	0
54	MG	1A	3240	1/1	0.97	0.17	64,64,64,64	0
54	MG	1A	3802	1/1	0.97	0.10	29,29,29,29	0
54	MG	1A	3717	1/1	0.97	0.07	48,48,48,48	0
54	MG	1E	302	1/1	0.97	0.09	41,41,41,41	0
54	MG	1A	3176	1/1	0.97	0.28	46,46,46,46	0
54	MG	1A	3203	1/1	0.97	0.17	40,40,40,40	0
54	MG	2Q	201	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3177	1/1	0.97	0.24	53,53,53,53	0
54	MG	1A	3807	1/1	0.97	0.04	57,57,57,57	0
54	MG	2A	3424	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3333	1/1	0.97	0.14	52,52,52,52	0
54	MG	1A	3334	1/1	0.97	0.05	28,28,28,28	0
54	MG	2T	202	1/1	0.97	0.19	68,68,68,68	0
54	MG	2A	3427	1/1	0.97	0.11	37,37,37,37	0
54	MG	2A	3609	1/1	0.97	0.14	62,62,62,62	0
54	MG	1F	303	1/1	0.97	0.16	34,34,34,34	0
54	MG	1A	3021	1/1	0.97	0.09	41,41,41,41	0
54	MG	2A	3263	1/1	0.97	0.07	52,52,52,52	0
54	MG	2A	3431	1/1	0.97	0.05	52,52,52,52	0
54	MG	1a	1747	1/1	0.97	0.10	54,54,54,54	0
54	MG	2A	3265	1/1	0.97	0.06	32,32,32,32	0
54	MG	1F	306	1/1	0.97	0.17	38,38,38,38	0
54	MG	2A	3267	1/1	0.97	0.08	52,52,52,52	0
54	MG	1F	307	1/1	0.97	0.06	37,37,37,37	0
54	MG	1a	1622	1/1	0.97	0.04	48,48,48,48	0
54	MG	1A	3336	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3099	1/1	0.97	0.21	36,36,36,36	0
54	MG	1A	3726	1/1	0.97	0.07	52,52,52,52	0
54	MG	1e	201	1/1	0.97	0.08	59,59,59,59	0
54	MG	1e	202	1/1	0.97	0.07	68,68,68,68	0
54	MG	1A	4010	1/1	0.97	0.04	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3626	1/1	0.97	0.04	60,60,60,60	0
54	MG	2k	201	1/1	0.97	0.09	57,57,57,57	0
54	MG	1a	1627	1/1	0.97	0.06	52,52,52,52	0
54	MG	1A	3814	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	3041	1/1	0.97	0.05	23,23,23,23	0
54	MG	1A	3287	1/1	0.97	0.10	18,18,18,18	0
54	MG	1A	3341	1/1	0.97	0.10	34,34,34,34	0
54	MG	1A	3582	1/1	0.97	0.09	28,28,28,28	0
54	MG	1a	1633	1/1	0.97	0.09	47,47,47,47	0
54	MG	1A	3734	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3026	1/1	0.97	0.18	32,32,32,32	0
54	MG	2a	3013	1/1	0.97	0.19	54,54,54,54	0
54	MG	1A	4018	1/1	0.97	0.07	50,50,50,50	0
54	MG	1A	3151	1/1	0.97	0.07	41,41,41,41	0
54	MG	2A	3133	1/1	0.97	0.06	51,51,51,51	0
54	MG	2a	3017	1/1	0.97	0.06	58,58,58,58	0
54	MG	1A	3083	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3923	1/1	0.97	0.07	57,57,57,57	0
54	MG	1H	202	1/1	0.97	0.09	59,59,59,59	0
58	ZN	2Y	202	1/1	0.97	0.05	97,97,97,97	0
54	MG	1A	3652	1/1	0.97	0.05	39,39,39,39	0
58	ZN	2n	102	1/1	0.97	0.06	102,102,102,102	0
54	MG	1D	304	1/1	0.98	0.06	46,46,46,46	0
54	MG	1A	3252	1/1	0.98	0.17	31,31,31,31	0
54	MG	1D	306	1/1	0.98	0.08	17,17,17,17	0
54	MG	2a	3081	1/1	0.98	0.06	74,74,74,74	0
54	MG	1D	307	1/1	0.98	0.04	40,40,40,40	0
54	MG	1D	308	1/1	0.98	0.10	33,33,33,33	0
54	MG	1A	3661	1/1	0.98	0.06	31,31,31,31	0
54	MG	1D	310	1/1	0.98	0.22	29,29,29,29	0
54	MG	1A	3013	1/1	0.98	0.04	26,26,26,26	0
54	MG	1a	1862	1/1	0.98	0.05	65,65,65,65	0
54	MG	1A	3455	1/1	0.98	0.06	31,31,31,31	0
54	MG	1a	1864	1/1	0.98	0.06	62,62,62,62	0
54	MG	2A	3169	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3861	1/1	0.98	0.05	34,34,34,34	0
54	MG	1A	3042	1/1	0.98	0.19	29,29,29,29	0
54	MG	2A	3638	1/1	0.98	0.08	40,40,40,40	0
54	MG	1A	3114	1/1	0.98	0.12	33,33,33,33	0
54	MG	2A	3641	1/1	0.98	0.07	63,63,63,63	0
54	MG	1A	3727	1/1	0.98	0.04	71,71,71,71	0
54	MG	1A	3033	1/1	0.98	0.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3292	1/1	0.98	0.06	51,51,51,51	0
54	MG	1E	301	1/1	0.98	0.18	45,45,45,45	0
54	MG	2A	3646	1/1	0.98	0.11	59,59,59,59	0
54	MG	1A	4021	1/1	0.98	0.07	30,30,30,30	0
54	MG	1A	3668	1/1	0.98	0.04	47,47,47,47	0
54	MG	2A	3070	1/1	0.98	0.07	28,28,28,28	0
54	MG	2A	3650	1/1	0.98	0.09	57,57,57,57	0
54	MG	2A	3288	1/1	0.98	0.07	35,35,35,35	0
54	MG	1A	3135	1/1	0.98	0.14	26,26,26,26	0
54	MG	1A	3732	1/1	0.98	0.05	57,57,57,57	0
54	MG	1A	3162	1/1	0.98	0.23	42,42,42,42	0
54	MG	1A	3373	1/1	0.98	0.11	36,36,36,36	0
54	MG	1E	308	1/1	0.98	0.07	62,62,62,62	0
54	MG	1A	3514	1/1	0.98	0.07	27,27,27,27	0
54	MG	1d	302	1/1	0.98	0.16	65,65,65,65	0
54	MG	2R	201	1/1	0.98	0.19	49,49,49,49	0
54	MG	1F	301	1/1	0.98	0.13	39,39,39,39	0
54	MG	1A	3415	1/1	0.98	0.04	31,31,31,31	0
54	MG	1A	3055	1/1	0.98	0.09	51,51,51,51	0
54	MG	2A	3662	1/1	0.98	0.04	57,57,57,57	0
54	MG	1F	305	1/1	0.98	0.06	38,38,38,38	0
54	MG	1A	3375	1/1	0.98	0.09	48,48,48,48	0
54	MG	2V	202	1/1	0.98	0.12	44,44,44,44	0
54	MG	1A	3877	1/1	0.98	0.05	46,46,46,46	0
54	MG	2A	3534	1/1	0.98	0.04	69,69,69,69	0
54	MG	17	101	1/1	0.98	0.10	38,38,38,38	0
54	MG	2A	3668	1/1	0.98	0.04	44,44,44,44	0
54	MG	2X	101	1/1	0.98	0.07	58,58,58,58	0
54	MG	2a	3129	1/1	0.98	0.05	65,65,65,65	0
54	MG	2a	3130	1/1	0.98	0.06	70,70,70,70	0
54	MG	2A	3303	1/1	0.98	0.06	27,27,27,27	0
54	MG	17	102	1/1	0.98	0.12	43,43,43,43	0
54	MG	2a	3133	1/1	0.98	0.05	76,76,76,76	0
54	MG	2A	3671	1/1	0.98	0.07	64,64,64,64	0
54	MG	1A	3068	1/1	0.98	0.05	31,31,31,31	0
54	MG	1F	309	1/1	0.98	0.15	34,34,34,34	0
54	MG	1A	3227	1/1	0.98	0.11	29,29,29,29	0
54	MG	1F	311	1/1	0.98	0.06	37,37,37,37	0
54	MG	17	107	1/1	0.98	0.06	52,52,52,52	0
54	MG	1A	3881	1/1	0.98	0.05	42,42,42,42	0
54	MG	1A	3742	1/1	0.98	0.04	23,23,23,23	0
54	MG	1A	3165	1/1	0.98	0.06	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	3744	1/1	0.98	0.09	53,53,53,53	0
54	MG	1A	3138	1/1	0.98	0.17	39,39,39,39	0
54	MG	1A	3623	1/1	0.98	0.06	47,47,47,47	0
54	MG	2A	3549	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	3044	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3966	1/1	0.98	0.09	49,49,49,49	0
54	MG	1A	3573	1/1	0.98	0.06	48,48,48,48	0
54	MG	1A	3231	1/1	0.98	0.20	39,39,39,39	0
54	MG	2A	3435	1/1	0.98	0.05	59,59,59,59	0
54	MG	1A	3009	1/1	0.98	0.05	35,35,35,35	0
54	MG	2a	3011	1/1	0.98	0.08	49,49,49,49	0
54	MG	1A	3169	1/1	0.98	0.15	31,31,31,31	0
54	MG	2A	3103	1/1	0.98	0.06	30,30,30,30	0
54	MG	1A	3687	1/1	0.98	0.14	31,31,31,31	0
54	MG	1A	3234	1/1	0.98	0.12	31,31,31,31	0
54	MG	2A	3325	1/1	0.98	0.10	34,34,34,34	0
54	MG	2A	3697	1/1	0.98	0.05	68,68,68,68	0
54	MG	1a	1610	1/1	0.98	0.33	56,56,56,56	0
54	MG	2A	3562	1/1	0.98	0.05	62,62,62,62	0
54	MG	2a	3162	1/1	0.98	0.07	79,79,79,79	0
54	MG	1A	3141	1/1	0.98	0.15	37,37,37,37	0
54	MG	1A	3690	1/1	0.98	0.05	51,51,51,51	0
54	MG	1A	3307	1/1	0.98	0.21	40,40,40,40	0
54	MG	2A	3703	1/1	0.98	0.07	55,55,55,55	0
54	MG	1A	3897	1/1	0.98	0.03	32,32,32,32	0
54	MG	1N	204	1/1	0.98	0.04	55,55,55,55	0
54	MG	1A	3977	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3001	1/1	0.98	0.04	40,40,40,40	0
54	MG	1A	3143	1/1	0.98	0.05	40,40,40,40	0
54	MG	2A	3335	1/1	0.98	0.06	37,37,37,37	0
54	MG	2A	3572	1/1	0.98	0.08	41,41,41,41	0
54	MG	2A	3573	1/1	0.98	0.05	58,58,58,58	0
54	MG	1A	3028	1/1	0.98	0.28	33,33,33,33	0
54	MG	1A	3349	1/1	0.98	0.07	28,28,28,28	0
54	MG	2A	3454	1/1	0.98	0.04	47,47,47,47	0
54	MG	2A	3013	1/1	0.98	0.07	26,26,26,26	0
54	MG	1A	3350	1/1	0.98	0.04	37,37,37,37	0
54	MG	1A	3762	1/1	0.98	0.14	38,38,38,38	0
54	MG	1A	3174	1/1	0.98	0.12	36,36,36,36	0
54	MG	1a	1721	1/1	0.98	0.12	63,63,63,63	0
54	MG	2A	3583	1/1	0.98	0.06	71,71,71,71	0
54	MG	2a	3184	1/1	0.98	0.06	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	3175	1/1	0.98	0.17	36,36,36,36	0
54	MG	1A	3436	1/1	0.98	0.04	34,34,34,34	0
54	MG	2A	3586	1/1	0.98	0.08	73,73,73,73	0
54	MG	1A	3122	1/1	0.98	0.05	67,67,67,67	0
54	MG	1a	1725	1/1	0.98	0.05	62,62,62,62	0
54	MG	1A	3146	1/1	0.98	0.31	39,39,39,39	0
54	MG	1A	3007	1/1	0.98	0.09	43,43,43,43	0
54	MG	1R	201	1/1	0.98	0.08	42,42,42,42	0
54	MG	1A	3091	1/1	0.98	0.05	24,24,24,24	0
54	MG	1A	3149	1/1	0.98	0.17	50,50,50,50	0
54	MG	1A	3442	1/1	0.98	0.05	18,18,18,18	0
54	MG	1B	212	1/1	0.98	0.08	47,47,47,47	0
54	MG	1A	3004	1/1	0.98	0.06	41,41,41,41	0
54	MG	1A	3919	1/1	0.98	0.04	19,19,19,19	0
54	MG	2A	3358	1/1	0.98	0.07	42,42,42,42	0
54	MG	1A	3708	1/1	0.98	0.04	37,37,37,37	0
54	MG	1a	1736	1/1	0.98	0.06	67,67,67,67	0
54	MG	1A	3545	1/1	0.98	0.07	44,44,44,44	0
54	MG	1a	1738	1/1	0.98	0.05	56,56,56,56	0
54	MG	1A	3842	1/1	0.98	0.04	33,33,33,33	0
54	MG	1A	3108	1/1	0.98	0.07	42,42,42,42	0
54	MG	2A	3481	1/1	0.98	0.07	57,57,57,57	0
54	MG	1A	3597	1/1	0.98	0.07	52,52,52,52	0
54	MG	1A	3445	1/1	0.98	0.05	43,43,43,43	0
54	MG	1A	3018	1/1	0.98	0.15	28,28,28,28	0
54	MG	1A	3040	1/1	0.98	0.09	35,35,35,35	0
54	MG	1A	3129	1/1	0.98	0.15	35,35,35,35	0
54	MG	1A	3850	1/1	0.98	0.08	44,44,44,44	0
54	MG	1A	3655	1/1	0.98	0.06	39,39,39,39	0
54	MG	2A	3257	1/1	0.98	0.08	21,21,21,21	0
54	MG	1A	3156	1/1	0.98	0.14	39,39,39,39	0
54	MG	1V	202	1/1	0.98	0.15	35,35,35,35	0
54	MG	1A	3286	1/1	0.98	0.07	22,22,22,22	0
58	ZN	1Y	501	1/1	0.98	0.04	58,58,58,58	0
54	MG	1a	1651	1/1	0.98	0.07	46,46,46,46	0
58	ZN	15	109	1/1	0.98	0.04	61,61,61,61	0
54	MG	1A	3658	1/1	0.98	0.05	54,54,54,54	0
54	MG	1A	3553	1/1	0.98	0.17	59,59,59,59	0
58	ZN	26	501	1/1	0.98	0.03	67,67,67,67	0
58	ZN	29	501	1/1	0.98	0.04	76,76,76,76	0
54	MG	2A	3157	1/1	0.98	0.18	54,54,54,54	0
59	SF4	1d	306	8/8	0.98	0.05	60,71,79,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	SF4	2d	302	8/8	0.98	0.05	71,83,87,87	0
54	MG	2A	3135	1/1	0.99	0.09	43,43,43,43	0
54	MG	2A	3527	1/1	0.99	0.07	54,54,54,54	0
54	MG	2A	3691	1/1	0.99	0.03	51,51,51,51	0
54	MG	1A	3302	1/1	0.99	0.07	47,47,47,47	0
54	MG	1B	223	1/1	0.99	0.06	58,58,58,58	0
54	MG	2A	3581	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3901	1/1	0.99	0.04	43,43,43,43	0
54	MG	1A	3902	1/1	0.99	0.06	28,28,28,28	0
54	MG	2A	3639	1/1	0.99	0.06	42,42,42,42	0
54	MG	1A	3110	1/1	0.99	0.13	35,35,35,35	0
54	MG	2A	3282	1/1	0.99	0.06	53,53,53,53	0
54	MG	2A	3141	1/1	0.99	0.07	61,61,61,61	0
54	MG	2a	3118	1/1	0.99	0.04	56,56,56,56	0
54	MG	2A	3587	1/1	0.99	0.04	46,46,46,46	0
54	MG	1A	3789	1/1	0.99	0.03	29,29,29,29	0
54	MG	2a	3121	1/1	0.99	0.10	67,67,67,67	0
54	MG	1A	3104	1/1	0.99	0.14	37,37,37,37	0
54	MG	1A	3089	1/1	0.99	0.04	42,42,42,42	0
54	MG	2a	3124	1/1	0.99	0.03	80,80,80,80	0
54	MG	1A	3090	1/1	0.99	0.16	26,26,26,26	0
54	MG	2A	3592	1/1	0.99	0.04	42,42,42,42	0
54	MG	1D	302	1/1	0.99	0.05	55,55,55,55	0
54	MG	1A	3069	1/1	0.99	0.07	35,35,35,35	0
54	MG	1A	3153	1/1	0.99	0.15	38,38,38,38	0
54	MG	1A	3847	1/1	0.99	0.03	26,26,26,26	0
54	MG	1A	3470	1/1	0.99	0.04	48,48,48,48	0
54	MG	1A	3912	1/1	0.99	0.03	49,49,49,49	0
54	MG	1A	3006	1/1	0.99	0.04	25,25,25,25	0
54	MG	1A	3472	1/1	0.99	0.03	57,57,57,57	0
54	MG	2A	3601	1/1	0.99	0.04	46,46,46,46	0
54	MG	1A	3473	1/1	0.99	0.06	39,39,39,39	0
54	MG	1A	3773	1/1	0.99	0.05	43,43,43,43	0
54	MG	1A	3774	1/1	0.99	0.05	43,43,43,43	0
54	MG	1A	3200	1/1	0.99	0.23	39,39,39,39	0
54	MG	1a	1841	1/1	0.99	0.03	63,63,63,63	0
54	MG	1A	3684	1/1	0.99	0.04	61,61,61,61	0
54	MG	1a	1716	1/1	0.99	0.06	46,46,46,46	0
54	MG	1A	3529	1/1	0.99	0.03	25,25,25,25	0
54	MG	1a	1718	1/1	0.99	0.09	40,40,40,40	0
54	MG	2A	3353	1/1	0.99	0.05	42,42,42,42	0
54	MG	1A	3130	1/1	0.99	0.32	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	3858	1/1	0.99	0.11	39,39,39,39	0
54	MG	1A	3626	1/1	0.99	0.08	29,29,29,29	0
54	MG	1A	3212	1/1	0.99	0.11	33,33,33,33	0
54	MG	1A	3733	1/1	0.99	0.05	42,42,42,42	0
54	MG	1A	3073	1/1	0.99	0.06	42,42,42,42	0
54	MG	1a	1852	1/1	0.99	0.08	40,40,40,40	0
54	MG	1B	213	1/1	0.99	0.04	39,39,39,39	0
54	MG	1A	3927	1/1	0.99	0.07	56,56,56,56	0
54	MG	1A	3461	1/1	0.99	0.03	52,52,52,52	0
54	MG	1A	3691	1/1	0.99	0.03	36,36,36,36	0
54	MG	1A	3865	1/1	0.99	0.06	55,55,55,55	0
54	MG	1a	1648	1/1	0.99	0.13	51,51,51,51	0
54	MG	2A	3129	1/1	0.99	0.04	33,33,33,33	0
58	ZN	19	103	1/1	0.99	0.03	50,50,50,50	0
58	ZN	1n	104	1/1	0.99	0.03	77,77,77,77	0
54	MG	2A	3369	1/1	0.99	0.04	51,51,51,51	0
54	MG	1A	3479	1/1	0.99	0.06	42,42,42,42	0
58	ZN	25	102	1/1	0.99	0.03	71,71,71,71	0
54	MG	1A	3447	1/1	0.99	0.04	32,32,32,32	0
54	MG	2A	3685	1/1	0.99	0.04	47,47,47,47	0
54	MG	1F	302	1/1	0.99	0.05	34,34,34,34	0
54	MG	1A	3898	1/1	0.99	0.04	42,42,42,42	0
54	MG	1A	3899	1/1	0.99	0.07	41,41,41,41	0
54	MG	2A	3357	1/1	1.00	0.05	34,34,34,34	0
54	MG	1A	3978	1/1	1.00	0.04	33,33,33,33	0
54	MG	1A	3879	1/1	1.00	0.07	35,35,35,35	0
54	MG	1A	3931	1/1	1.00	0.04	47,47,47,47	0
54	MG	2A	3475	1/1	1.00	0.08	37,37,37,37	0
58	ZN	16	501	1/1	1.00	0.05	48,48,48,48	0
54	MG	1A	3338	1/1	1.00	0.05	34,34,34,34	0
54	MG	1A	3454	1/1	1.00	0.05	28,28,28,28	0

6.5 Other polymers

There are no such residues in this entry.