



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 30, 2026 – 02:15 PM UTC

PDB ID : 6CFK / pdb\_00006cfk  
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with D-histidyl-CAM and bound to protein Y (YfiA) at 2.7Å resolution  
Authors : Tereshchenkov, A.G.; Dobosz-Bartoszek, M.; Osterman, I.A.; Marks, J.; Sergeeva, V.A.; Kasatsky, P.; Komarova, E.S.; Stavrianidi, A.N.; Rodin, I.A.; Konevega, A.L.; Sergiev, P.V.; Sumbatyan, N.V.; Mankin, A.S.; Bogdanov, A.A.; Polikanov, Y.S.  
Deposited on : 2018-02-15  
Resolution : 2.70 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](mailto: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>.

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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)

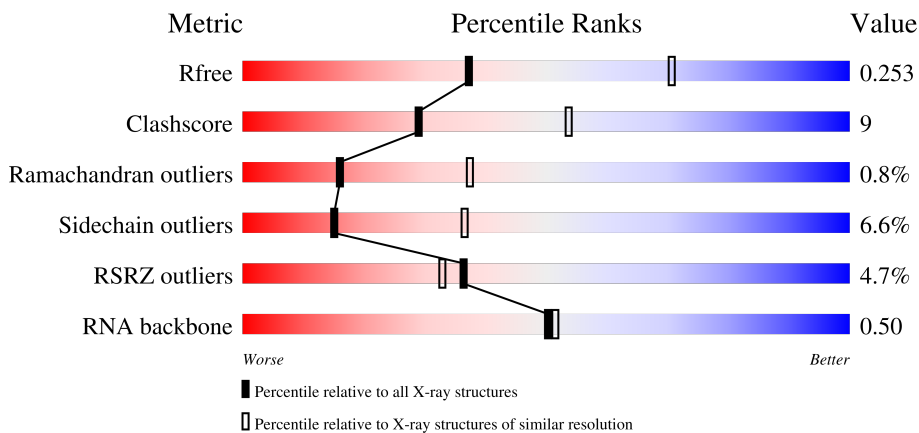
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)


























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  $\geq 3$ , 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	
1	2A	2915	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	1B	121	 74% 21% ..
2	2B	121	 7% 59% 35% 6% ..
3	1D	276	 79% 17% .
3	2D	276	 79% 17% .
4	1E	206	 75% 21% ..
4	2E	206	 73% 22% ..
5	1F	210	 70% 22% 5% .
5	2F	210	 66% 27% ..
6	1G	182	 2% 62% 33% 5% ..
6	2G	182	 14% 59% 36% 5% ..
7	1H	180	 71% 24% ..
7	2H	180	 6% 66% 27% . ..
8	1I	148	 3% 70% 26% ..
8	2I	148	 7% 67% 28% ..
9	1N	140	 83% 14% .
9	2N	140	 81% 17% .
10	1O	122	 80% 20% .
10	2O	122	 77% 21% .
11	1P	150	 75% 23% ..
11	2P	150	 2% 79% 19% ..
12	1Q	141	 76% 22% .
12	2Q	141	 2% 67% 30% .
13	1R	118	 81% 18% .
13	2R	118	 75% 20% .
14	1S	112	 81% 14% ..

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Mol	Chain	Length	Quality of chain
14	2S	112	14% 56% 40% ..
15	1T	146	3% 68% 18% 10%
15	2T	146	% 64% 21% 10%
16	1U	118	78% 19% ..
16	2U	118	% 75% 22% ..
17	1V	101	76% 22% .
17	2V	101	72% 24% ..
18	1W	113	81% 16% ..
18	2W	113	% 78% 18% ..
19	1X	96	% 73% 22% ..
19	2X	96	% 76% 19% ..
20	1Y	110	% 72% 22% ..
20	2Y	110	5% 68% 27% ..
21	1Z	206	% 77% 20% ..
21	2Z	206	4% 72% 23% ..
22	10	85	74% 16% 9%
22	20	85	2% 74% 15% 9%
23	11	98	% 78% 18% ..
23	21	98	2% 71% 24% ..
24	12	72	% 82% 14% ..
24	22	72	76% 18% ..
25	13	60	77% 17% 5% .
25	23	60	2% 65% 28% 5% .
26	14	71	20% 62% 28% 7% .
26	24	71	18% 41% 49% 7% .

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Mol	Chain	Length	Quality of chain
27	15	60	68% 27% ..
27	25	60	82% 15% ..
28	16	54	63% 31% ..
28	26	54	2% 72% 22% ..
29	17	49	2% 73% 22% ..
29	27	49	4% 88% 10% ..
30	18	65	69% 28% ..
30	28	65	2% 72% 23% ..
31	19	37	73% 24% ..
31	29	37	3% 57% 43% ..
32	1a	1521	2% 56% 35% 7% ..
32	2a	1521	4% 51% 39% 8% ..
33	1b	256	11% 56% 29% 5% 10%
33	2b	256	18% 55% 32% 2% 10%
34	1c	239	6% 67% 18% 2% 14%
34	2c	239	15% 59% 26% 2% 14%
35	1d	209	6% 61% 36% 2% ..
35	2d	209	5% 70% 27% 2% ..
36	1e	162	62% 27% 2% 9%
36	2e	162	2% 66% 25% 2% 9%
37	1f	101	% 75% 20% ..
37	2f	101	84% 12% ..
38	1g	156	2% 74% 24% ..
38	2g	156	6% 73% 23% ..
39	1h	138	% 72% 25% ..

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Mol	Chain	Length	Quality of chain
39	2h	138	73% 23%
40	1i	128	57% 42% 11%
40	2i	128	53% 41% 33%
41	1j	105	64% 27% 8% 10%
41	2j	105	56% 33% 9% 50%
42	1k	129	72% 15% 12%
42	2k	129	69% 18% 12% 6%
43	1l	132	74% 15% 8% 2%
43	2l	132	73% 18% 8% 2%
44	1m	126	60% 30% 8% 6%
44	2m	126	55% 34% 10% 17%
45	1n	61	74% 23% 5%
45	2n	61	61% 38% 36%
46	1o	89	70% 27% 3%
46	2o	89	75% 21% 2%
47	1p	88	61% 32% 7% 15%
47	2p	88	59% 32% 7% 7%
48	1q	105	68% 25% 6% 2%
48	2q	105	71% 22% 6% 2%
49	1r	88	66% 11% 23%
49	2r	88	56% 19% 23%
50	1s	93	67% 20% 11% 2%
50	2s	93	52% 32% 5% 11%
51	1t	106	64% 24% 9% 8%
51	2t	106	63% 25% 8% 8%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	2A	3215	-	-	-	X

## 2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 295438 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
			Total	C	N	O	P			
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
			Total	C	N	O	P			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
10	2O	122	933	588	171	170	4	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
42	2k	114	833	519	156	155	3	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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	1024	Total	Mg	0	0
			1024	1024		
54	1B	29	Total	Mg	0	0
			29	29		
54	1D	13	Total	Mg	0	0
			13	13		
54	1E	7	Total	Mg	0	0
			7	7		
54	1F	13	Total	Mg	0	0
			13	13		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	3	Total	Mg	0	0
			3	3		
54	1O	2	Total	Mg	0	0
			2	2		
54	1P	3	Total	Mg	0	0
			3	3		
54	1Q	4	Total	Mg	0	0
			4	4		
54	1R	3	Total	Mg	0	0
			3	3		
54	1S	1	Total	Mg	0	0
			1	1		
54	1T	3	Total	Mg	0	0
			3	3		
54	1U	2	Total	Mg	0	0
			2	2		
54	1V	3	Total	Mg	0	0
			3	3		
54	1W	2	Total	Mg	0	0
			2	2		
54	1X	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1Z	1	Total Mg 1 1	0	0
54	10	6	Total Mg 6 6	0	0
54	11	3	Total Mg 3 3	0	0
54	13	2	Total Mg 2 2	0	0
54	14	1	Total Mg 1 1	0	0
54	15	3	Total Mg 3 3	0	0
54	17	2	Total Mg 2 2	0	0
54	18	1	Total Mg 1 1	0	0
54	19	2	Total Mg 2 2	0	0
54	1a	255	Total Mg 255 255	0	0
54	1b	1	Total Mg 1 1	0	0
54	1d	6	Total Mg 6 6	0	0
54	1e	2	Total Mg 2 2	0	0
54	1f	2	Total Mg 2 2	0	0
54	1g	3	Total Mg 3 3	0	0
54	1h	2	Total Mg 2 2	0	0
54	1i	1	Total Mg 1 1	0	0
54	1l	2	Total Mg 2 2	0	0
54	1n	1	Total Mg 1 1	0	0
54	1o	1	Total Mg 1 1	0	0
54	1t	1	Total Mg 1 1	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
54	1y	4	Total Mg 4 4	0	0
54	2A	721	Total Mg 721 721	0	0
54	2B	19	Total Mg 19 19	0	0
54	2D	8	Total Mg 8 8	0	0
54	2E	6	Total Mg 6 6	0	0
54	2F	3	Total Mg 3 3	0	0
54	2G	3	Total Mg 3 3	0	0
54	2I	1	Total Mg 1 1	0	0
54	2N	1	Total Mg 1 1	0	0
54	2O	1	Total Mg 1 1	0	0
54	2P	2	Total Mg 2 2	0	0
54	2Q	2	Total Mg 2 2	0	0
54	2R	1	Total Mg 1 1	0	0
54	2T	4	Total Mg 4 4	0	0
54	2V	1	Total Mg 1 1	0	0
54	2W	2	Total Mg 2 2	0	0
54	2X	1	Total Mg 1 1	0	0
54	20	1	Total Mg 1 1	0	0
54	21	1	Total Mg 1 1	0	0
54	25	1	Total Mg 1 1	0	0
54	28	3	Total Mg 3 3	0	0

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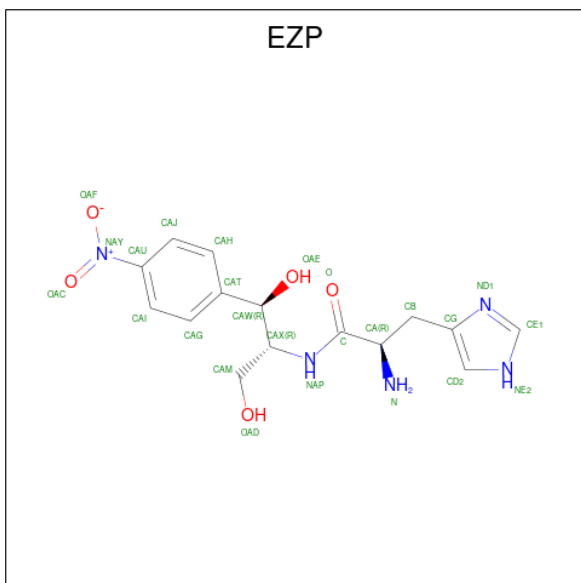
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	2a	151	Total Mg 151 151	0	0
54	2e	1	Total Mg 1 1	0	0
54	2f	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2p	1	Total Mg 1 1	0	0
54	2q	1	Total Mg 1 1	0	0
54	2r	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0

- Molecule 55 is POTASSIUM ION (CCD ID: K) (formula: K).

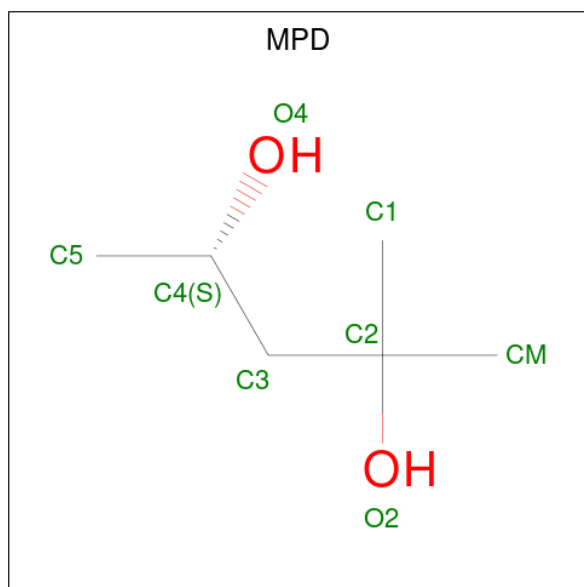
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1A	1	Total K 1 1	0	0
55	2A	1	Total K 1 1	0	0

- Molecule 56 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-D-histidinamide (CCD ID: EZP) (formula: C<sub>15</sub>H<sub>19</sub>N<sub>5</sub>O<sub>5</sub>).



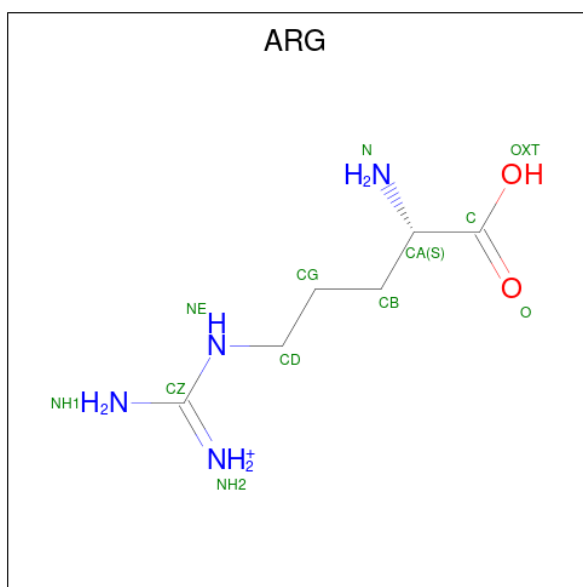
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
56	1A	1	25	15	5	5	0	0
56	2A	1	25	15	5	5	0	0

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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

- Molecule 58 is ARGinine (CCD ID: ARG) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>4</sub>O<sub>2</sub>).



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

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

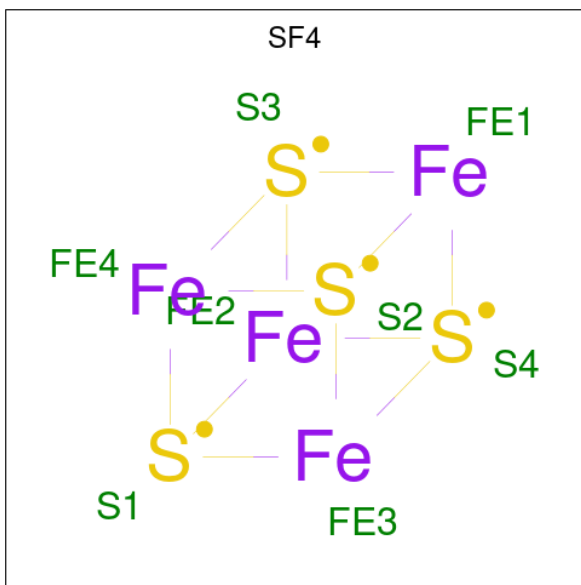
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0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

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

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2980	Total O 2980 2980	0	0
61	1B	105	Total O 105 105	0	0
61	1D	116	Total O 116 116	0	0
61	1E	76	Total O 76 76	0	0
61	1F	63	Total O 63 63	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	22	Total 22	O 22	0	0
61	1H	16	Total 16	O 16	0	0
61	1I	7	Total 7	O 7	0	0
61	1N	50	Total 50	O 50	0	0
61	1O	22	Total 22	O 22	0	0
61	1P	58	Total 58	O 58	0	0
61	1Q	42	Total 42	O 42	0	0
61	1R	37	Total 37	O 37	0	0
61	1S	13	Total 13	O 13	0	0
61	1T	42	Total 42	O 42	0	0
61	1U	45	Total 45	O 45	0	0
61	1V	37	Total 37	O 37	0	0
61	1W	24	Total 24	O 24	0	0
61	1X	24	Total 24	O 24	0	0
61	1Y	15	Total 15	O 15	0	0
61	1Z	14	Total 14	O 14	0	0
61	10	22	Total 22	O 22	0	0
61	11	28	Total 28	O 28	0	0
61	12	14	Total 14	O 14	0	0
61	13	22	Total 22	O 22	0	0
61	14	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	15	26	Total O 26 26	0	0
61	16	17	Total O 17 17	0	0
61	17	14	Total O 14 14	0	0
61	18	30	Total O 30 30	0	0
61	19	8	Total O 8 8	0	0
61	1a	261	Total O 261 261	0	0
61	1b	1	Total O 1 1	0	0
61	1d	9	Total O 9 9	0	0
61	1e	6	Total O 6 6	0	0
61	1f	3	Total O 3 3	0	0
61	1h	1	Total O 1 1	0	0
61	1i	1	Total O 1 1	0	0
61	1j	1	Total O 1 1	0	0
61	1k	1	Total O 1 1	0	0
61	1l	4	Total O 4 4	0	0
61	1n	1	Total O 1 1	0	0
61	1o	5	Total O 5 5	0	0
61	1p	3	Total O 3 3	0	0
61	1y	5	Total O 5 5	0	0
61	2A	1686	Total O 1686 1686	0	0
61	2B	65	Total O 65 65	0	0

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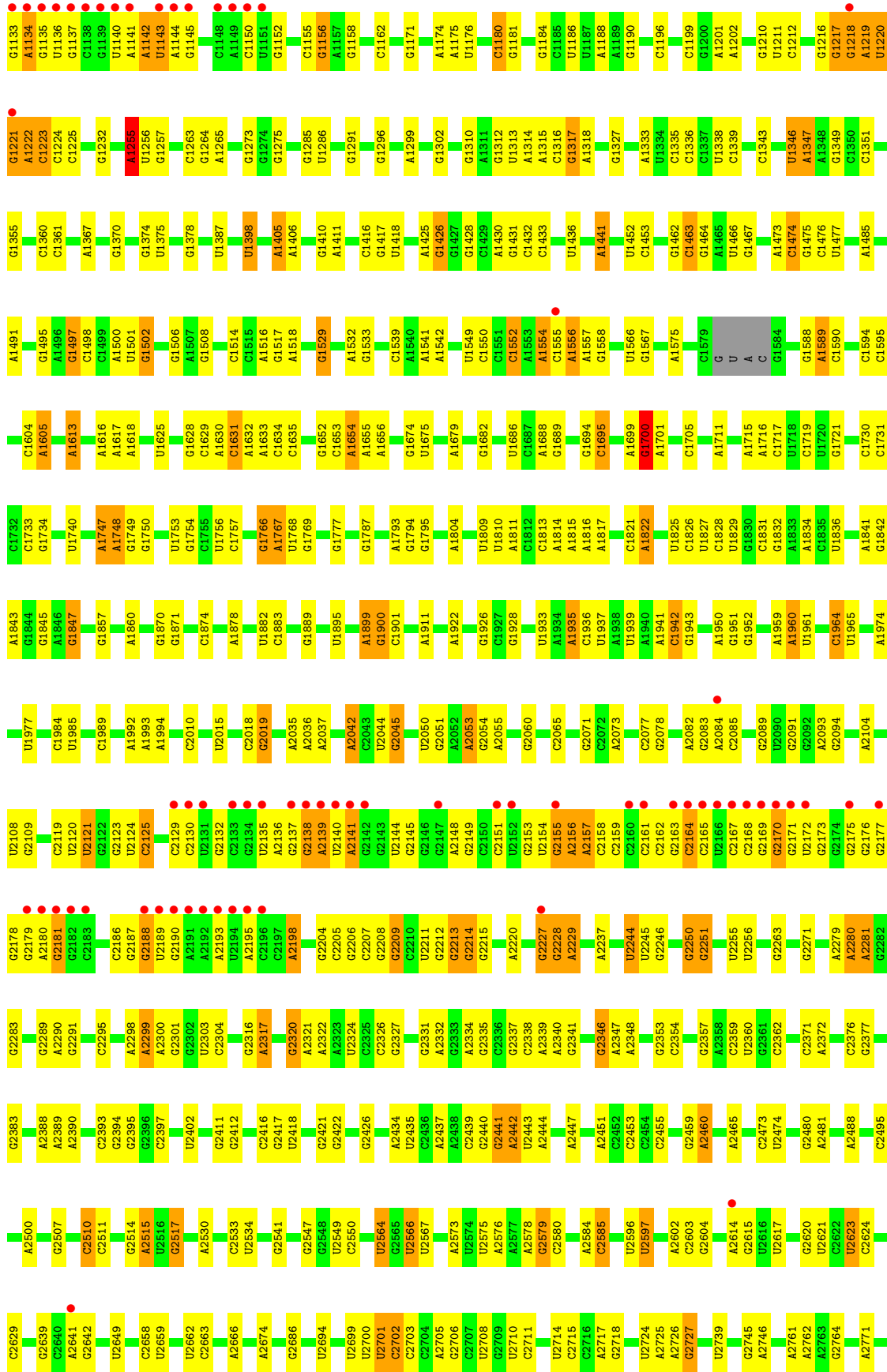
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2D	52	Total 52	O 52	0	0
61	2E	25	Total 25	O 25	0	0
61	2F	21	Total 21	O 21	0	0
61	2G	7	Total 7	O 7	0	0
61	2H	4	Total 4	O 4	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	6	Total 6	O 6	0	0
61	2O	22	Total 22	O 22	0	0
61	2P	23	Total 23	O 23	0	0
61	2Q	30	Total 30	O 30	0	0
61	2R	21	Total 21	O 21	0	0
61	2S	8	Total 8	O 8	0	0
61	2T	10	Total 10	O 10	0	0
61	2U	14	Total 14	O 14	0	0
61	2V	9	Total 9	O 9	0	0
61	2W	21	Total 21	O 21	0	0
61	2X	9	Total 9	O 9	0	0
61	2Y	3	Total 3	O 3	0	0
61	2Z	15	Total 15	O 15	0	0
61	20	13	Total 13	O 13	0	0
61	21	24	Total 24	O 24	0	0

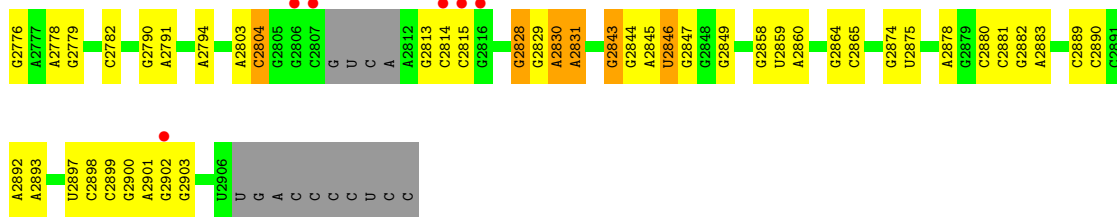
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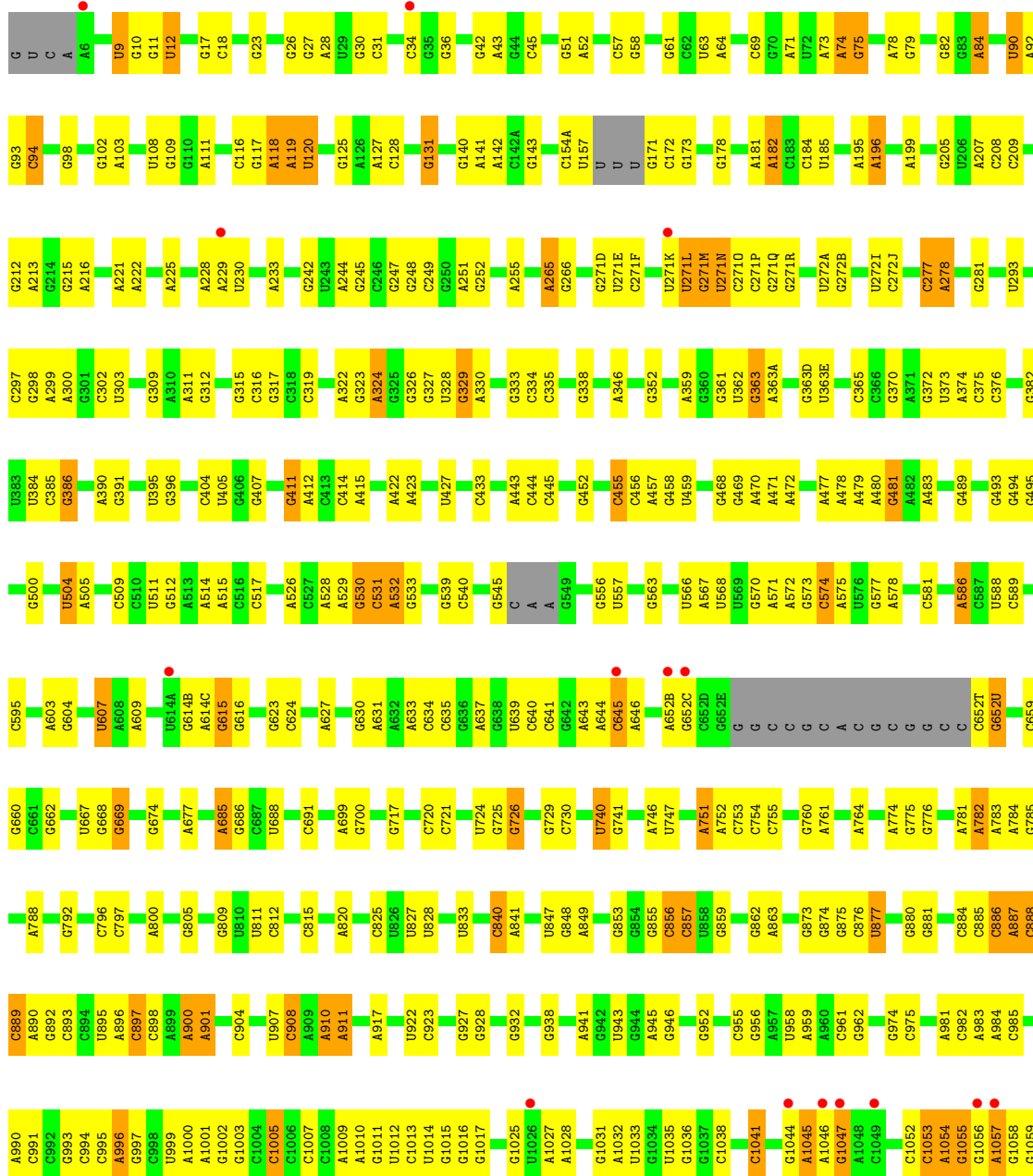
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	22	5	Total 5	O 5	0	0
61	23	3	Total 3	O 3	0	0
61	24	2	Total 2	O 2	0	0
61	25	9	Total 9	O 9	0	0
61	26	6	Total 6	O 6	0	0
61	27	7	Total 7	O 7	0	0
61	28	15	Total 15	O 15	0	0
61	29	2	Total 2	O 2	0	0
61	2a	100	Total 100	O 100	0	0
61	2d	6	Total 6	O 6	0	0
61	2e	1	Total 1	O 1	0	0
61	2f	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	1	Total 1	O 1	0	0
61	2m	1	Total 1	O 1	0	0
61	2o	2	Total 2	O 2	0	0
61	2p	1	Total 1	O 1	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	4	Total 4	O 4	0	0
61	2y	1	Total 1	O 1	0	0



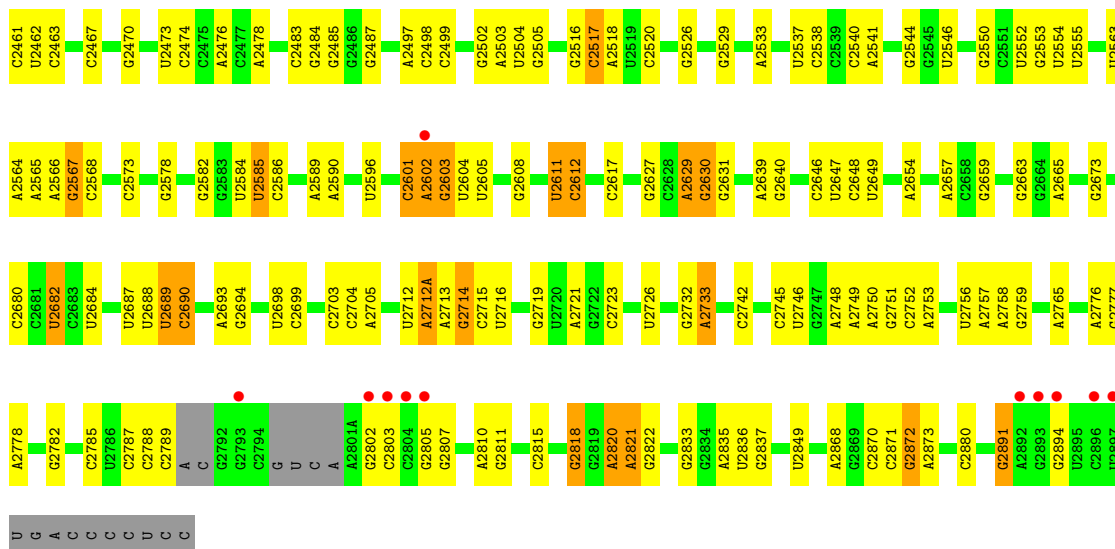




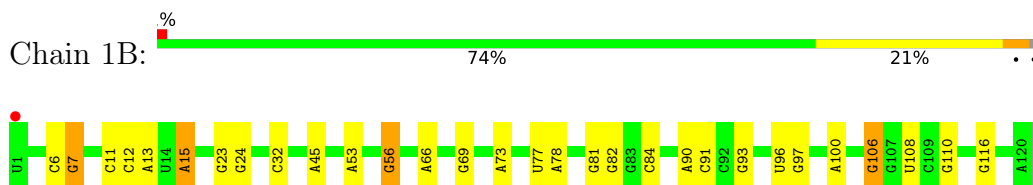
● Molecule 1: 23S Ribosomal RNA



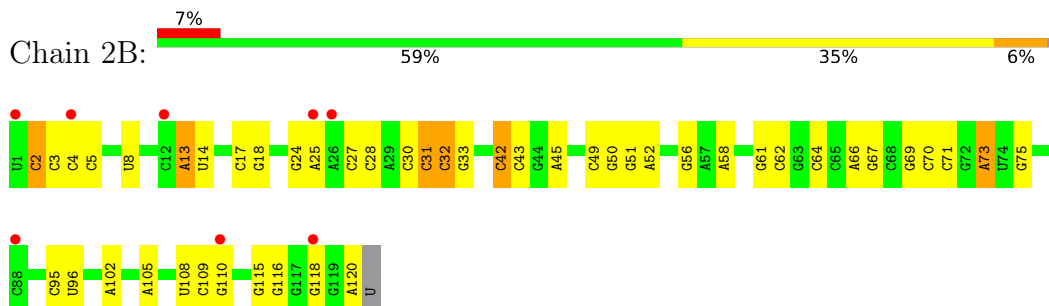
C2364	A2287	G2177	A2117	A1900	C1781	C1858	G1538	C1446	G1324	G1229	A1126	U1060
G2365	A2288	C2178	U2118	A1901	C1782	A1664	G1539	G1447	C1327	G1229	A1129	G1062
A2366	G2289	C2179	A2119	C1902	A1783	A1665	U1540	G1448	G1328	G1235	A1130	U1063
G2375	A2292	U2180	G2120	G1906	A1784	A1666	G1541	A1449	U1341	G1236	A1131	C1064
A2376	C2293	G2181	U2121	G1907	A1785	A1667	A1542	C1450A	A1342	A1237	C1135	U1065
A2377	C2294	C2182	U2122	G1910	A1786	G1667	C1543	C1450A	U1341	A1237	C1136	U1066
A2378	C2295	G2183	G2123	G1911	A1791	A1668	C1547	G1485	A1342	U1240	C1137	A1067
A2379	U2296	C2184	G2124	U1912	G1792	A1669	C1587	G1485	U1352	A1241	G1138	G1068
G2383	C2297	C2185	A2125	A1913	G1793	C1674	C1550	G1489	G1356	A1246	G1138	A1069
G2384	G2298	U2186	A2126	A1913	C1793	G1675	C1557	G1489	U1356	A1246	U1141	A1070
G2385	G2299	G2187	G2038	C1914	U1794	C1676	U1558	C1487	A1359	A1253	U1142	G1071
G2386	G2302	U2189	C2039	U1915	C1795	U1680	A1558	C1487	A1360	A1254	U1142A	A1073
G2387	G2303	G2190	C2040	A1916	U1796	A1689	U1589	A1471	A1360	U1255	G1170	A1074
A2388	G2304	G2191	C2043	U1917	C1797	C1686	C1586	A1482	G1364	U1256	C1153	G1075
G2389	A2305	C2192	A2051	C1920	U1798	G1687	A1566	G1482	A1365	G1256	C1153	A1076
U2401	G2306	G2193	A2051	G1921	C1800	U1688	A1365	A1486	A1366	C1257	G1154	U1077
C2402	G2307	A2194	A2051	G1921	G1801	U1688	A1366	A1487	A1367	G1260	A1155	U1078
U2406	G2308	A2195	C2055	G1929	A1802	G1596	C1577	G1488	G1368	G1261	U1165	G1079
G2407	A2309	C2136	G2056	G1930	A1803	A1700	U1577	A1489	U1165	G1271	C1166	C1080
G2410	A2310	C2137	G2060	A1937	G1807	A1701	A1579	U1489	A1371	U1272	C1166	U1081
U2411	A2311	C2138	A2060	A1938	G1807	A1702	A1580	A1490	U1372	G1264	U1167	U1082
C2402	G2313	G2139	G2061	U1938	A1815	G1703	C1582	A1491	U1372	A1265	G1168	U1083
U2406	C2314	C2140	A2062	U1939	G1816	G1703	G1582	C1493	A1379	G1266	G1169	A1084
G2407	G2315	G2141	G2069	C1942	G1817	G1707	A1583	A1494	G1380	G1271	G1171	A1085
G2410	C2316	C2142	G2070	C1942	U1818	C1708	C1584	A1495	A1384	U1272	G	A1086
G2414	G2317	U2144	G2074	U1946	G1826	U1709	A1586	A1496	A1384	U1273	A	G1087
C2417	G2318	C2145	U2074	C1947	G1827	C1710	A1587	A1497	G1385	A1274	U	U1088
U2418	G2319	C2146	U2075	C1827	G1828	U1720	C1588	C1498	C1386	A1274	C	G1089
A2419	G2320	G2147	U2079	A1952	A1829	U1721	U1589	U1503	A1382	A1278	A	U1090
G2420	A2321	G2148	U2086	A1953	G1832	A1722	U1590	C1504	U1392	G1281	C1178	G1091
G2421	G2322	G2149	G2087	G1954	C1830	A1722	A1591	C1506	U1394	G1281	C1179	C1092
A2422	C2323	U2150	U2086	U1955	C1831	G1740	G1595	A1509A	A1405	A1287	C1180	U1093
U2423	G2324	C2151	G2087	C1832	G1832	A1741	A1596	G1510	U1405	U1288	C1181	U1094
C2424	C2325	G2152	U2092	G1835	G1835	G1746	A1597	A1508	U1406	U1288	G1186	A1095
A2425	G2251	C2153	U2092	G1835	G1835	G1746	A1598	C1509	A1406	C1291	G1187	U1097
G2429	G2252	G2154	G2093	C1962	U1839	G1748	C1598	A1509A	C1409	U1292	U1188	A1098
A2430	C2253	C2155	G2094	U1967	G1839	A1749	C1599	A1509B	G1410	C1293	A1189	G1099
A2431	A2334	G2156	G2094	C1967	G1839	G1750	G1595	G1510	C1411	C1293	G1195	U1101
A2435	C2343	G2157	U2096	C1967	G1842	G1750	A1609	U1514	G1413	C1297	G1203	A1102
A2459	U2344	G2158	U2096	A1970	A1847	G1754	A1610	G1515	G1416	U1300	A1204	C1104
C2440	U2344	C2159	U2096	A1971	A1848	A1755	A1614	G1518	C1417	A1302	U1205	U1105
C2441	A2336	G2160	G2100	U1991	G1858	G1756	A1614	U1519	U1420	G1303	G1210	C1109
G2445	A2336	C2161	G2101	G1992	G1858	G1756	A1614	U1519	U1421	G1303	G1211	G1110
A2448	C2343	C2162	C2103	U1993	U1864	G1762	U1629	G1526	A1427	A1308	G1212	G1112
C2449	U2344	C2163	G2104	C1996	U1864	G1763	U1629	G1526	C1428	A1308	G1212	U1113
C2441	C2347	G2165	G2105	G1997	A1876	G1764	A1631A	G1527	G1429	A1308	G1212	G1114
G2445	C2350	U2167	G2106	G1997	A1877	G1764	A1631A	A1528	C1430	A1308	G1212	G1115
A2448	G2354	G2168	C2108	A2001	G1878	C1771	U1639	A1528A	G1429	A1308	G1212	G1116
G2454	C2355	A2170	U2109	G2002	G1878	A1772	C1640	G1529	G1431	A1308	G1212	G1117
U2459	G2356	G2171	C2111	A2014	C1882	A1773	G1647	G1533	U1431	A1308	G1212	G1117
G2454	U2357	U2172	G2112	A2014	C1882	G1776	C1648	U	G1442	A1308	G1212	G1117
A2459	C2358	A2173	U2113	A2020	A1889	U1777	A1654	A	A1445	A1322	G1225	G1122
U2460	A2286	C2174	A2114	G2021	A1890	U1778	A1654	C1536	A1445A	A1322	G1225	G1125
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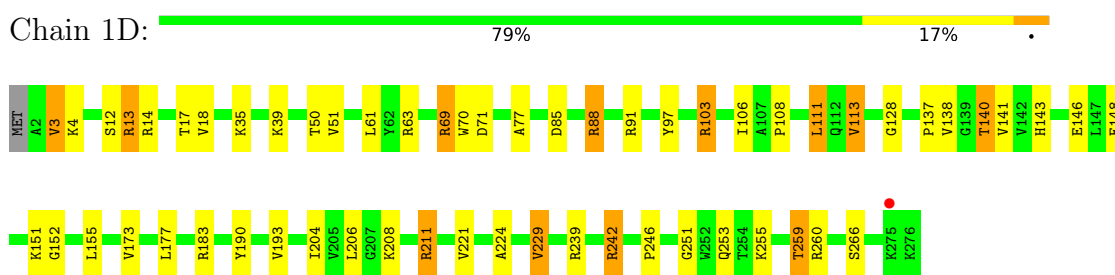
● Molecule 2: 5S Ribosomal RNA



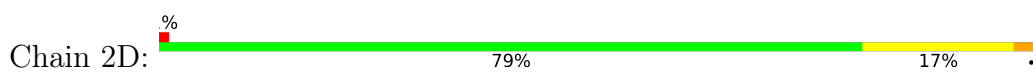
● Molecule 2: 5S Ribosomal RNA



● Molecule 3: 50S ribosomal protein L2

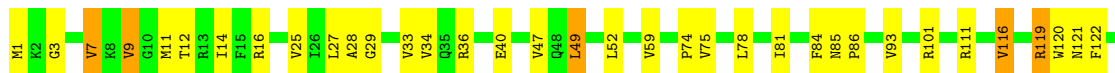
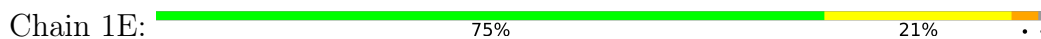


● Molecule 3: 50S ribosomal protein L2

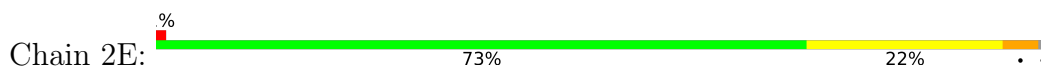




- Molecule 4: 50S ribosomal protein L3



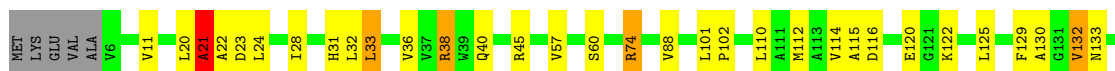
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

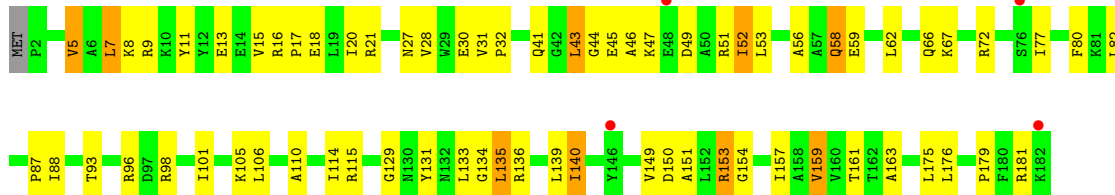


- Molecule 5: 50S ribosomal protein L4



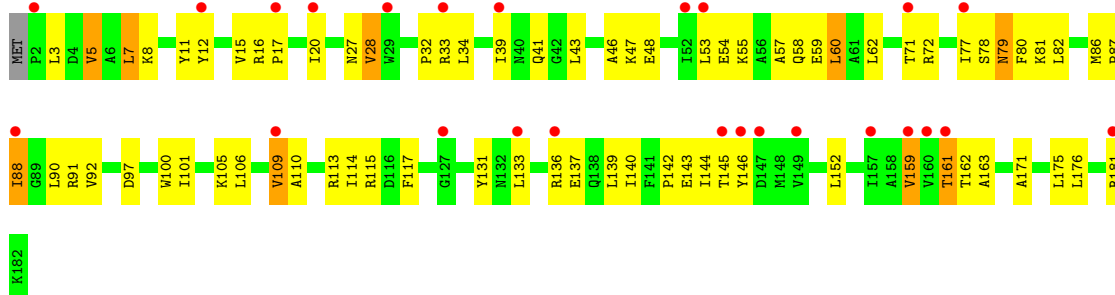
- Molecule 6: 50S ribosomal protein L5

Chain 1G:  2% 62% 33% 5%



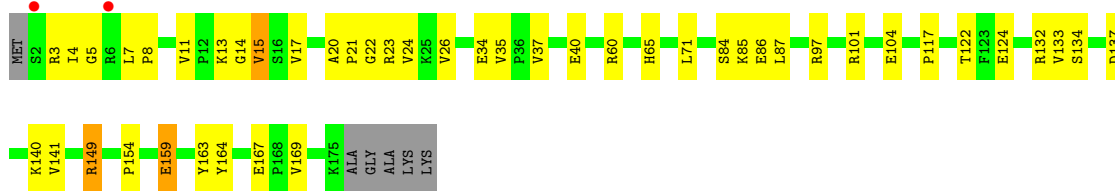
- Molecule 6: 50S ribosomal protein L5

Chain 2G:  14% 59% 36% 5%



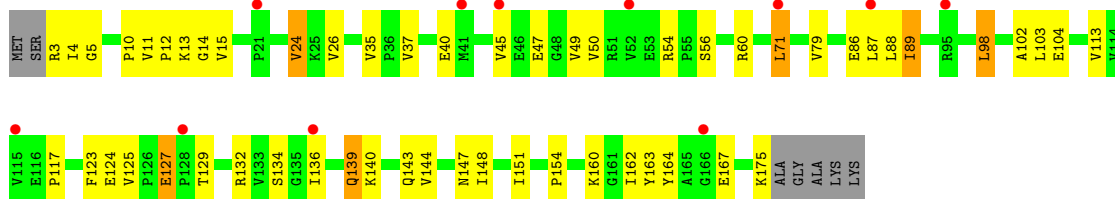
- Molecule 7: 50S ribosomal protein L6

Chain 1H:  71% 24%



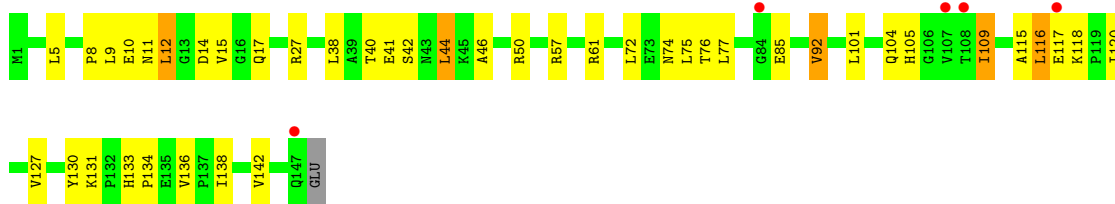
- Molecule 7: 50S ribosomal protein L6

Chain 2H:  6% 66% 27%

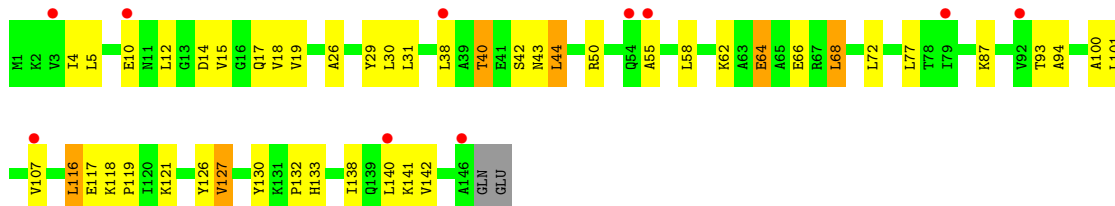


- Molecule 8: 50S ribosomal protein L9

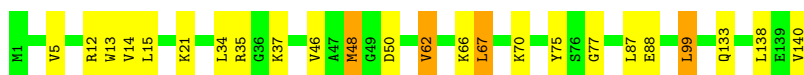
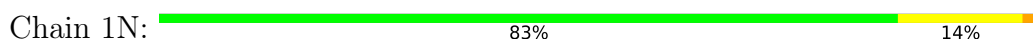
Chain 1I:  3% 70% 26%



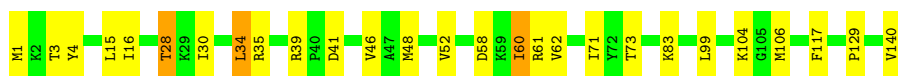
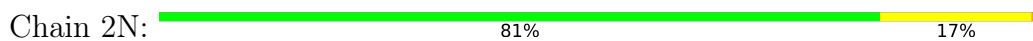
• Molecule 8: 50S ribosomal protein L9



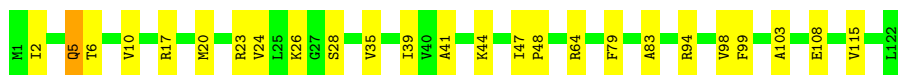
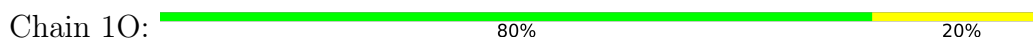
• Molecule 9: 50S ribosomal protein L13



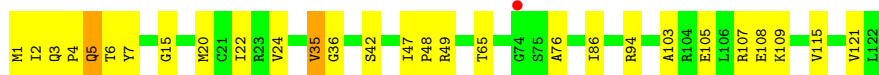
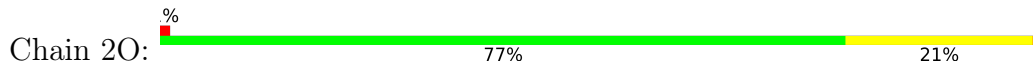
• Molecule 9: 50S ribosomal protein L13



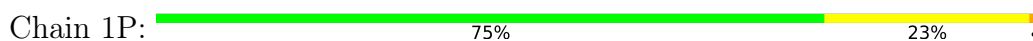
• Molecule 10: 50S ribosomal protein L14

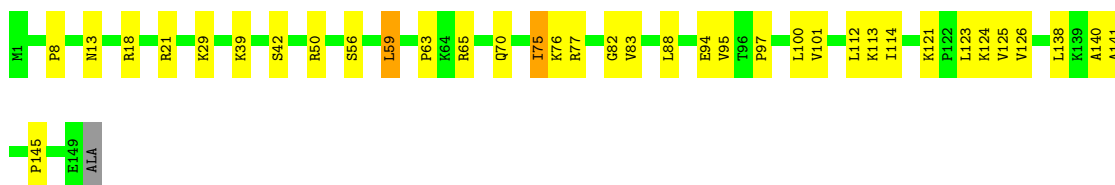


• Molecule 10: 50S ribosomal protein L14

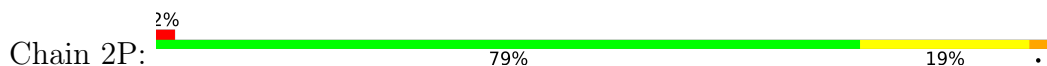


• Molecule 11: 50S ribosomal protein L15

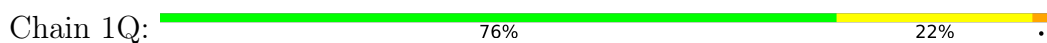




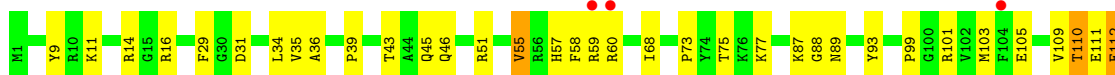
- Molecule 11: 50S ribosomal protein L15



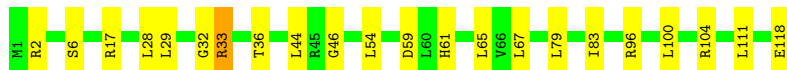
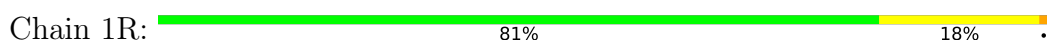
- Molecule 12: 50S ribosomal protein L16



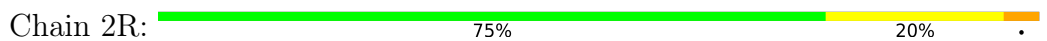
- Molecule 12: 50S ribosomal protein L16



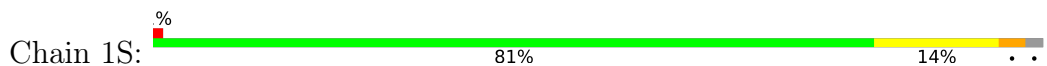
- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17

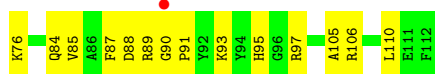
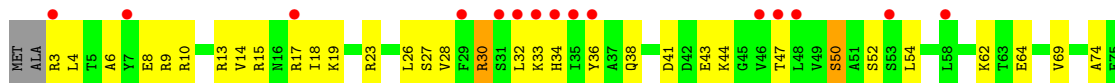


- Molecule 14: 50S ribosomal protein L18

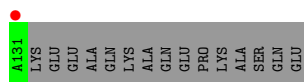




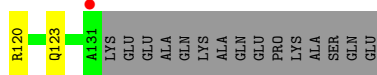
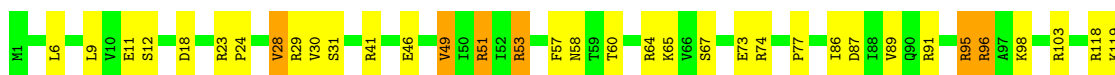
• Molecule 14: 50S ribosomal protein L18



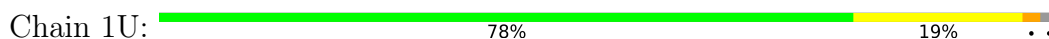
• Molecule 15: 50S ribosomal protein L19



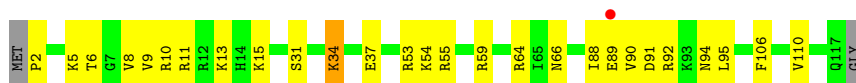
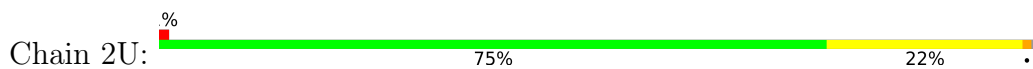
• Molecule 15: 50S ribosomal protein L19




• Molecule 16: 50S ribosomal protein L20

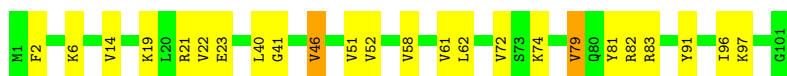


• Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  76% 22%




- Molecule 17: 50S ribosomal protein L21

Chain 2V:  72% 24%




- Molecule 18: 50S ribosomal protein L22

Chain 1W:  81% 16%




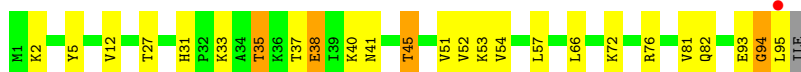
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  78% 18%




- Molecule 19: 50S ribosomal protein L23

Chain 1X:  73% 22%




- Molecule 19: 50S ribosomal protein L23

Chain 2X:  76% 19%

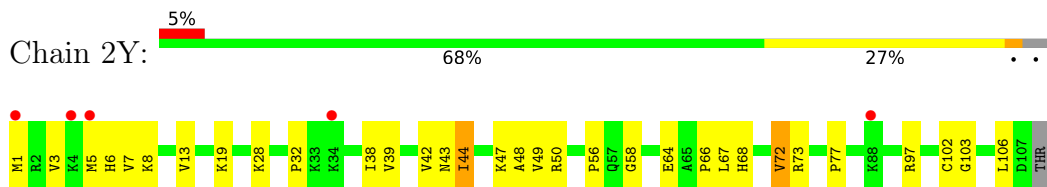


- Molecule 20: 50S ribosomal protein L24

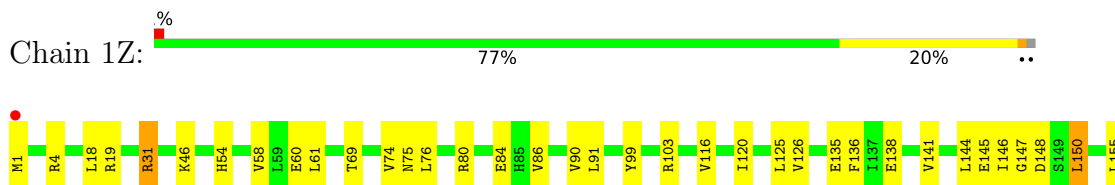
Chain 1Y:  72% 22%



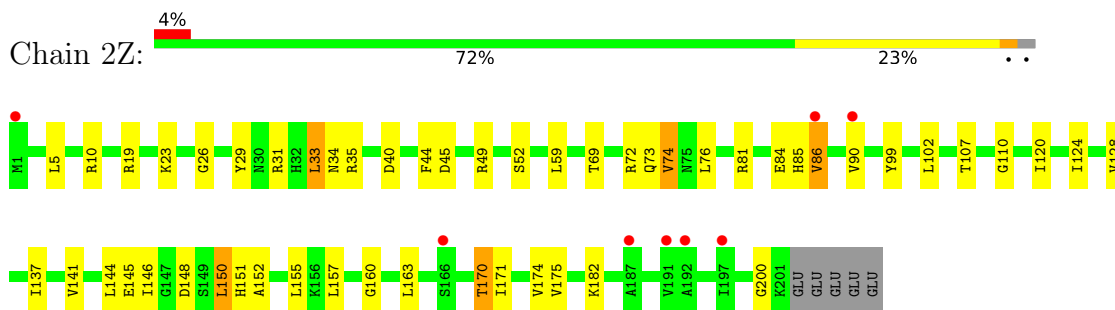
- Molecule 20: 50S ribosomal protein L24



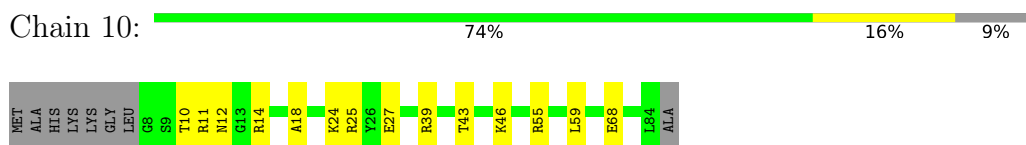
- Molecule 21: 50S ribosomal protein L25



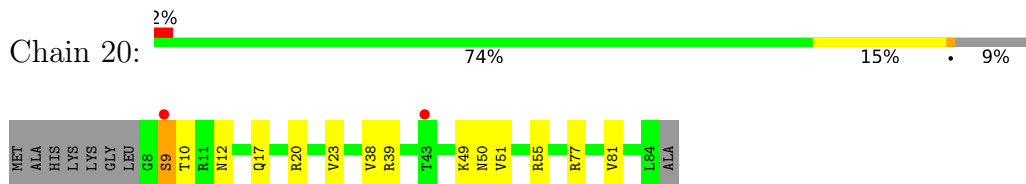
- Molecule 21: 50S ribosomal protein L25



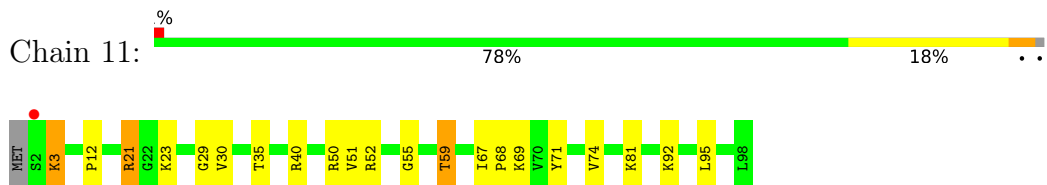
- Molecule 22: 50S ribosomal protein L27



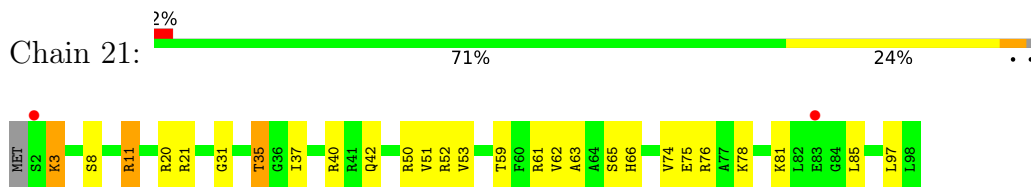
- Molecule 22: 50S ribosomal protein L27



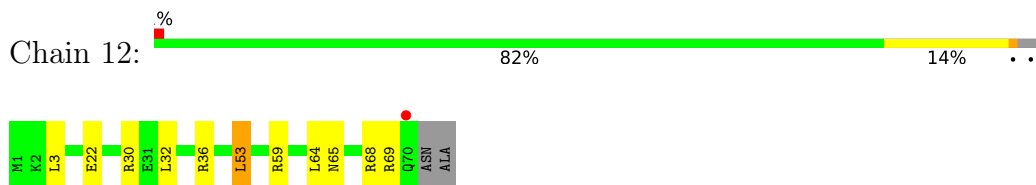
- Molecule 23: 50S ribosomal protein L28



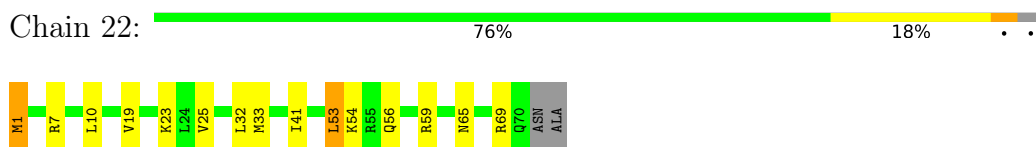
- Molecule 23: 50S ribosomal protein L28



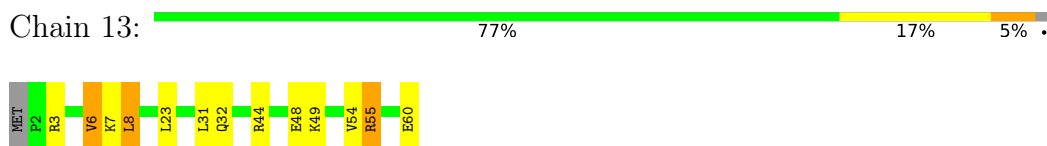
- Molecule 24: 50S ribosomal protein L29



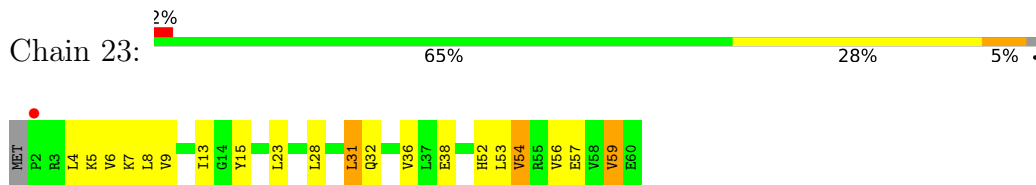
- Molecule 24: 50S ribosomal protein L29



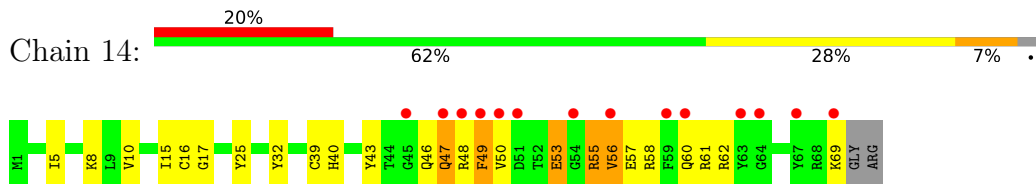
- Molecule 25: 50S ribosomal protein L30



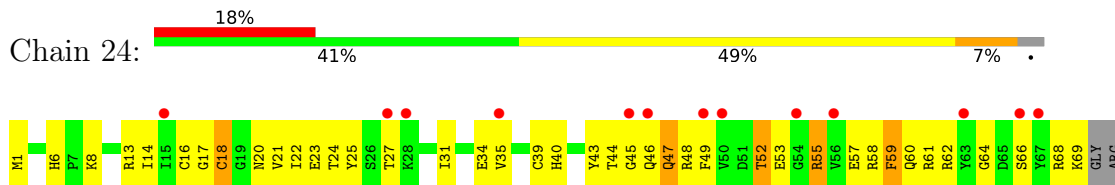
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31




- Molecule 27: 50S ribosomal protein L32

Chain 15:  68% 27% ..



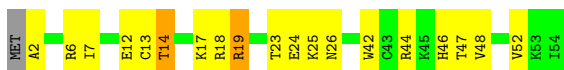
- Molecule 27: 50S ribosomal protein L32

Chain 25:  82% 15% ..




- Molecule 28: 50S ribosomal protein L33

Chain 16:  63% 31% ..




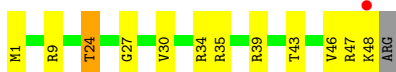
- Molecule 28: 50S ribosomal protein L33

Chain 26:  2% 72% 22% ..




- Molecule 29: 50S ribosomal protein L34

Chain 17:  2% 73% 22% ..



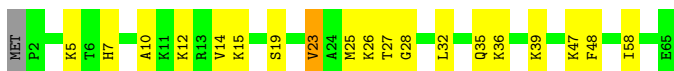
- Molecule 29: 50S ribosomal protein L34

Chain 27:  4% 88% 10% ..

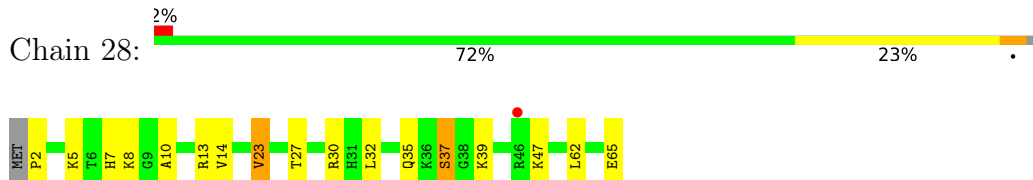


- Molecule 30: 50S ribosomal protein L35

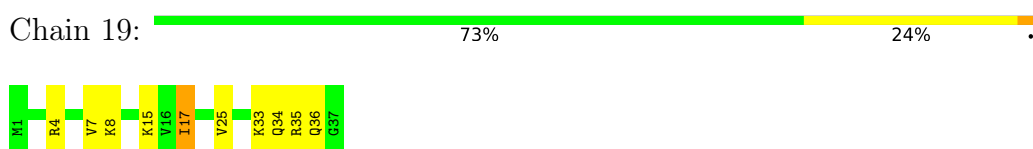
Chain 18:  69% 28% ..



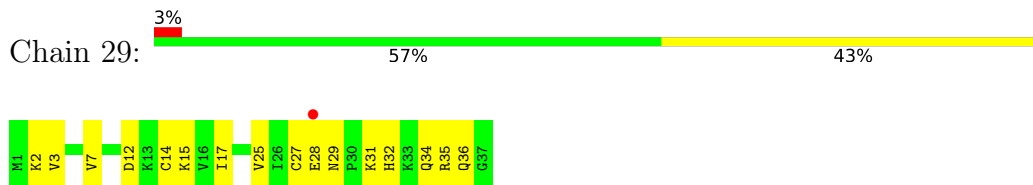
• Molecule 30: 50S ribosomal protein L35



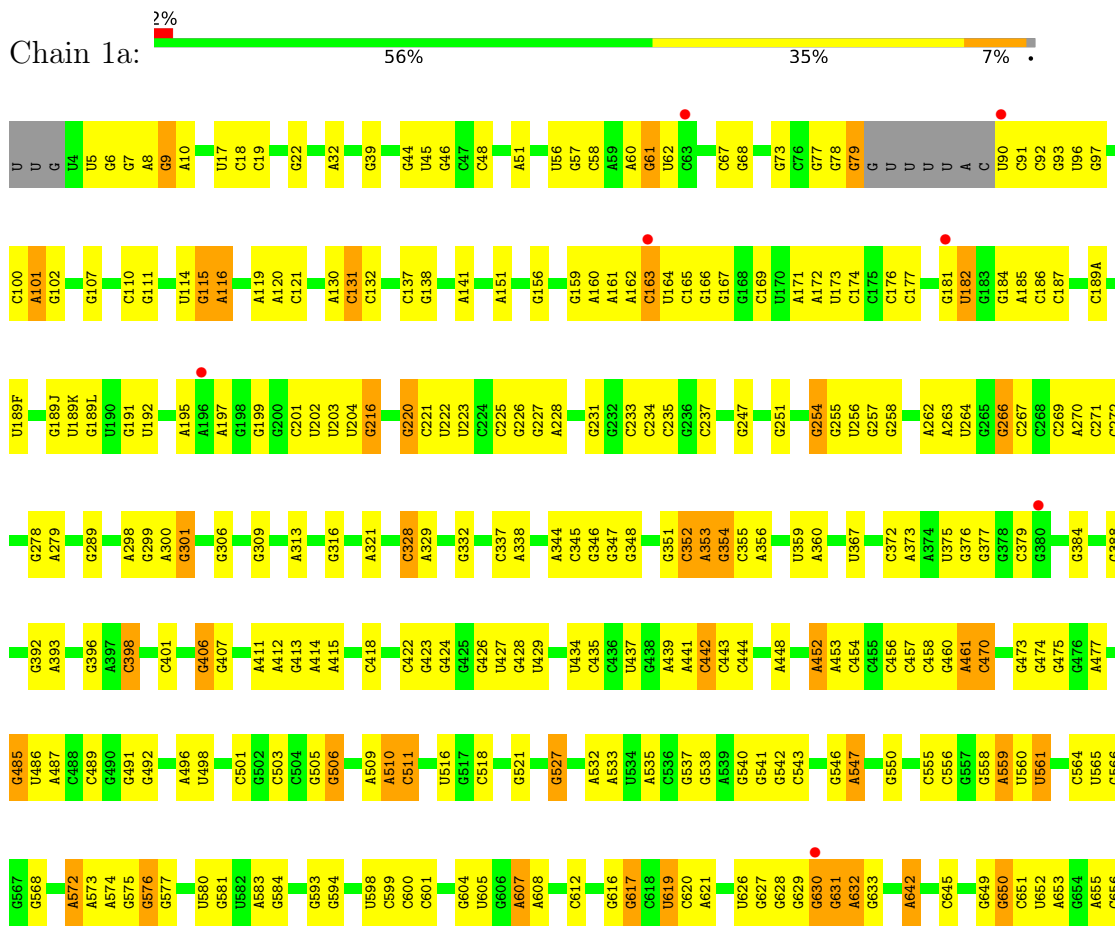
• Molecule 31: 50S ribosomal protein L36

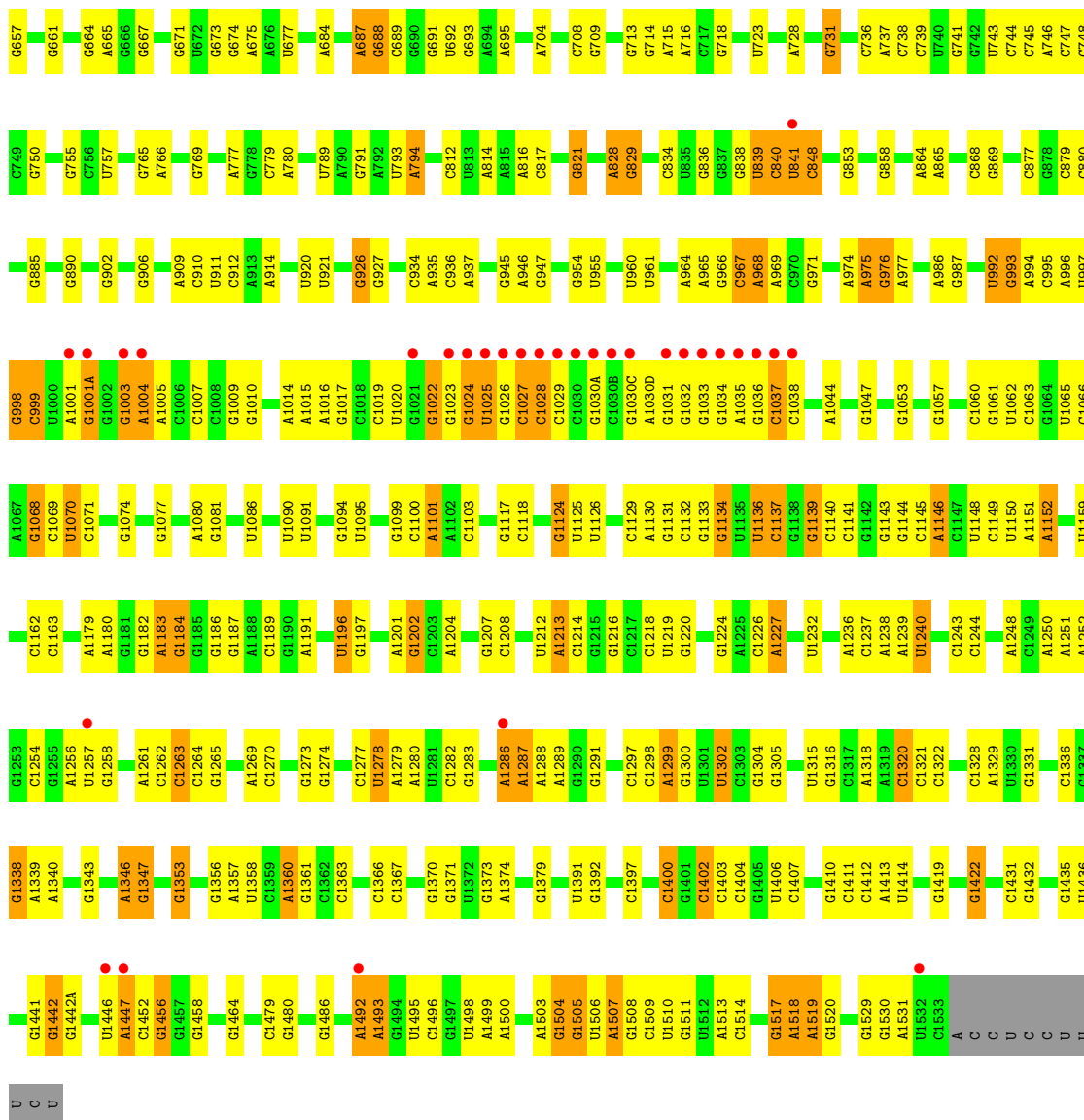


• Molecule 31: 50S ribosomal protein L36

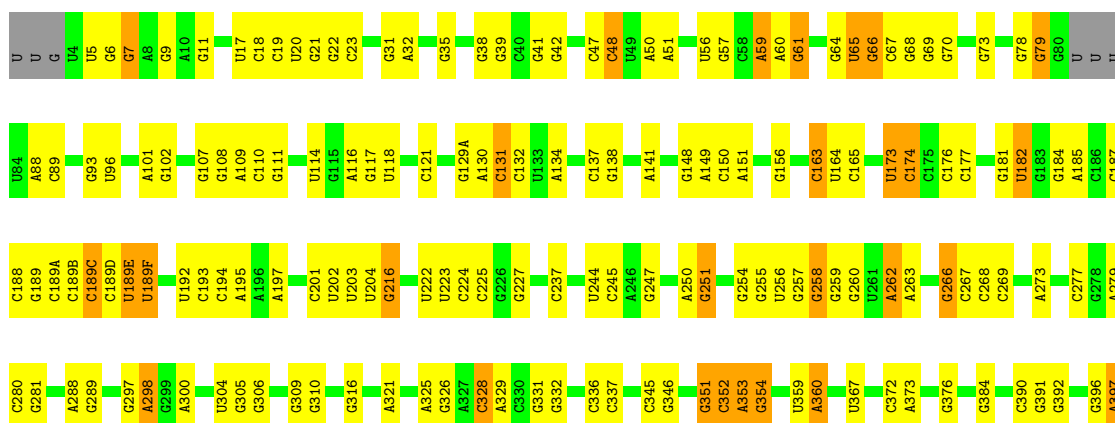


• Molecule 32: 16S Ribosomal RNA

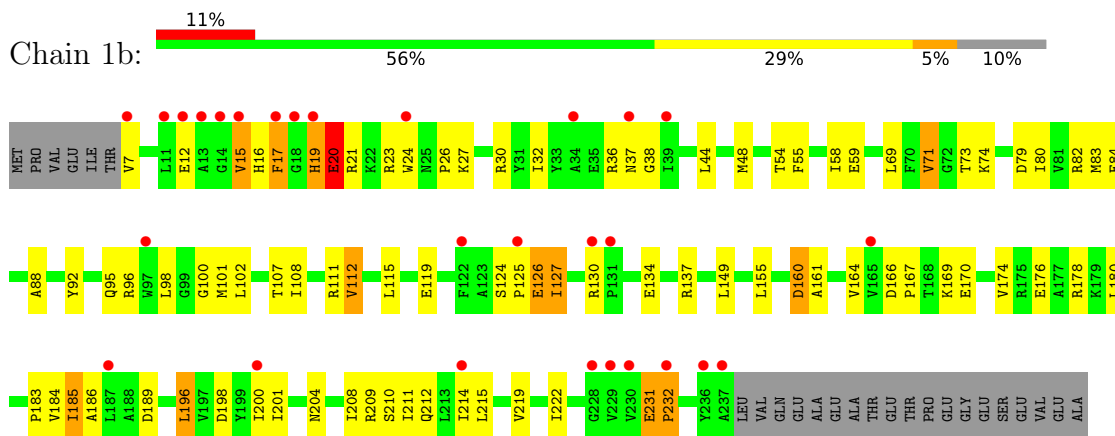




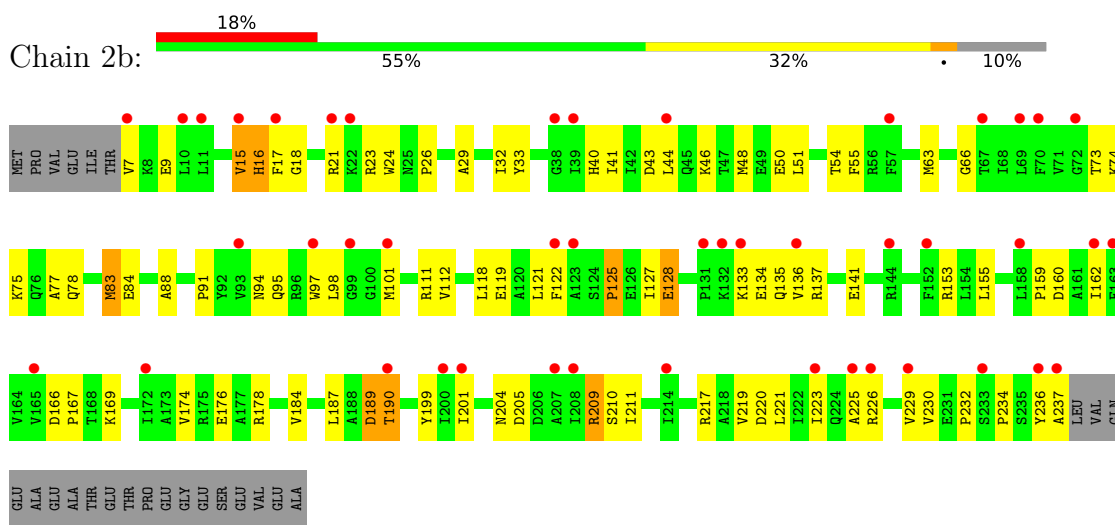
• Molecule 32: 16S Ribosomal RNA



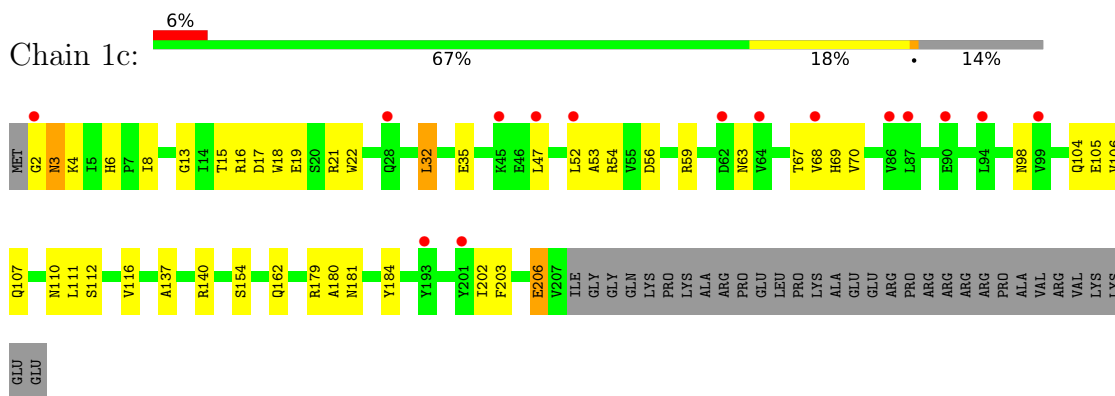




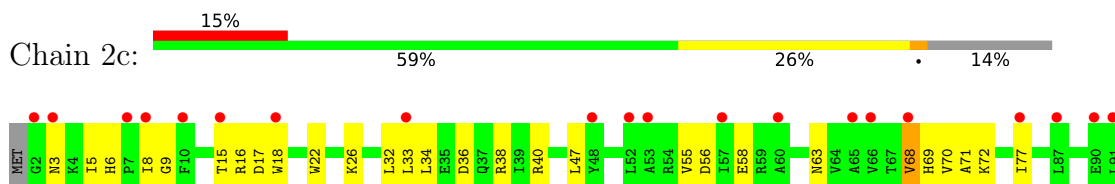
• Molecule 33: 30S ribosomal protein S2

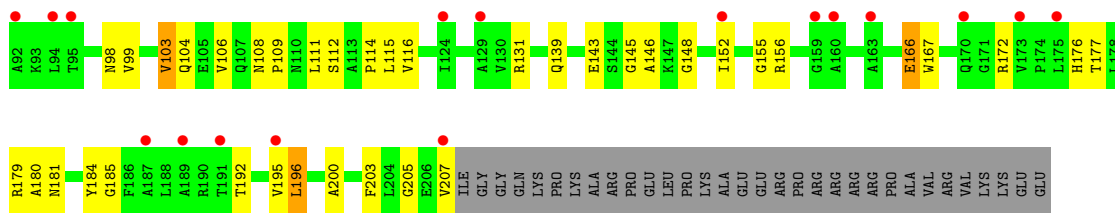


• Molecule 34: 30S ribosomal protein S3

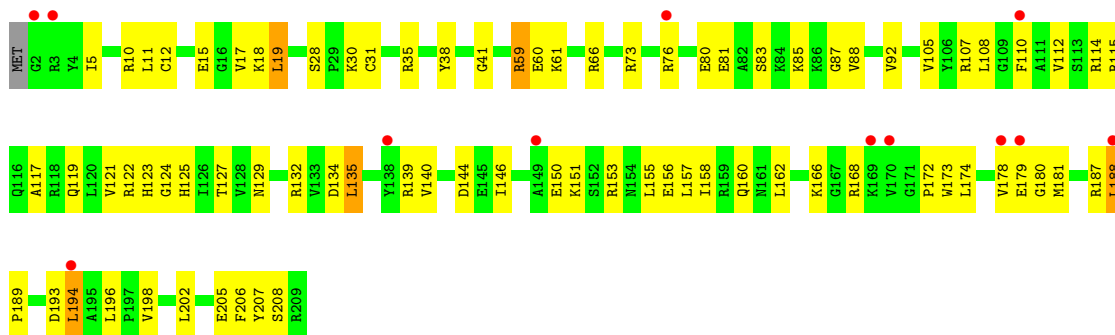


• Molecule 34: 30S ribosomal protein S3

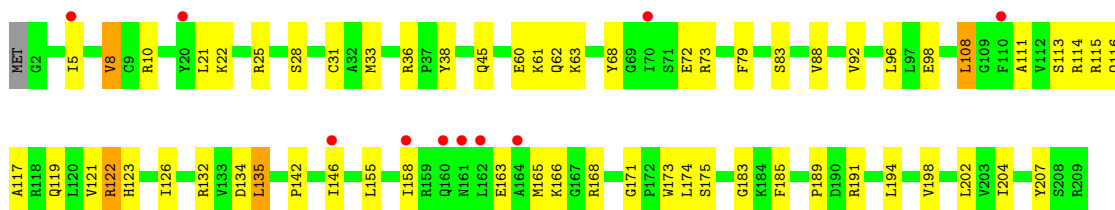




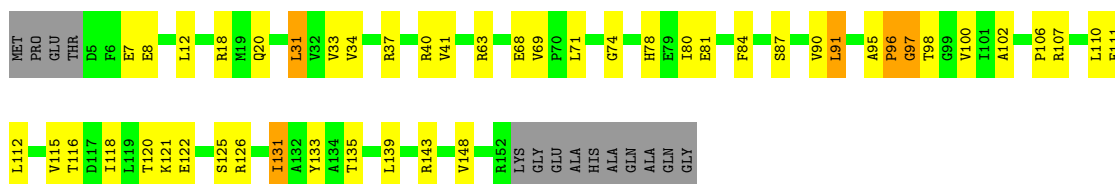
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

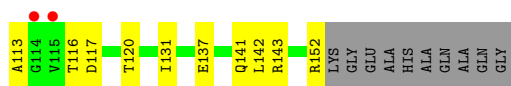


• Molecule 36: 30S ribosomal protein S5

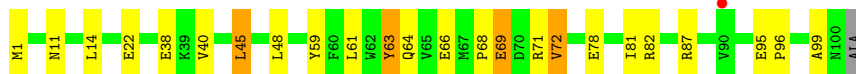
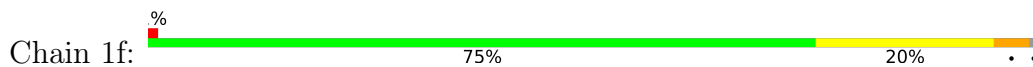


• Molecule 36: 30S ribosomal protein S5

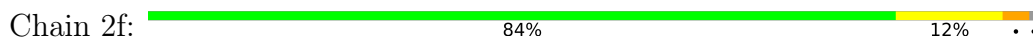




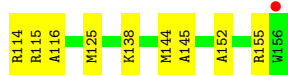
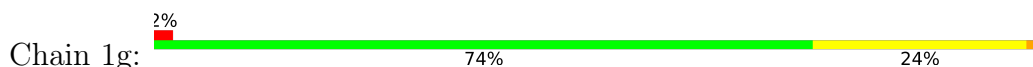
• Molecule 37: 30S ribosomal protein S6



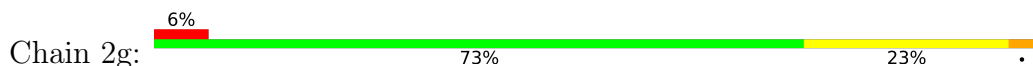
• Molecule 37: 30S ribosomal protein S6



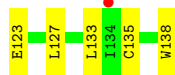
• Molecule 38: 30S ribosomal protein S7



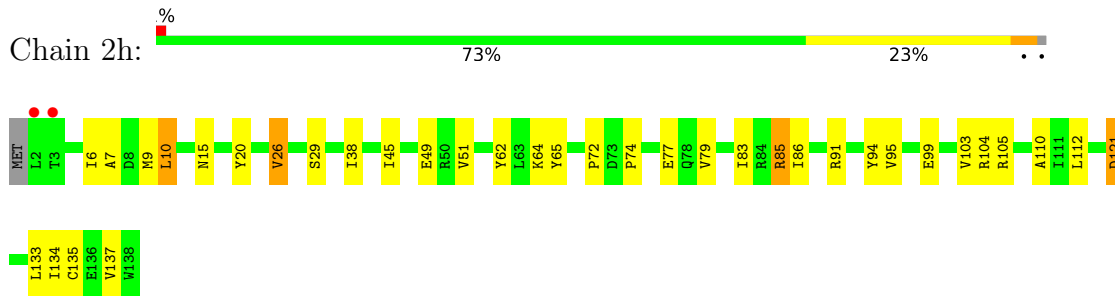
• Molecule 38: 30S ribosomal protein S7



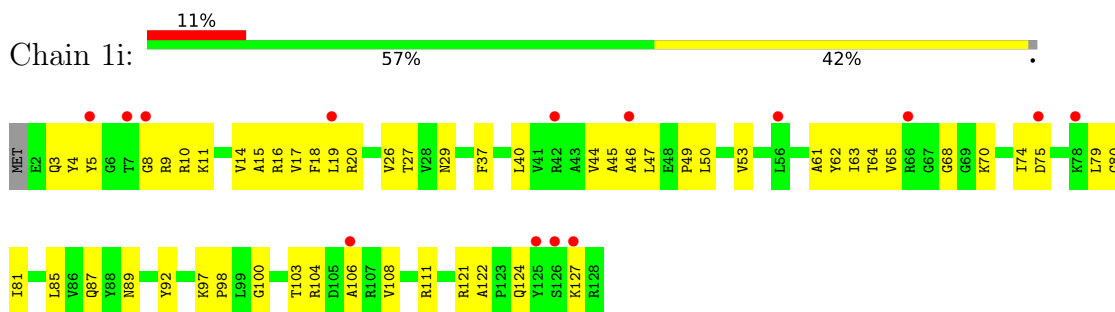
• Molecule 39: 30S ribosomal protein S8



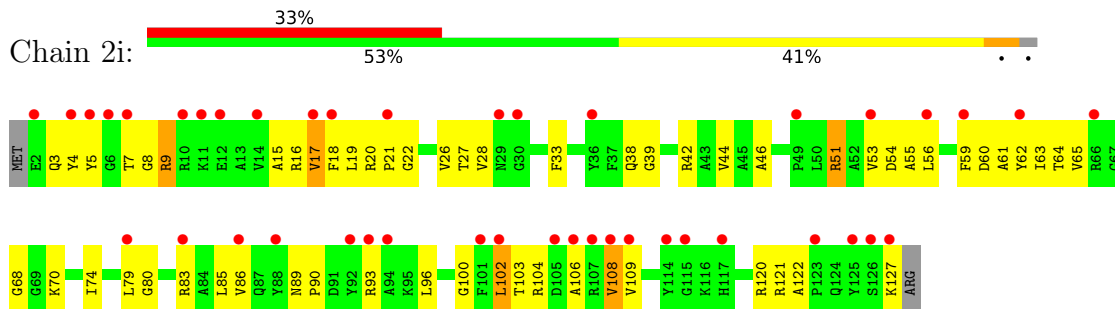
• Molecule 39: 30S ribosomal protein S8



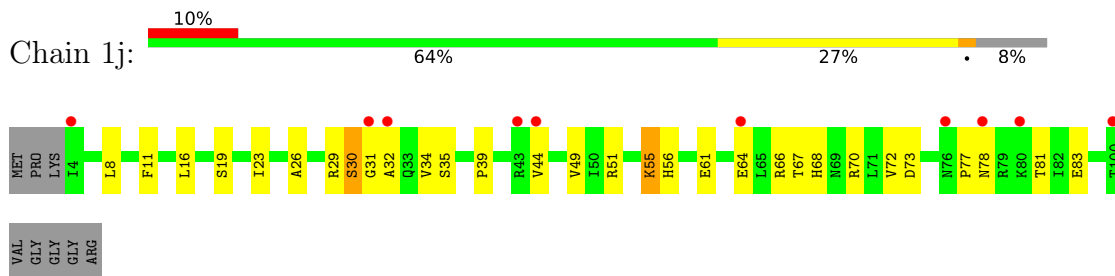
• Molecule 40: 30S ribosomal protein S9



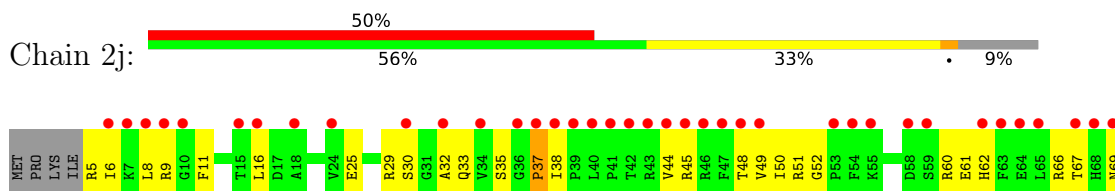
• Molecule 40: 30S ribosomal protein S9

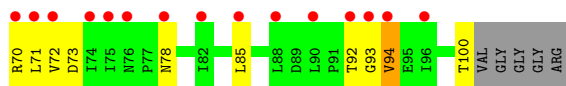


• Molecule 41: 30S ribosomal protein S10



• Molecule 41: 30S ribosomal protein S10

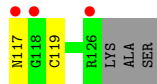




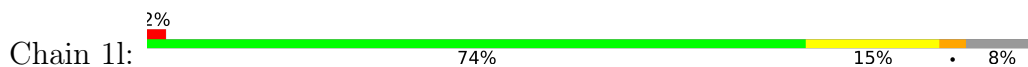
• Molecule 42: 30S ribosomal protein S11



• Molecule 42: 30S ribosomal protein S11



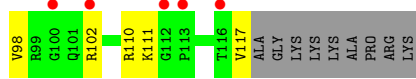
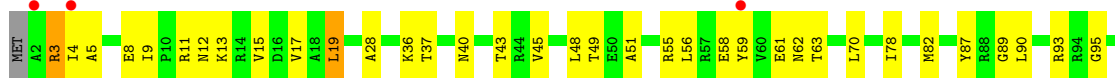
• Molecule 43: 30S ribosomal protein S12



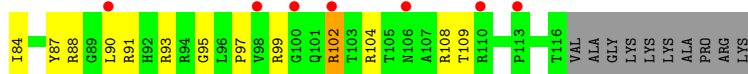
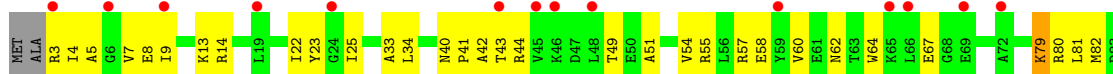
• Molecule 43: 30S ribosomal protein S12



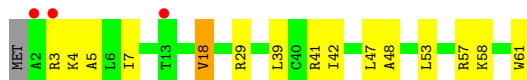
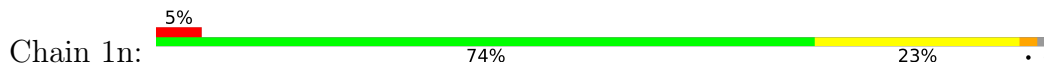
• Molecule 44: 30S ribosomal protein S13



• Molecule 44: 30S ribosomal protein S13



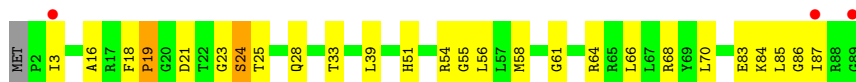
- Molecule 45: 30S ribosomal protein S14 type Z



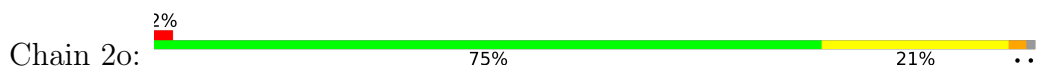
- Molecule 45: 30S ribosomal protein S14 type Z



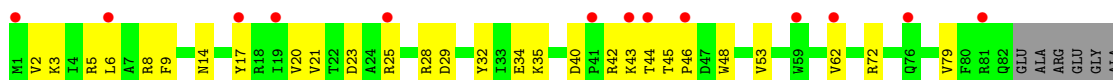
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15

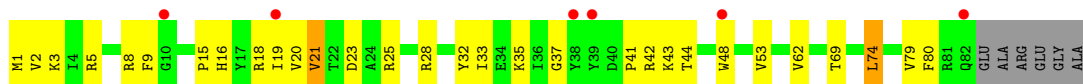


- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16

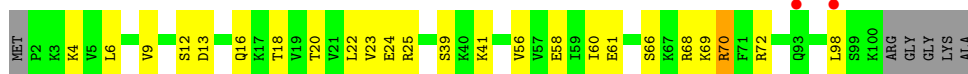




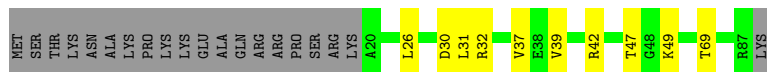
• Molecule 48: 30S ribosomal protein S17



• Molecule 48: 30S ribosomal protein S17



• Molecule 49: 30S ribosomal protein S18



• Molecule 49: 30S ribosomal protein S18

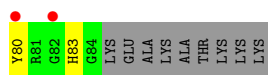


• Molecule 50: 30S ribosomal protein S19



• Molecule 50: 30S ribosomal protein S19

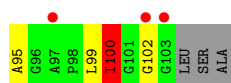
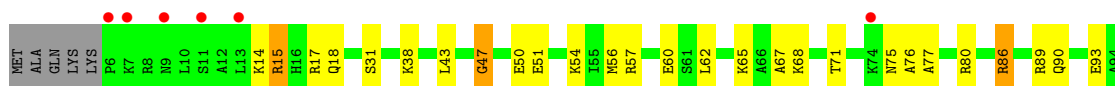




• Molecule 51: 30S ribosomal protein S20



• Molecule 51: 30S ribosomal protein S20



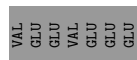
• Molecule 52: 30S ribosomal protein Thx



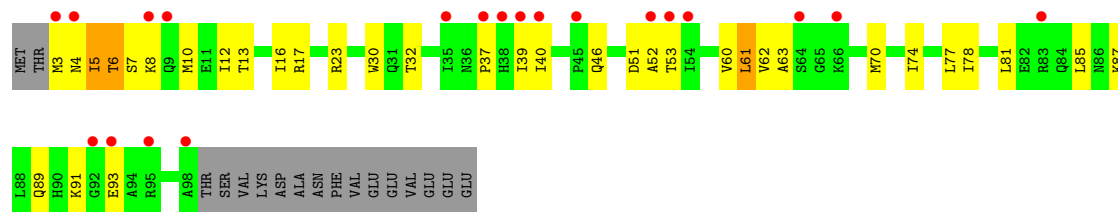
• Molecule 52: 30S ribosomal protein Thx



• 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, $\alpha$ , $\beta$ , $\gamma$	210.09Å 449.12Å 621.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.92 – 2.70 121.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (121.92-2.70) 99.2 (121.92-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.206 , 0.253 0.207 , 0.253	Depositor DCC
$R_{free}$ test set	79057 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtrriage
Anisotropy	0.142	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	295438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, 7MG, MPD, 2MA, 2MU, UR3, M2G, K, 5MU, 4OC, 5MC, 0TD, MA6, EZP, OMG, MG, SF4, ZN, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1A	0.29	0/69029	0.47	2/107746 (0.0%)
1	2A	0.23	0/68901	0.43	2/107544 (0.0%)
2	1B	0.24	0/2876	0.43	0/4486
2	2B	0.20	0/2878	0.38	0/4490
3	1D	0.29	0/2181	0.53	0/2940
3	2D	0.25	0/2186	0.52	2/2944 (0.1%)
4	1E	0.29	0/1592	0.52	0/2149
4	2E	0.24	0/1592	0.51	0/2149
5	1F	0.27	0/1619	0.50	0/2193
5	2F	0.22	0/1615	0.48	2/2188 (0.1%)
6	1G	0.22	0/1451	0.47	1/1961 (0.1%)
6	2G	0.23	0/1449	0.47	0/1957
7	1H	0.23	0/1356	0.45	0/1834
7	2H	0.20	0/1350	0.43	0/1826
8	1I	0.23	0/1109	0.47	0/1512
8	2I	0.19	0/1091	0.40	0/1490
9	1N	0.29	0/1148	0.48	0/1547
9	2N	0.20	0/1144	0.43	0/1543
10	1O	0.27	0/943	0.50	0/1269
10	2O	0.22	0/943	0.47	0/1269
11	1P	0.29	0/1152	0.52	0/1533
11	2P	0.23	0/1152	0.48	0/1533
12	1Q	0.28	0/1143	0.50	0/1527
12	2Q	0.21	0/1143	0.44	0/1527
13	1R	0.29	0/982	0.51	0/1312
13	2R	0.26	0/982	0.53	0/1312
14	1S	0.23	0/887	0.50	0/1180
14	2S	0.23	0/880	0.48	0/1172
15	1T	0.26	0/1105	0.52	0/1477
15	2T	0.23	0/1097	0.48	0/1468
16	1U	0.31	0/977	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.22	0/977	0.41	0/1301
17	1V	0.28	0/786	0.51	0/1053
17	2V	0.22	0/782	0.43	0/1049
18	1W	0.27	0/897	0.46	0/1205
18	2W	0.24	0/897	0.46	0/1205
19	1X	0.29	0/764	0.52	0/1025
19	2X	0.22	0/764	0.48	0/1025
20	1Y	0.28	0/823	0.64	2/1099 (0.2%)
20	2Y	0.21	0/823	0.44	0/1100
21	1Z	0.22	0/1620	0.45	0/2200
21	2Z	0.21	0/1590	0.45	1/2162 (0.0%)
22	10	0.27	0/616	0.52	0/821
22	20	0.27	0/616	0.47	0/821
23	11	0.28	0/761	0.47	0/1013
23	21	0.25	0/766	0.45	0/1018
24	12	0.23	0/590	0.46	0/781
24	22	0.22	0/594	0.50	1/785 (0.1%)
25	13	0.27	0/474	0.49	0/635
25	23	0.21	0/469	0.41	0/630
26	14	0.29	0/559	0.61	0/754
26	24	0.28	0/549	0.65	1/741 (0.1%)
27	15	0.30	0/473	0.55	0/639
27	25	0.26	0/469	0.48	0/635
28	16	0.27	0/460	0.51	0/613
28	26	0.24	0/456	0.43	0/608
29	17	0.34	0/426	0.59	0/561
29	27	0.26	0/426	0.51	0/561
30	18	0.30	0/525	0.50	0/691
30	28	0.23	0/525	0.45	0/691
31	19	0.31	0/310	0.50	0/407
31	29	0.23	0/310	0.43	0/407
32	1a	0.21	0/35795	0.40	0/55864
32	2a	0.20	0/35890	0.40	1/56012 (0.0%)
33	1b	0.24	0/1876	0.49	2/2533 (0.1%)
33	2b	0.27	0/1860	0.53	2/2518 (0.1%)
34	1c	0.21	0/1582	0.43	0/2137
34	2c	0.24	0/1566	0.45	0/2119
35	1d	0.22	0/1695	0.47	0/2274
35	2d	0.22	0/1698	0.47	0/2277
36	1e	0.23	0/1149	0.47	0/1548
36	2e	0.23	0/1149	0.50	1/1548 (0.1%)
37	1f	0.22	0/827	0.45	0/1120
37	2f	0.21	0/829	0.45	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.19	0/1254	0.43	0/1683
38	2g	0.20	0/1248	0.39	0/1676
39	1h	0.20	0/1118	0.43	0/1506
39	2h	0.21	0/1108	0.44	0/1494
40	1i	0.18	0/1005	0.46	0/1351
40	2i	0.23	0/985	0.48	0/1329
41	1j	0.27	0/732	0.46	0/993
41	2j	0.23	0/723	0.45	0/984
42	1k	0.22	0/849	0.44	0/1150
42	2k	0.24	0/848	0.54	1/1149 (0.1%)
43	1l	0.20	0/937	0.44	0/1260
43	2l	0.22	0/937	0.49	1/1260 (0.1%)
44	1m	0.20	0/924	0.44	0/1242
44	2m	0.28	0/905	0.59	1/1217 (0.1%)
45	1n	0.22	0/501	0.43	0/664
45	2n	0.23	0/501	0.43	0/664
46	1o	0.21	0/739	0.46	0/985
46	2o	0.19	0/739	0.43	0/985
47	1p	0.23	0/697	0.52	0/939
47	2p	0.23	0/693	0.47	0/935
48	1q	0.22	0/836	0.45	0/1117
48	2q	0.19	0/836	0.40	0/1117
49	1r	0.21	0/560	0.43	0/746
49	2r	0.19	0/560	0.42	0/746
50	1s	0.21	0/663	0.46	0/895
50	2s	0.19	0/660	0.42	0/893
51	1t	0.21	0/734	0.49	1/969 (0.1%)
51	2t	0.20	0/736	0.44	0/976
52	1u	0.16	0/203	0.42	0/266
52	2u	0.27	0/203	0.56	0/266
53	1y	0.28	0/776	0.41	0/1048
53	2y	0.18	0/761	0.38	0/1030
All	All	0.24	0/309937	0.44	24/463223 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
19	1X	0	1
26	24	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2m	5	ALA	CB-CA-C	-10.07	103.53	117.23
20	1Y	102	CYS	CA-C-O	8.42	122.83	117.94
24	22	41	ILE	N-CA-C	-7.54	105.20	112.29
3	2D	98	VAL	N-CA-C	-7.14	103.71	113.00
1	2A	1992	G	C2'-C3'-O3'	6.69	119.54	109.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	1X	93	GLU	Peptide
33	1b	127	ILE	Peptide
33	1b	231	GLU	Peptide
26	24	18	CYS	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	31201	585	0
1	2A	61758	0	31149	725	0
2	1B	2572	0	1305	17	0
2	2B	2573	0	1306	34	0
3	1D	2131	0	2207	48	0
3	2D	2136	0	2218	36	0
4	1E	1559	0	1618	33	0
4	2E	1559	0	1618	39	0
5	1F	1584	0	1625	35	0
5	2F	1580	0	1619	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	1G	1426	0	1445	42	0
6	2G	1424	0	1441	50	0
7	1H	1330	0	1407	26	0
7	2H	1324	0	1402	40	0
8	1I	1094	0	1127	35	0
8	2I	1076	0	1094	29	0
9	1N	1121	0	1195	18	0
9	2N	1117	0	1184	16	0
10	1O	933	0	996	15	0
10	2O	933	0	996	19	0
11	1P	1135	0	1212	30	0
11	2P	1135	0	1212	22	0
12	1Q	1122	0	1179	25	0
12	2Q	1122	0	1179	28	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	18	0
14	1S	877	0	938	16	0
14	2S	870	0	923	36	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	27	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	23	0
17	1V	775	0	841	12	0
17	2V	771	0	830	21	0
18	1W	886	0	940	11	0
18	2W	886	0	940	14	0
19	1X	750	0	814	16	0
19	2X	750	0	814	12	0
20	1Y	810	0	892	18	0
20	2Y	810	0	887	24	0
21	1Z	1587	0	1598	23	0
21	2Z	1557	0	1564	36	0
22	10	608	0	622	10	0
22	20	608	0	622	12	0
23	11	754	0	823	14	0
23	21	759	0	837	20	0
24	12	588	0	643	10	0
24	22	592	0	654	9	0
25	13	469	0	518	11	0
25	23	464	0	514	16	0
26	14	546	0	522	17	0
26	24	536	0	514	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	15	459	0	476	11	0
27	25	455	0	465	9	0
28	16	453	0	473	11	0
28	26	449	0	469	10	0
29	17	418	0	467	10	0
29	27	418	0	467	4	0
30	18	517	0	582	16	0
30	28	517	0	582	12	0
31	19	307	0	335	8	0
31	29	307	0	335	10	0
32	1a	32246	0	16296	430	0
32	2a	32331	0	16339	509	0
33	1b	1842	0	1862	50	0
33	2b	1825	0	1828	57	0
34	1c	1558	0	1557	32	0
34	2c	1542	0	1517	48	0
35	1d	1665	0	1687	62	0
35	2d	1668	0	1703	48	0
36	1e	1133	0	1191	35	0
36	2e	1133	0	1191	26	0
37	1f	814	0	808	15	0
37	2f	816	0	808	11	0
38	1g	1235	0	1249	27	0
38	2g	1229	0	1238	26	0
39	1h	1098	0	1143	27	0
39	2h	1088	0	1126	25	0
40	1i	986	0	990	41	0
40	2i	966	0	953	47	0
41	1j	719	0	672	20	0
41	2j	710	0	661	29	0
42	1k	834	0	838	10	0
42	2k	833	0	836	12	0
43	1l	932	0	981	18	0
43	2l	932	0	981	17	0
44	1m	914	0	954	23	0
44	2m	895	0	920	33	0
45	1n	492	0	529	13	0
45	2n	492	0	529	24	0
46	1o	728	0	760	21	0
46	2o	728	0	760	15	0
47	1p	681	0	697	20	0
47	2p	677	0	686	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	1q	823	0	891	25	0
48	2q	823	0	891	17	0
49	1r	555	0	618	6	0
49	2r	555	0	618	14	0
50	1s	648	0	658	17	0
50	2s	645	0	635	34	0
51	1t	732	0	809	20	0
51	2t	733	0	795	20	0
52	1u	199	0	208	6	0
52	2u	199	0	208	7	0
53	1y	764	0	786	16	0
53	2y	749	0	757	29	0
54	10	6	0	0	0	0
54	11	3	0	0	0	0
54	13	2	0	0	0	0
54	14	1	0	0	0	0
54	15	3	0	0	0	0
54	17	2	0	0	0	0
54	18	1	0	0	0	0
54	19	2	0	0	0	0
54	1A	1024	0	0	0	0
54	1B	29	0	0	0	0
54	1D	13	0	0	0	0
54	1E	7	0	0	0	0
54	1F	13	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	3	0	0	0	0
54	1O	2	0	0	0	0
54	1P	3	0	0	0	0
54	1Q	4	0	0	0	0
54	1R	3	0	0	0	0
54	1S	1	0	0	0	0
54	1T	3	0	0	0	0
54	1U	2	0	0	0	0
54	1V	3	0	0	0	0
54	1W	2	0	0	0	0
54	1X	2	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	255	0	0	0	0
54	1b	1	0	0	0	0
54	1d	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
54	1l	2	0	0	0	0
54	1n	1	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	1	0	0	0	0
54	21	1	0	0	0	0
54	25	1	0	0	0	0
54	28	3	0	0	0	0
54	2A	721	0	0	0	0
54	2B	19	0	0	0	0
54	2D	8	0	0	0	0
54	2E	6	0	0	0	0
54	2F	3	0	0	0	0
54	2G	3	0	0	0	0
54	2I	1	0	0	0	0
54	2N	1	0	0	0	0
54	2O	1	0	0	0	0
54	2P	2	0	0	0	0
54	2Q	2	0	0	0	0
54	2R	1	0	0	0	0
54	2T	4	0	0	0	0
54	2V	1	0	0	0	0
54	2W	2	0	0	0	0
54	2X	1	0	0	0	0
54	2a	151	0	0	0	0
54	2e	1	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2p	1	0	0	0	0
54	2q	1	0	0	0	0
54	2r	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	1	0	0	0	0
55	2A	1	0	0	0	0
56	1A	25	0	0	0	0
56	2A	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	18	8	0	14	1	0
57	1A	8	0	14	0	0
57	1T	8	0	14	1	0
57	1a	8	0	14	2	0
57	2A	16	0	28	2	0
57	2B	8	0	14	0	0
58	1B	12	0	12	3	0
58	1F	12	0	12	3	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	1	0
61	10	22	0	0	0	0
61	11	28	0	0	0	0
61	12	14	0	0	2	0
61	13	22	0	0	2	0
61	14	2	0	0	0	0
61	15	26	0	0	0	0
61	16	17	0	0	1	0
61	17	14	0	0	2	0
61	18	30	0	0	0	0
61	19	8	0	0	1	0
61	1A	2980	0	0	97	0
61	1B	105	0	0	3	0
61	1D	116	0	0	6	0
61	1E	76	0	0	4	0
61	1F	63	0	0	5	0
61	1G	22	0	0	0	0
61	1H	16	0	0	0	0
61	1I	7	0	0	1	0
61	1N	50	0	0	0	0
61	1O	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1P	58	0	0	4	0
61	1Q	42	0	0	4	0
61	1R	37	0	0	0	0
61	1S	13	0	0	1	0
61	1T	42	0	0	3	0
61	1U	45	0	0	4	0
61	1V	37	0	0	1	0
61	1W	24	0	0	0	0
61	1X	24	0	0	1	0
61	1Y	15	0	0	1	0
61	1Z	14	0	0	0	0
61	1a	261	0	0	16	0
61	1b	1	0	0	0	0
61	1d	9	0	0	2	0
61	1e	6	0	0	1	0
61	1f	3	0	0	0	0
61	1h	1	0	0	0	0
61	1i	1	0	0	0	0
61	1j	1	0	0	0	0
61	1k	1	0	0	0	0
61	1l	4	0	0	0	0
61	1n	1	0	0	1	0
61	1o	5	0	0	1	0
61	1p	3	0	0	0	0
61	1y	5	0	0	0	0
61	20	13	0	0	2	0
61	21	24	0	0	5	0
61	22	5	0	0	0	0
61	23	3	0	0	1	0
61	24	2	0	0	0	0
61	25	9	0	0	1	0
61	26	6	0	0	1	0
61	27	7	0	0	0	0
61	28	15	0	0	1	0
61	29	2	0	0	0	0
61	2A	1686	0	0	85	0
61	2B	65	0	0	6	0
61	2D	52	0	0	2	0
61	2E	25	0	0	1	0
61	2F	21	0	0	3	0
61	2G	7	0	0	0	0
61	2H	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2I	4	0	0	0	0
61	2N	6	0	0	0	0
61	2O	22	0	0	0	0
61	2P	23	0	0	0	0
61	2Q	30	0	0	0	0
61	2R	21	0	0	1	0
61	2S	8	0	0	2	0
61	2T	10	0	0	0	0
61	2U	14	0	0	2	0
61	2V	9	0	0	0	0
61	2W	21	0	0	0	0
61	2X	9	0	0	0	0
61	2Y	3	0	0	0	0
61	2Z	15	0	0	3	0
61	2a	100	0	0	6	0
61	2d	6	0	0	1	0
61	2e	1	0	0	0	0
61	2f	1	0	0	0	0
61	2j	2	0	0	1	0
61	2l	1	0	0	0	0
61	2m	1	0	0	0	0
61	2o	2	0	0	0	0
61	2p	1	0	0	0	0
61	2q	1	0	0	0	0
61	2r	4	0	0	1	0
61	2y	1	0	0	0	0
All	All	295438	0	194513	4034	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 9.

The worst 5 of 4034 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:1128:U:H3	1:1A:1132:A:N6	1.36	1.23
1:1A:2159:C:N4	1:1A:2176:G:H1	1.50	1.09
32:1a:78:G:H1	32:1a:91:C:N4	1.57	1.02
1:2A:2139:C:N4	1:2A:2152:G:H1	1.56	1.01
1:1A:2331:G:H22	14:1S:3:ARG:HD3	1.23	1.01

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%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24	48
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24	48
5	1F	201/210 (96%)	191 (95%)	9 (4%)	1 (0%)	24	48
5	2F	201/210 (96%)	191 (95%)	7 (4%)	3 (2%)	8	22
6	1G	179/182 (98%)	163 (91%)	15 (8%)	1 (1%)	21	44
6	2G	179/182 (98%)	166 (93%)	10 (6%)	3 (2%)	7	19
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21	44
7	2H	171/180 (95%)	152 (89%)	19 (11%)	0	100	100
8	1I	145/148 (98%)	129 (89%)	15 (10%)	1 (1%)	18	41
8	2I	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	9	23
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	18	41
10	1O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	37
10	2O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	37
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	41
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18	41
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18	41
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	14	35
14	2S	108/112 (96%)	96 (89%)	12 (11%)	0	100	100
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	12	32
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	32
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	29
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11	29
20	1Y	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
21	1Z	201/206 (98%)	189 (94%)	12 (6%)	0	100	100
21	2Z	199/206 (97%)	183 (92%)	16 (8%)	0	100	100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	20	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	29
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	29
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	1 (2%)	1 (2%)	6	18
26	14	67/71 (94%)	52 (78%)	12 (18%)	3 (4%)	2	4
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	1
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	55 (96%)	1 (2%)	1 (2%)	6	18
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	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%)	200 (87%)	20 (9%)	9 (4%)	2	5
33	2b	229/256 (90%)	200 (87%)	22 (10%)	7 (3%)	3	8
34	1c	204/239 (85%)	191 (94%)	12 (6%)	1 (0%)	24	48
34	2c	204/239 (85%)	172 (84%)	29 (14%)	3 (2%)	8	22
35	1d	206/209 (99%)	192 (93%)	13 (6%)	1 (0%)	24	48
35	2d	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	24	48
36	1e	146/162 (90%)	141 (97%)	3 (2%)	2 (1%)	9	23
36	2e	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
38	1g	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	18	41
38	2g	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	9	25
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	18	41
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	37
40	2i	124/128 (97%)	111 (90%)	10 (8%)	3 (2%)	4	12
41	1j	95/105 (90%)	77 (81%)	15 (16%)	3 (3%)	3	7
41	2j	94/105 (90%)	80 (85%)	12 (13%)	2 (2%)	5	15
42	1k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	14	35
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	14	35
43	1l	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
43	2l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
44	1m	114/126 (90%)	104 (91%)	8 (7%)	2 (2%)	6	18
44	2m	112/126 (89%)	98 (88%)	12 (11%)	2 (2%)	6	18
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	1 (1%)	3 (4%)	3	6
46	2o	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	10	27
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	9	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	68 (85%)	11 (14%)	1 (1%)	9	25
48	1q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	4	11
50	2s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
51	1t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	5	15
51	2t	96/106 (91%)	89 (93%)	3 (3%)	4 (4%)	2	4
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	16 (76%)	4 (19%)	1 (5%)	2	3
53	1y	95/113 (84%)	90 (95%)	5 (5%)	0	100	100
53	2y	94/113 (83%)	88 (94%)	6 (6%)	0	100	100
All	All	11629/12354 (94%)	10827 (93%)	706 (6%)	96 (1%)	16	37

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	14	47	GLN
26	14	55	ARG
33	1b	21	ARG
4	2E	51	PHE
6	2G	78	SER

### 5.3.2 Protein sidechains [i](#)

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%)	192 (90%)	22 (10%)	7	18
3	2D	215/218 (99%)	195 (91%)	20 (9%)	8	21
4	1E	164/166 (99%)	150 (92%)	14 (8%)	10	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	150 (92%)	14 (8%)	10	25
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8	21
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	21
6	1G	144/156 (92%)	128 (89%)	16 (11%)	6	15
6	2G	142/156 (91%)	127 (89%)	15 (11%)	6	17
7	1H	144/148 (97%)	137 (95%)	7 (5%)	22	49
7	2H	143/148 (97%)	133 (93%)	10 (7%)	14	34
8	1I	111/124 (90%)	101 (91%)	10 (9%)	9	23
8	2I	108/124 (87%)	101 (94%)	7 (6%)	15	37
9	1N	119/119 (100%)	112 (94%)	7 (6%)	18	42
9	2N	118/119 (99%)	110 (93%)	8 (7%)	14	35
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22	48
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36	66
11	1P	115/116 (99%)	109 (95%)	6 (5%)	21	47
11	2P	115/116 (99%)	108 (94%)	7 (6%)	17	40
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	20	45
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	31	60
13	1R	101/101 (100%)	91 (90%)	10 (10%)	7	19
13	2R	101/101 (100%)	89 (88%)	12 (12%)	5	13
14	1S	87/88 (99%)	80 (92%)	7 (8%)	11	28
14	2S	85/88 (97%)	78 (92%)	7 (8%)	10	27
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	34
15	2T	113/127 (89%)	105 (93%)	8 (7%)	13	33
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15	37
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26	54
17	1V	81/82 (99%)	73 (90%)	8 (10%)	7	19
17	2V	80/82 (98%)	75 (94%)	5 (6%)	16	39
18	1W	90/92 (98%)	80 (89%)	10 (11%)	6	15
18	2W	90/92 (98%)	81 (90%)	9 (10%)	7	19
19	1X	77/78 (99%)	72 (94%)	5 (6%)	15	37
19	2X	77/78 (99%)	72 (94%)	5 (6%)	15	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	86/91 (94%)	78 (91%)	8 (9%)	8	21
20	2Y	86/91 (94%)	82 (95%)	4 (5%)	23	51
21	1Z	169/179 (94%)	153 (90%)	16 (10%)	8	20
21	2Z	165/179 (92%)	158 (96%)	7 (4%)	26	55
22	10	61/67 (91%)	58 (95%)	3 (5%)	22	49
22	20	61/67 (91%)	60 (98%)	1 (2%)	55	80
23	11	79/83 (95%)	75 (95%)	4 (5%)	21	48
23	21	81/83 (98%)	77 (95%)	4 (5%)	22	49
24	12	65/67 (97%)	64 (98%)	1 (2%)	57	81
24	22	66/67 (98%)	63 (96%)	3 (4%)	24	52
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	29
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	41
26	14	58/63 (92%)	55 (95%)	3 (5%)	21	47
26	24	54/63 (86%)	53 (98%)	1 (2%)	50	77
27	15	51/52 (98%)	44 (86%)	7 (14%)	3	9
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	41
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	29
28	26	50/52 (96%)	46 (92%)	4 (8%)	11	28
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	12
29	27	41/42 (98%)	40 (98%)	1 (2%)	43	72
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	32
30	28	54/55 (98%)	49 (91%)	5 (9%)	8	21
31	19	34/34 (100%)	32 (94%)	2 (6%)	18	42
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	42
33	1b	191/220 (87%)	177 (93%)	14 (7%)	13	32
33	2b	187/220 (85%)	178 (95%)	9 (5%)	23	50
34	1c	144/188 (77%)	138 (96%)	6 (4%)	26	55
34	2c	140/188 (74%)	132 (94%)	8 (6%)	18	43
35	1d	171/181 (94%)	161 (94%)	10 (6%)	18	42
35	2d	172/181 (95%)	166 (96%)	6 (4%)	32	61
36	1e	114/123 (93%)	109 (96%)	5 (4%)	25	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	114/123 (93%)	107 (94%)	7 (6%)	17	40
37	1f	85/90 (94%)	79 (93%)	6 (7%)	13	33
37	2f	85/90 (94%)	82 (96%)	3 (4%)	32	61
38	1g	120/127 (94%)	114 (95%)	6 (5%)	22	48
38	2g	119/127 (94%)	112 (94%)	7 (6%)	18	42
39	1h	116/119 (98%)	109 (94%)	7 (6%)	17	41
39	2h	114/119 (96%)	104 (91%)	10 (9%)	9	23
40	1i	91/99 (92%)	89 (98%)	2 (2%)	45	74
40	2i	88/99 (89%)	82 (93%)	6 (7%)	14	35
41	1j	68/92 (74%)	66 (97%)	2 (3%)	37	67
41	2j	68/92 (74%)	65 (96%)	3 (4%)	25	53
42	1k	83/99 (84%)	78 (94%)	5 (6%)	17	41
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	20
43	1l	96/108 (89%)	91 (95%)	5 (5%)	21	47
43	2l	96/108 (89%)	93 (97%)	3 (3%)	35	65
44	1m	90/101 (89%)	84 (93%)	6 (7%)	15	36
44	2m	87/101 (86%)	82 (94%)	5 (6%)	18	43
45	1n	49/50 (98%)	47 (96%)	2 (4%)	27	56
45	2n	49/50 (98%)	48 (98%)	1 (2%)	48	76
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21	48
46	2o	78/80 (98%)	77 (99%)	1 (1%)	61	83
47	1p	69/74 (93%)	66 (96%)	3 (4%)	26	54
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9	23
48	1q	94/97 (97%)	90 (96%)	4 (4%)	26	54
48	2q	94/97 (97%)	90 (96%)	4 (4%)	26	54
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32	62
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	18
50	1s	68/80 (85%)	67 (98%)	1 (2%)	57	81
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	23
51	1t	71/82 (87%)	67 (94%)	4 (6%)	19	44
51	2t	70/82 (85%)	63 (90%)	7 (10%)	7	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	44
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	44
53	1y	82/98 (84%)	75 (92%)	7 (8%)	10	25
53	2y	79/98 (81%)	74 (94%)	5 (6%)	16	39
All	All	9524/10260 (93%)	8896 (93%)	628 (7%)	15	36

5 of 628 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	2V	79	VAL
41	2j	94	VAL
19	2X	57	LEU
17	2V	72	VAL
33	2b	112	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
37	2f	100	ASN
38	2g	56	GLN
45	2n	49	HIS
35	1d	45	GLN
34	1c	162	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	421 (14%)	29 (1%)
1	2A	2858/2915 (98%)	493 (17%)	36 (1%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	119/121 (98%)	18 (15%)	0
32	1a	1497/1521 (98%)	234 (15%)	0
32	2a	1501/1521 (98%)	262 (17%)	0
All	All	8959/9114 (98%)	1439 (16%)	65 (0%)

5 of 1439 RNA backbone outliers are listed below:

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

5 of 65 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	2288	A
1	2A	2321	G
1	1A	2418	U
1	1A	2250	G
1	2A	2406	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
32	5MC	1a	1400	32	19,22,23	1.80	3 (15%)	26,32,35	1.18	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.71	2 (10%)	26,32,35	1.21	3 (11%)
32	4OC	1a	1402	32	20,23,24	0.72	0	25,32,35	0.99	2 (8%)
32	5MC	2a	1407	32	19,22,23	1.63	3 (15%)	26,32,35	1.18	3 (11%)
1	5MU	1A	1937	1	19,22,23	1.44	5 (26%)	27,32,35	2.22	8 (29%)
1	2MU	1A	2564	54,1	19,22,24	1.34	4 (21%)	25,31,36	1.87	6 (24%)
32	7MG	1a	527	54,32	23,26,27	1.40	3 (13%)	27,39,42	2.43	6 (22%)
32	PSU	1a	516	54,32	18,21,22	1.40	2 (11%)	21,30,33	1.93	4 (19%)
32	PSU	2a	516	54,32	18,21,22	1.33	2 (11%)	21,30,33	2.07	5 (23%)
1	PSU	1A	2617	54,1	18,21,22	1.39	3 (16%)	21,30,33	1.94	5 (23%)
32	5MC	2a	1404	32	19,22,23	1.76	3 (15%)	26,32,35	1.24	4 (15%)
1	5MU	2A	1939	1	19,22,23	1.45	5 (26%)	27,32,35	2.30	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	UR3	1a	1498	32	19,22,23	0.96	1 (5%)	26,32,35	1.85	4 (15%)
32	2MG	1a	1207	32	23,26,27	1.24	2 (8%)	33,38,41	2.46	10 (30%)
43	0TD	2l	92	43	8,9,10	4.44	1 (12%)	6,11,13	4.29	3 (50%)
1	4OC	1A	1942	1	19,22,24	0.80	0	25,31,35	0.90	1 (4%)
1	PSU	1A	1933	1	18,21,22	1.39	2 (11%)	21,30,33	2.18	5 (23%)
32	MA6	1a	1518	32	23,26,27	1.56	5 (21%)	33,38,41	2.21	12 (36%)
1	PSU	2A	2605	1	18,21,22	1.41	3 (16%)	21,30,33	1.96	5 (23%)
1	5MU	1A	1961	54,1	19,22,23	1.44	5 (26%)	27,32,35	2.21	6 (22%)
1	5MC	1A	1984	54,1	19,22,23	1.65	3 (15%)	26,32,35	1.22	4 (15%)
32	5MC	1a	1404	32	19,22,23	1.68	3 (15%)	26,32,35	1.14	3 (11%)
32	2MG	2a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.07	8 (24%)
1	OMG	1A	2263	54,1	23,26,27	1.27	3 (13%)	32,38,41	2.07	6 (18%)
32	MA6	2a	1519	32	23,26,27	1.56	5 (21%)	33,38,41	2.40	13 (39%)
32	M2G	1a	966	32	24,27,28	1.28	3 (12%)	33,40,43	1.83	6 (18%)
43	0TD	1l	92	43	8,9,10	4.56	1 (12%)	6,11,13	3.20	3 (50%)
32	4OC	2a	1402	32	20,23,24	0.77	0	25,32,35	1.11	1 (4%)
1	5MC	2A	1942	1	19,22,23	1.70	3 (15%)	26,32,35	1.20	2 (7%)
32	MA6	1a	1519	32	23,26,27	1.56	5 (21%)	33,38,41	2.20	11 (33%)
1	5MU	2A	1915	1	19,22,23	1.43	4 (21%)	27,32,35	2.21	8 (29%)
1	4OC	2A	1920	1	19,22,24	0.80	0	25,31,35	0.95	1 (4%)
32	5MC	2a	967	32	19,22,23	2.03	3 (15%)	26,32,35	1.19	3 (11%)
1	2MA	1A	2515	54,1	22,25,26	1.45	5 (22%)	32,37,40	2.36	7 (21%)
32	UR3	2a	1498	54,32	19,22,23	0.95	1 (5%)	26,32,35	1.79	3 (11%)
1	5MC	1A	1964	54,1	19,22,23	1.47	3 (15%)	26,32,35	1.11	2 (7%)
1	5MC	2A	1962	54,1	19,22,23	1.53	3 (15%)	26,32,35	1.09	2 (7%)
1	OMG	2A	2251	54,1	23,26,27	1.17	3 (13%)	32,38,41	2.01	7 (21%)
32	MA6	2a	1518	32	23,26,27	1.64	4 (17%)	33,38,41	2.23	12 (36%)
32	M2G	2a	966	32	24,27,28	1.38	4 (16%)	33,40,43	1.83	5 (15%)
1	PSU	1A	1939	1	18,21,22	1.35	2 (11%)	21,30,33	1.87	4 (19%)
32	5MC	1a	967	32	19,22,23	1.59	3 (15%)	26,32,35	1.14	2 (7%)
32	7MG	2a	527	54,32	23,26,27	1.34	4 (17%)	27,39,42	2.58	5 (18%)
32	5MC	2a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.21	2 (7%)
1	2MU	2A	2552	54,1	19,22,24	1.23	3 (15%)	25,31,36	2.02	6 (24%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	2.09	3 (14%)
1	2MA	2A	2503	54,1	22,25,26	1.41	5 (22%)	32,37,40	2.35	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	2A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.06	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
32	5MC	1a	1407	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	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	2/7/25/26	0/2/2/2
1	2MU	1A	2564	54,1	-	0/9/27/28	0/2/2/2
32	7MG	1a	527	54,32	-	1/7/37/38	0/3/3/3
32	PSU	1a	516	54,32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	54,32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	54,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
43	0TD	2l	92	43	-	1/7/12/14	-
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	3/11/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	54,1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	54,1	-	2/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	OMG	1A	2263	54,1	-	1/9/27/28	0/3/3/3
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
43	0TD	1l	92	43	-	3/7/12/14	-
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	54,1	-	2/7/25/26	0/3/3/3
32	UR3	2a	1498	54,32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	54,1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	54,1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	54,1	-	0/9/27/28	0/3/3/3
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	54,32	-	0/7/37/38	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	54,1	-	1/7/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2

The worst 5 of 137 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.47	1.69	1.82
43	2l	92	0TD	CB-SB	-12.21	1.70	1.82
32	2a	967	5MC	C5-C4	7.77	1.50	1.44
32	1a	1400	5MC	C5-C4	6.69	1.49	1.44
32	2a	1404	5MC	C5-C4	6.56	1.49	1.44

The worst 5 of 242 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-9.81	84.73	102.36
1	1A	2515	2MA	C5-C4-N3	-8.66	118.06	127.18
32	2a	527	7MG	N9-C4-N3	8.50	137.92	125.46
32	1a	527	7MG	N9-C4-N3	8.21	137.50	125.46
1	2A	2503	2MA	C5-C4-N3	-7.68	119.09	127.18

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C1'-N1-C2
1	1A	1937	5MU	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1518	MA6	C5-C6-N6-C9

There are no ring outliers.

23 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1400	5MC	2	0
32	1a	1402	4OC	1	0
1	1A	2564	2MU	1	0
32	1a	527	7MG	1	0
1	2A	1939	5MU	2	0
43	2l	92	0TD	1	0
1	1A	1942	4OC	1	0
32	1a	1518	MA6	1	0
32	2a	1207	2MG	3	0
32	2a	1519	MA6	1	0
43	1l	92	0TD	1	0
32	2a	1402	4OC	3	0
32	1a	1519	MA6	2	0
1	2A	1915	5MU	1	0
32	2a	967	5MC	1	0
1	1A	2515	2MA	1	0
1	1A	1964	5MC	1	0
1	2A	2251	OMG	1	0
32	2a	1518	MA6	1	0
32	1a	967	5MC	1	0
32	2a	1400	5MC	2	0
1	2A	1917	PSU	1	0
1	2A	1911	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2389 ligands modelled in this entry, 2376 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
57	MPD	18	102	-	7,7,7	0.31	0	9,10,10	0.38	0
57	MPD	2B	3020	-	7,7,7	0.31	0	9,10,10	0.31	0
58	ARG	1B	228	54	10,11,11	0.76	1 (10%)	9,13,13	1.07	1 (11%)
57	MPD	1T	204	-	7,7,7	0.35	0	9,10,10	0.37	0
56	EZP	1A	3987	-	26,26,26	2.59	3 (11%)	32,35,35	1.55	4 (12%)
57	MPD	2A	3711	-	7,7,7	0.32	0	9,10,10	0.27	0
58	ARG	1F	314	-	10,11,11	0.72	0	9,13,13	0.86	1 (11%)
57	MPD	2A	3710	-	7,7,7	0.41	0	9,10,10	0.33	0
60	SF4	2d	501	35	0,12,12	-	-	-	-	-
57	MPD	1A	3988	-	7,7,7	0.31	0	9,10,10	0.28	0
60	SF4	1d	302	35	0,12,12	-	-	-	-	-
56	EZP	2A	3709	-	26,26,26	3.25	3 (11%)	32,35,35	0.85	1 (3%)
57	MPD	1a	1854	-	7,7,7	0.41	0	9,10,10	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	18	102	-	-	3/5/5/5	-
57	MPD	2B	3020	-	-	5/5/5/5	-
58	ARG	1B	228	54	-	4/11/11/11	-
57	MPD	1T	204	-	-	1/5/5/5	-
56	EZP	1A	3987	-	-	8/24/26/26	0/2/2/2
57	MPD	2A	3711	-	-	3/5/5/5	-
58	ARG	1F	314	-	-	3/11/11/11	-
57	MPD	2A	3710	-	-	0/5/5/5	-
60	SF4	2d	501	35	-	-	0/6/5/5
57	MPD	1A	3988	-	-	3/5/5/5	-
60	SF4	1d	302	35	-	-	0/6/5/5
56	EZP	2A	3709	-	-	8/24/26/26	0/2/2/2
57	MPD	1a	1854	-	-	3/5/5/5	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2A	3709	EZP	OAC-NAY	13.29	1.45	1.22
56	1A	3987	EZP	OAC-NAY	9.03	1.38	1.22
56	2A	3709	EZP	CAT-CAW	-8.15	1.39	1.51
56	1A	3987	EZP	CAT-CAW	-7.51	1.40	1.51
56	1A	3987	EZP	CAU-NAY	-4.66	1.34	1.45

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	3987	EZP	CAT-CAW-CAX	4.85	120.42	111.72
56	1A	3987	EZP	CAW-CAX-NAP	4.58	118.30	110.03
58	1B	228	ARG	OXT-C-O	-2.67	118.01	124.08
58	1F	314	ARG	OXT-C-O	-2.43	118.57	124.08
56	2A	3709	EZP	CAW-CAX-NAP	2.39	114.35	110.03

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	1A	3987	EZP	NAP-C-CA-CB
56	1A	3987	EZP	O-C-CA-CB
56	1A	3987	EZP	C-CA-CB-CG
56	2A	3709	EZP	NAP-C-CA-N
56	2A	3709	EZP	NAP-C-CA-CB

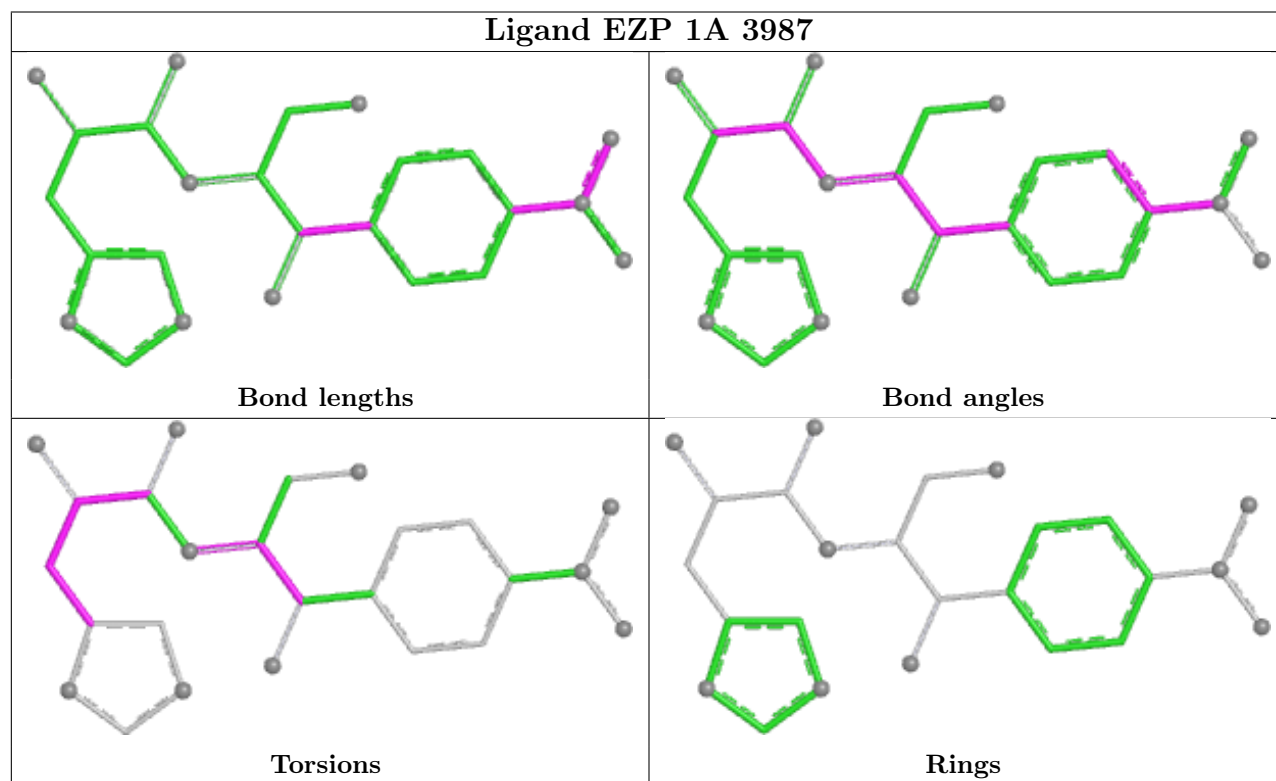
There are no ring outliers.

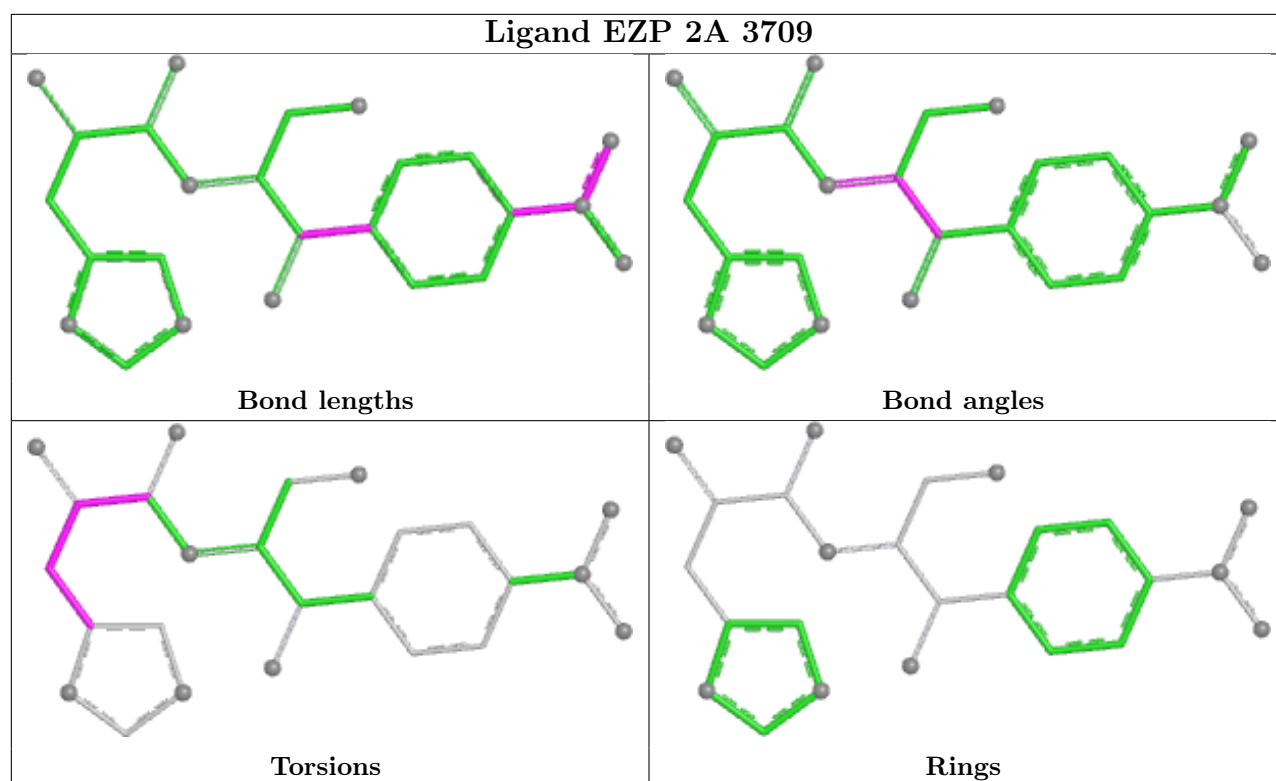
7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	18	102	MPD	1	0
58	1B	228	ARG	3	0
57	1T	204	MPD	1	0
58	1F	314	ARG	3	0
57	2A	3710	MPD	2	0
60	2d	501	SF4	1	0
57	1a	1854	MPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1A	2861/2915 (98%)	-0.65	114 (3%) 42 38	15, 31, 89, 105	0
1	2A	2856/2915 (97%)	-0.19	134 (4%) 36 33	27, 50, 92, 103	0
2	1B	120/121 (99%)	-0.53	1 (0%) 82 81	24, 44, 58, 80	0
2	2B	120/121 (99%)	0.72	8 (6%) 24 21	52, 74, 83, 90	0
3	1D	275/276 (99%)	-0.35	1 (0%) 88 87	17, 32, 46, 65	0
3	2D	275/276 (99%)	-0.01	2 (0%) 84 83	26, 44, 56, 76	0
4	1E	204/206 (99%)	-0.28	1 (0%) 87 86	16, 34, 55, 70	0
4	2E	204/206 (99%)	0.14	3 (1%) 72 70	29, 50, 66, 79	0
5	1F	203/210 (96%)	-0.22	1 (0%) 87 86	16, 35, 60, 83	0
5	2F	203/210 (96%)	0.25	0 100 100	29, 60, 72, 85	0
6	1G	181/182 (99%)	0.33	4 (2%) 62 59	39, 56, 72, 80	0
6	2G	181/182 (99%)	1.21	25 (13%) 6 5	68, 77, 85, 89	0
7	1H	174/180 (96%)	0.01	2 (1%) 78 76	32, 46, 59, 64	0
7	2H	173/180 (96%)	0.97	11 (6%) 25 22	62, 75, 82, 86	0
8	1I	147/148 (99%)	0.57	5 (3%) 48 44	34, 66, 76, 83	0
8	2I	146/148 (98%)	0.85	10 (6%) 23 20	51, 69, 81, 84	0
9	1N	140/140 (100%)	-0.34	0 100 100	22, 32, 53, 67	0
9	2N	140/140 (100%)	0.23	0 100 100	43, 57, 71, 76	0
10	1O	122/122 (100%)	-0.33	0 100 100	23, 34, 50, 58	0
10	2O	122/122 (100%)	0.15	1 (0%) 82 81	38, 51, 61, 69	0
11	1P	149/150 (99%)	-0.20	0 100 100	15, 38, 58, 71	0
11	2P	149/150 (99%)	0.28	3 (2%) 65 62	32, 59, 77, 80	0
12	1Q	141/141 (100%)	-0.30	0 100 100	21, 35, 46, 62	0
12	2Q	141/141 (100%)	0.46	3 (2%) 63 61	40, 57, 67, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	-0.42	0 100 100	21, 29, 44, 50	0
13	2R	118/118 (100%)	-0.07	0 100 100	31, 44, 55, 65	0
14	1S	110/112 (98%)	0.03	1 (0%) 81 80	34, 45, 56, 65	0
14	2S	110/112 (98%)	1.17	16 (14%) 6 5	59, 69, 76, 81	0
15	1T	131/146 (89%)	-0.13	4 (3%) 51 48	28, 38, 62, 75	0
15	2T	131/146 (89%)	0.13	1 (0%) 82 81	41, 52, 70, 76	0
16	1U	116/118 (98%)	-0.52	0 100 100	18, 25, 39, 57	0
16	2U	116/118 (98%)	0.25	1 (0%) 81 80	33, 52, 67, 74	0
17	1V	101/101 (100%)	-0.47	0 100 100	15, 35, 54, 67	0
17	2V	101/101 (100%)	0.38	0 100 100	31, 62, 72, 77	0
18	1W	112/113 (99%)	-0.47	0 100 100	19, 27, 46, 75	0
18	2W	112/113 (99%)	0.01	1 (0%) 81 80	29, 43, 59, 84	0
19	1X	95/96 (98%)	-0.25	1 (1%) 78 76	23, 32, 58, 68	0
19	2X	95/96 (98%)	0.43	1 (1%) 78 76	43, 54, 69, 74	0
20	1Y	107/110 (97%)	0.02	1 (0%) 81 80	29, 42, 62, 67	0
20	2Y	107/110 (97%)	0.91	5 (4%) 36 33	49, 63, 73, 82	0
21	1Z	203/206 (98%)	0.10	2 (0%) 79 78	35, 51, 66, 76	0
21	2Z	201/206 (97%)	0.89	8 (3%) 42 38	57, 71, 79, 88	0
22	10	77/85 (90%)	-0.25	0 100 100	24, 31, 48, 54	0
22	20	77/85 (90%)	0.60	2 (2%) 57 54	43, 57, 67, 72	0
23	11	97/98 (98%)	0.02	1 (1%) 79 78	22, 39, 61, 69	0
23	21	97/98 (98%)	0.32	2 (2%) 63 61	35, 49, 71, 73	0
24	12	70/72 (97%)	-0.12	1 (1%) 73 72	29, 44, 57, 78	0
24	22	70/72 (97%)	0.49	0 100 100	53, 64, 71, 73	0
25	13	59/60 (98%)	-0.41	0 100 100	20, 30, 55, 63	0
25	23	59/60 (98%)	0.36	1 (1%) 69 67	45, 55, 69, 77	0
26	14	69/71 (97%)	0.89	14 (20%) 3 2	50, 69, 86, 90	0
26	24	69/71 (97%)	1.37	13 (18%) 3 3	70, 83, 88, 91	0
27	15	59/60 (98%)	-0.50	0 100 100	17, 27, 44, 54	0
27	25	59/60 (98%)	-0.17	0 100 100	29, 44, 59, 68	0
28	16	53/54 (98%)	-0.45	0 100 100	28, 36, 48, 55	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.20	1 (1%) 66 63	46, 54, 63, 68	0
29	17	48/49 (97%)	-0.32	1 (2%) 63 61	17, 24, 49, 58	0
29	27	48/49 (97%)	-0.07	2 (4%) 40 37	28, 36, 58, 65	0
30	18	64/65 (98%)	-0.47	0 100 100	23, 28, 34, 47	0
30	28	64/65 (98%)	0.21	1 (1%) 70 68	38, 49, 56, 63	0
31	19	37/37 (100%)	-0.29	0 100 100	22, 32, 49, 53	0
31	29	37/37 (100%)	0.76	1 (2%) 56 53	50, 60, 68, 69	0
32	1a	1488/1521 (97%)	0.10	38 (2%) 57 54	32, 62, 89, 104	0
32	2a	1492/1521 (98%)	0.42	61 (4%) 41 37	42, 71, 91, 103	0
33	1b	231/256 (90%)	0.94	28 (12%) 8 7	61, 74, 83, 88	0
33	2b	231/256 (90%)	1.30	45 (19%) 3 2	66, 80, 86, 90	0
34	1c	206/239 (86%)	0.74	15 (7%) 21 18	53, 67, 77, 81	0
34	2c	206/239 (86%)	1.34	37 (17%) 3 3	70, 79, 84, 91	0
35	1d	208/209 (99%)	0.75	12 (5%) 29 25	51, 66, 75, 81	0
35	2d	208/209 (99%)	0.93	10 (4%) 35 32	55, 68, 77, 79	0
36	1e	148/162 (91%)	0.28	0 100 100	46, 59, 69, 80	0
36	2e	148/162 (91%)	0.75	4 (2%) 56 53	57, 68, 76, 83	0
37	1f	100/101 (99%)	0.41	1 (1%) 79 78	43, 60, 70, 74	0
37	2f	100/101 (99%)	0.31	0 100 100	52, 62, 70, 76	0
38	1g	155/156 (99%)	0.49	3 (1%) 66 63	56, 65, 76, 85	0
38	2g	155/156 (99%)	0.87	10 (6%) 25 22	68, 74, 81, 87	0
39	1h	137/138 (99%)	0.41	2 (1%) 72 70	51, 62, 71, 74	0
39	2h	137/138 (99%)	0.67	2 (1%) 72 70	58, 69, 74, 82	0
40	1i	127/128 (99%)	1.05	14 (11%) 10 9	52, 73, 79, 82	0
40	2i	126/128 (98%)	1.74	42 (33%) 1 1	67, 80, 85, 87	0
41	1j	97/105 (92%)	1.03	10 (10%) 12 10	52, 72, 83, 86	0
41	2j	96/105 (91%)	2.17	53 (55%) 0 0	71, 80, 85, 87	0
42	1k	114/129 (88%)	0.27	1 (0%) 81 80	39, 58, 69, 73	0
42	2k	114/129 (88%)	0.72	8 (7%) 22 19	50, 66, 75, 81	0
43	1l	121/132 (91%)	0.20	3 (2%) 58 55	42, 54, 65, 70	0
43	2l	121/132 (91%)	0.63	3 (2%) 58 55	54, 62, 69, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	116/126 (92%)	0.82	8 (6%) 23 20	52, 68, 75, 79	0
44	2m	114/126 (90%)	1.42	21 (18%) 3 3	73, 80, 85, 87	0
45	1n	60/61 (98%)	0.84	3 (5%) 34 30	57, 64, 72, 79	0
45	2n	60/61 (98%)	1.90	22 (36%) 1 0	71, 79, 85, 88	0
46	1o	88/89 (98%)	0.58	3 (3%) 48 44	43, 60, 71, 77	0
46	2o	88/89 (98%)	0.69	2 (2%) 61 58	54, 67, 75, 78	0
47	1p	82/88 (93%)	1.36	13 (15%) 5 4	55, 67, 77, 80	0
47	2p	82/88 (93%)	1.03	6 (7%) 21 18	55, 65, 75, 82	0
48	1q	99/105 (94%)	0.65	2 (2%) 65 62	48, 63, 72, 73	0
48	2q	99/105 (94%)	0.58	2 (2%) 65 62	53, 63, 73, 79	0
49	1r	68/88 (77%)	0.24	0 100 100	51, 60, 73, 76	0
49	2r	68/88 (77%)	0.45	1 (1%) 72 70	59, 67, 74, 76	0
50	1s	83/93 (89%)	0.74	2 (2%) 59 56	59, 70, 76, 79	0
50	2s	83/93 (89%)	1.55	22 (26%) 1 1	70, 82, 86, 88	0
51	1t	96/106 (90%)	1.00	9 (9%) 14 12	53, 66, 76, 82	0
51	2t	98/106 (92%)	0.66	9 (9%) 14 12	53, 64, 75, 77	0
52	1u	23/27 (85%)	0.94	0 100 100	61, 66, 69, 72	0
52	2u	23/27 (85%)	2.45	14 (60%) 0 0	73, 76, 80, 82	0
53	1y	97/113 (85%)	0.47	4 (4%) 41 37	45, 56, 67, 71	0
53	2y	96/113 (84%)	1.38	20 (20%) 2 2	60, 72, 79, 83	0
All	All	20766/21468 (96%)	0.18	976 (4%) 36 33	15, 57, 84, 105	0

The worst 5 of 976 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1133	G	9.1
45	2n	2	ALA	8.8
1	1A	1110	C	7.0
1	2A	2602	A	6.9
51	1t	103	GLY	6.8

## 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
32	2MG	2a	1207	24/25	0.82	0.12	76,86,91,102	0
1	5MU	1A	1937	21/22	0.83	0.12	67,74,83,94	0
1	5MU	2A	1915	21/22	0.85	0.11	76,82,88,101	0
1	PSU	2A	1917	20/21	0.86	0.10	71,78,90,90	0
32	PSU	2a	516	20/21	0.87	0.11	71,76,80,84	0
43	0TD	1l	92	10/11	0.88	0.13	50,54,59,76	0
1	PSU	2A	1911	20/21	0.89	0.09	56,70,76,78	0
43	0TD	2l	92	10/11	0.89	0.14	60,65,71,95	0
1	PSU	1A	1939	20/21	0.90	0.09	62,68,77,77	0
32	M2G	2a	966	25/26	0.90	0.16	57,67,81,92	0
32	5MC	2a	967	21/22	0.91	0.16	63,68,77,88	0
32	2MG	1a	1207	24/25	0.92	0.10	56,66,69,71	0
1	4OC	2A	1920	21/23	0.93	0.10	61,65,72,73	0
32	7MG	2a	527	24/25	0.93	0.11	61,67,73,74	0
32	5MC	2a	1400	21/22	0.94	0.13	65,70,73,74	0
32	4OC	2a	1402	22/23	0.94	0.11	53,63,68,71	0
1	PSU	1A	1933	20/21	0.94	0.08	55,62,65,66	0
32	5MC	1a	967	21/22	0.95	0.11	53,58,65,71	0
32	PSU	1a	516	20/21	0.95	0.08	56,60,64,65	0
32	5MC	2a	1404	21/22	0.95	0.09	51,60,63,66	0
32	5MC	2a	1407	21/22	0.95	0.10	50,60,64,68	0
32	MA6	2a	1518	24/25	0.95	0.11	51,61,66,67	0
32	7MG	1a	527	24/25	0.95	0.09	42,51,54,59	0
32	UR3	1a	1498	21/22	0.96	0.08	43,46,52,60	0
32	MA6	1a	1519	24/25	0.96	0.09	37,43,46,49	0
32	4OC	1a	1402	22/23	0.96	0.09	42,47,55,56	0
32	UR3	2a	1498	21/22	0.96	0.08	52,58,63,66	0
1	5MC	2A	1942	21/22	0.96	0.08	36,48,53,54	0
32	MA6	2a	1519	24/25	0.96	0.10	51,60,64,67	0
32	5MC	1a	1407	21/22	0.96	0.08	36,45,49,56	0
1	5MC	1A	1964	21/22	0.97	0.06	26,32,38,47	0
32	MA6	1a	1518	24/25	0.97	0.09	34,41,46,51	0
1	5MU	2A	1939	21/22	0.97	0.08	29,36,41,43	0
32	5MC	1a	1400	21/22	0.97	0.08	40,45,49,51	0
1	5MC	2A	1962	21/22	0.97	0.08	33,43,48,58	0
1	2MA	2A	2503	23/24	0.97	0.08	24,30,35,37	0
1	2MU	2A	2552	21/23	0.97	0.08	30,36,39,41	0
32	M2G	1a	966	25/26	0.97	0.08	51,53,58,61	0
32	5MC	1a	1404	21/22	0.97	0.08	35,44,46,49	0
1	4OC	1A	1942	21/23	0.97	0.09	39,54,59,60	0
1	OMG	1A	2263	24/25	0.98	0.06	15,21,23,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	2MA	1A	2515	23/24	0.98	0.07	16,20,24,31	0
1	PSU	2A	2605	20/21	0.98	0.07	29,35,39,44	0
1	2MU	1A	2564	21/23	0.98	0.06	20,26,28,29	0
1	PSU	1A	2617	20/21	0.98	0.07	18,22,28,28	0
1	5MU	1A	1961	21/22	0.98	0.07	18,24,27,32	0
1	5MC	1A	1984	21/22	0.98	0.07	25,33,37,45	0
1	OMG	2A	2251	24/25	0.98	0.07	32,36,38,39	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, 95<sup>th</sup> 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	1851	1/1	0.36	0.40	94,94,94,94	0
54	MG	1a	1752	1/1	0.47	0.31	71,71,71,71	0
54	MG	2A	3318	1/1	0.54	0.21	78,78,78,78	0
54	MG	1a	1846	1/1	0.59	0.23	74,74,74,74	0
54	MG	2A	3466	1/1	0.59	0.22	68,68,68,68	0
54	MG	1A	3957	1/1	0.62	0.21	79,79,79,79	0
54	MG	2A	3219	1/1	0.63	0.17	74,74,74,74	0
54	MG	2A	3685	1/1	0.64	0.19	75,75,75,75	0
54	MG	1A	3082	1/1	0.65	0.14	55,55,55,55	0
54	MG	2A	3197	1/1	0.65	0.16	73,73,73,73	0
54	MG	2B	3015	1/1	0.65	0.13	74,74,74,74	0
54	MG	2A	3586	1/1	0.66	0.29	84,84,84,84	0
54	MG	2A	3676	1/1	0.67	0.26	66,66,66,66	0
54	MG	2A	3171	1/1	0.68	0.15	58,58,58,58	0
54	MG	1A	3434	1/1	0.68	0.16	44,44,44,44	0
54	MG	1A	3721	1/1	0.68	0.12	25,25,25,25	0
54	MG	2A	3648	1/1	0.69	0.26	73,73,73,73	0
54	MG	2A	3215	1/1	0.69	0.55	73,73,73,73	0
54	MG	2A	3548	1/1	0.70	0.18	54,54,54,54	0
54	MG	2B	3003	1/1	0.70	0.26	74,74,74,74	0
54	MG	1A	3937	1/1	0.70	0.14	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	3167	1/1	0.71	0.22	74,74,74,74	0
54	MG	1a	1828	1/1	0.71	0.18	62,62,62,62	0
54	MG	1a	1840	1/1	0.71	0.16	45,45,45,45	0
54	MG	2A	3355	1/1	0.71	0.18	46,46,46,46	0
54	MG	1A	3941	1/1	0.72	0.15	68,68,68,68	0
54	MG	1a	1817	1/1	0.72	0.23	57,57,57,57	0
54	MG	1A	3191	1/1	0.72	0.19	51,51,51,51	0
54	MG	1a	1704	1/1	0.72	0.23	77,77,77,77	0
54	MG	2A	3370	1/1	0.72	0.23	70,70,70,70	0
54	MG	2A	3454	1/1	0.72	0.36	70,70,70,70	0
54	MG	1a	1845	1/1	0.72	0.19	78,78,78,78	0
54	MG	1a	1754	1/1	0.73	0.24	68,68,68,68	0
54	MG	2A	3251	1/1	0.73	0.25	60,60,60,60	0
54	MG	2a	1700	1/1	0.73	0.19	48,48,48,48	0
54	MG	2A	3388	1/1	0.74	0.21	51,51,51,51	0
54	MG	2A	3413	1/1	0.74	0.28	63,63,63,63	0
54	MG	1a	1751	1/1	0.74	0.17	69,69,69,69	0
54	MG	2A	3338	1/1	0.74	0.17	53,53,53,53	0
54	MG	1A	3934	1/1	0.74	0.24	50,50,50,50	0
54	MG	2I	3001	1/1	0.74	0.15	71,71,71,71	0
54	MG	1A	3942	1/1	0.74	0.23	73,73,73,73	0
54	MG	1A	3875	1/1	0.75	0.18	49,49,49,49	0
54	MG	1l	3002	1/1	0.75	0.10	72,72,72,72	0
54	MG	1A	3327	1/1	0.75	0.18	33,33,33,33	0
54	MG	1A	3602	1/1	0.75	0.17	54,54,54,54	0
54	MG	2B	3014	1/1	0.75	0.12	71,71,71,71	0
54	MG	2A	3467	1/1	0.75	0.29	79,79,79,79	0
54	MG	1A	3364	1/1	0.75	0.08	13,13,13,13	0
54	MG	1A	3837	1/1	0.75	0.20	56,56,56,56	0
54	MG	2a	1719	1/1	0.75	0.28	67,67,67,67	0
54	MG	2a	1729	1/1	0.75	0.18	64,64,64,64	0
54	MG	1a	1700	1/1	0.76	0.31	65,65,65,65	0
54	MG	2G	3003	1/1	0.76	0.15	79,79,79,79	0
54	MG	1A	3575	1/1	0.76	0.19	65,65,65,65	0
54	MG	2A	3493	1/1	0.76	0.17	55,55,55,55	0
54	MG	1a	1737	1/1	0.76	0.10	62,62,62,62	0
54	MG	2a	1725	1/1	0.76	0.20	64,64,64,64	0
54	MG	1a	1755	1/1	0.76	0.17	68,68,68,68	0
54	MG	2j	8001	1/1	0.76	0.12	82,82,82,82	0
58	ARG	1F	314	12/12	0.76	0.17	47,65,78,79	0
54	MG	1A	3404	1/1	0.77	0.22	65,65,65,65	0
54	MG	2A	3398	1/1	0.77	0.15	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	3198	1/1	0.77	0.26	60,60,60,60	0
54	MG	2A	3426	1/1	0.77	0.16	58,58,58,58	0
54	MG	1A	3794	1/1	0.77	0.14	53,53,53,53	0
54	MG	1a	1766	1/1	0.77	0.29	67,67,67,67	0
54	MG	1f	3001	1/1	0.77	0.23	64,64,64,64	0
54	MG	1A	3597	1/1	0.77	0.27	62,62,62,62	0
54	MG	2A	3142	1/1	0.77	0.16	68,68,68,68	0
54	MG	2A	3567	1/1	0.77	0.15	40,40,40,40	0
54	MG	2A	3579	1/1	0.77	0.36	65,65,65,65	0
54	MG	1A	3379	1/1	0.77	0.26	73,73,73,73	0
54	MG	1A	3921	1/1	0.77	0.22	58,58,58,58	0
54	MG	14	502	1/1	0.78	0.15	72,72,72,72	0
54	MG	1a	1608	1/1	0.78	0.12	63,63,63,63	0
54	MG	2A	3385	1/1	0.78	0.15	47,47,47,47	0
54	MG	2A	3115	1/1	0.78	0.22	63,63,63,63	0
54	MG	2B	3002	1/1	0.78	0.19	71,71,71,71	0
54	MG	1a	1686	1/1	0.78	0.27	61,61,61,61	0
54	MG	1a	1783	1/1	0.78	0.23	64,64,64,64	0
54	MG	1a	1807	1/1	0.78	0.30	67,67,67,67	0
54	MG	1a	1810	1/1	0.78	0.16	63,63,63,63	0
54	MG	1A	3499	1/1	0.78	0.18	50,50,50,50	0
54	MG	1a	1701	1/1	0.78	0.12	71,71,71,71	0
54	MG	2a	1703	1/1	0.78	0.28	61,61,61,61	0
54	MG	2A	3489	1/1	0.78	0.23	69,69,69,69	0
54	MG	1A	3501	1/1	0.78	0.28	59,59,59,59	0
54	MG	1A	3730	1/1	0.78	0.13	26,26,26,26	0
54	MG	1A	3908	1/1	0.78	0.13	52,52,52,52	0
54	MG	1A	3748	1/1	0.78	0.15	68,68,68,68	0
54	MG	2A	3673	1/1	0.79	0.25	68,68,68,68	0
54	MG	2A	3675	1/1	0.79	0.12	73,73,73,73	0
54	MG	1a	1767	1/1	0.79	0.17	58,58,58,58	0
54	MG	2A	3425	1/1	0.79	0.23	68,68,68,68	0
54	MG	1a	1778	1/1	0.79	0.24	60,60,60,60	0
54	MG	2A	3450	1/1	0.79	0.13	55,55,55,55	0
54	MG	1A	3649	1/1	0.79	0.15	58,58,58,58	0
54	MG	1a	1802	1/1	0.79	0.38	62,62,62,62	0
54	MG	1a	1803	1/1	0.79	0.26	64,64,64,64	0
54	MG	1A	3817	1/1	0.79	0.16	65,65,65,65	0
54	MG	1A	3577	1/1	0.79	0.15	26,26,26,26	0
54	MG	2A	3506	1/1	0.79	0.13	63,63,63,63	0
54	MG	1A	3567	1/1	0.79	0.22	62,62,62,62	0
54	MG	2A	3170	1/1	0.79	0.13	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	3887	1/1	0.79	0.10	69,69,69,69	0
54	MG	2A	3393	1/1	0.79	0.19	55,55,55,55	0
54	MG	1A	3177	1/1	0.79	0.14	51,51,51,51	0
54	MG	2A	3335	1/1	0.80	0.13	56,56,56,56	0
54	MG	2A	3451	1/1	0.80	0.21	49,49,49,49	0
54	MG	1A	3969	1/1	0.80	0.20	45,45,45,45	0
54	MG	1a	1835	1/1	0.80	0.15	67,67,67,67	0
54	MG	2B	3001	1/1	0.80	0.13	68,68,68,68	0
54	MG	1D	302	1/1	0.80	0.20	42,42,42,42	0
54	MG	1a	1843	1/1	0.80	0.17	78,78,78,78	0
54	MG	2B	3007	1/1	0.80	0.13	71,71,71,71	0
54	MG	1A	3138	1/1	0.80	0.26	59,59,59,59	0
54	MG	1a	1702	1/1	0.80	0.15	52,52,52,52	0
54	MG	1a	1759	1/1	0.80	0.20	64,64,64,64	0
54	MG	2A	3551	1/1	0.80	0.18	61,61,61,61	0
54	MG	20	101	1/1	0.80	0.24	75,75,75,75	0
54	MG	25	502	1/1	0.80	0.18	59,59,59,59	0
54	MG	2a	1664	1/1	0.80	0.15	61,61,61,61	0
54	MG	1a	1808	1/1	0.80	0.21	74,74,74,74	0
54	MG	2A	3569	1/1	0.80	0.21	51,51,51,51	0
54	MG	1A	3422	1/1	0.80	0.12	41,41,41,41	0
54	MG	1a	1681	1/1	0.80	0.13	60,60,60,60	0
54	MG	2A	3602	1/1	0.80	0.20	46,46,46,46	0
54	MG	2a	1742	1/1	0.80	0.34	65,65,65,65	0
54	MG	2A	3646	1/1	0.80	0.13	60,60,60,60	0
54	MG	2A	3429	1/1	0.80	0.14	59,59,59,59	0
54	MG	2A	3386	1/1	0.81	0.15	68,68,68,68	0
54	MG	1A	3745	1/1	0.81	0.22	60,60,60,60	0
54	MG	2A	3534	1/1	0.81	0.25	65,65,65,65	0
54	MG	1A	3935	1/1	0.81	0.13	55,55,55,55	0
54	MG	1a	1662	1/1	0.81	0.22	56,56,56,56	0
54	MG	2A	3555	1/1	0.81	0.16	61,61,61,61	0
54	MG	1h	3002	1/1	0.81	0.16	64,64,64,64	0
54	MG	2A	3419	1/1	0.81	0.23	59,59,59,59	0
54	MG	2A	3242	1/1	0.81	0.13	63,63,63,63	0
54	MG	1a	1731	1/1	0.81	0.27	56,56,56,56	0
54	MG	2A	3274	1/1	0.81	0.15	53,53,53,53	0
54	MG	2a	1672	1/1	0.81	0.33	62,62,62,62	0
54	MG	2a	1687	1/1	0.81	0.29	67,67,67,67	0
54	MG	1a	1773	1/1	0.81	0.20	61,61,61,61	0
54	MG	1a	1674	1/1	0.81	0.18	65,65,65,65	0
54	MG	2A	3662	1/1	0.81	0.16	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3672	1/1	0.81	0.14	55,55,55,55	0
54	MG	2a	1726	1/1	0.81	0.33	62,62,62,62	0
54	MG	1A	3131	1/1	0.81	0.11	48,48,48,48	0
54	MG	2a	1736	1/1	0.81	0.31	61,61,61,61	0
54	MG	1A	3411	1/1	0.81	0.18	46,46,46,46	0
54	MG	1F	311	1/1	0.81	0.19	45,45,45,45	0
54	MG	2A	3193	1/1	0.81	0.13	47,47,47,47	0
54	MG	2A	3108	1/1	0.82	0.19	62,62,62,62	0
54	MG	2A	3288	1/1	0.82	0.20	49,49,49,49	0
54	MG	1a	1830	1/1	0.82	0.35	66,66,66,66	0
54	MG	1A	3618	1/1	0.82	0.21	42,42,42,42	0
54	MG	2A	3605	1/1	0.82	0.15	62,62,62,62	0
54	MG	2A	3619	1/1	0.82	0.21	66,66,66,66	0
54	MG	2A	3635	1/1	0.82	0.23	64,64,64,64	0
54	MG	2a	1669	1/1	0.82	0.39	63,63,63,63	0
54	MG	1A	3398	1/1	0.82	0.15	26,26,26,26	0
54	MG	1G	3002	1/1	0.82	0.10	66,66,66,66	0
54	MG	1A	3473	1/1	0.82	0.14	63,63,63,63	0
54	MG	1A	3796	1/1	0.82	0.15	45,45,45,45	0
54	MG	1a	1617	1/1	0.82	0.13	58,58,58,58	0
54	MG	2A	3504	1/1	0.82	0.12	60,60,60,60	0
54	MG	1A	3256	1/1	0.82	0.24	51,51,51,51	0
54	MG	2A	3202	1/1	0.82	0.20	62,62,62,62	0
54	MG	1f	3002	1/1	0.82	0.14	53,53,53,53	0
54	MG	1a	1772	1/1	0.82	0.25	57,57,57,57	0
54	MG	1A	3832	1/1	0.82	0.21	57,57,57,57	0
57	MPD	2B	3020	8/8	0.82	0.23	61,66,69,79	0
54	MG	1y	3004	1/1	0.82	0.19	76,76,76,76	0
54	MG	2A	3503	1/1	0.83	0.23	54,54,54,54	0
54	MG	1A	3764	1/1	0.83	0.13	44,44,44,44	0
54	MG	1a	1634	1/1	0.83	0.26	69,69,69,69	0
54	MG	2A	3515	1/1	0.83	0.15	54,54,54,54	0
54	MG	1a	1637	1/1	0.83	0.23	67,67,67,67	0
54	MG	2A	3177	1/1	0.83	0.17	56,56,56,56	0
54	MG	1A	3906	1/1	0.83	0.17	55,55,55,55	0
54	MG	2D	301	1/1	0.83	0.21	56,56,56,56	0
54	MG	2A	3195	1/1	0.83	0.19	54,54,54,54	0
54	MG	2A	3389	1/1	0.83	0.17	47,47,47,47	0
54	MG	1a	1790	1/1	0.83	0.17	60,60,60,60	0
54	MG	2I	101	1/1	0.83	0.12	67,67,67,67	0
54	MG	1a	1665	1/1	0.83	0.17	59,59,59,59	0
54	MG	2a	1603	1/1	0.83	0.19	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	1641	1/1	0.83	0.40	66,66,66,66	0
54	MG	1A	3786	1/1	0.83	0.17	40,40,40,40	0
54	MG	1a	1680	1/1	0.83	0.18	70,70,70,70	0
54	MG	1A	3124	1/1	0.83	0.11	40,40,40,40	0
54	MG	2a	1677	1/1	0.83	0.20	53,53,53,53	0
54	MG	1R	203	1/1	0.83	0.15	34,34,34,34	0
54	MG	2a	1689	1/1	0.83	0.27	62,62,62,62	0
54	MG	2a	1693	1/1	0.83	0.21	55,55,55,55	0
54	MG	2a	1699	1/1	0.83	0.24	71,71,71,71	0
54	MG	2A	3633	1/1	0.83	0.11	43,43,43,43	0
54	MG	1A	3950	1/1	0.83	0.13	80,80,80,80	0
54	MG	2A	3252	1/1	0.83	0.23	61,61,61,61	0
54	MG	2A	3647	1/1	0.83	0.23	57,57,57,57	0
54	MG	2A	3261	1/1	0.83	0.16	43,43,43,43	0
54	MG	2A	3656	1/1	0.83	0.20	48,48,48,48	0
54	MG	1a	1822	1/1	0.83	0.28	60,60,60,60	0
54	MG	1A	3457	1/1	0.83	0.12	64,64,64,64	0
54	MG	1a	1768	1/1	0.83	0.19	69,69,69,69	0
57	MPD	2A	3711	8/8	0.83	0.25	48,60,64,64	0
54	MG	2A	3332	1/1	0.83	0.10	65,65,65,65	0
54	MG	2A	3150	1/1	0.83	0.20	62,62,62,62	0
54	MG	1A	3485	1/1	0.84	0.10	47,47,47,47	0
54	MG	2B	3005	1/1	0.84	0.17	61,61,61,61	0
54	MG	2A	3545	1/1	0.84	0.21	53,53,53,53	0
54	MG	2B	3008	1/1	0.84	0.16	66,66,66,66	0
54	MG	1A	3508	1/1	0.84	0.12	29,29,29,29	0
54	MG	1S	8001	1/1	0.84	0.17	62,62,62,62	0
54	MG	10	105	1/1	0.84	0.14	59,59,59,59	0
54	MG	1A	3905	1/1	0.84	0.14	53,53,53,53	0
54	MG	1d	307	1/1	0.84	0.10	89,89,89,89	0
54	MG	2A	3412	1/1	0.84	0.10	61,61,61,61	0
54	MG	2A	3216	1/1	0.84	0.20	54,54,54,54	0
54	MG	2A	3589	1/1	0.84	0.24	57,57,57,57	0
54	MG	28	8003	1/1	0.84	0.17	56,56,56,56	0
54	MG	1a	1794	1/1	0.84	0.25	67,67,67,67	0
54	MG	2a	1614	1/1	0.84	0.22	74,74,74,74	0
54	MG	2a	1630	1/1	0.84	0.12	62,62,62,62	0
54	MG	2a	1637	1/1	0.84	0.22	63,63,63,63	0
54	MG	2A	3236	1/1	0.84	0.11	61,61,61,61	0
54	MG	2a	1655	1/1	0.84	0.36	63,63,63,63	0
54	MG	2A	3610	1/1	0.84	0.20	51,51,51,51	0
54	MG	1A	3947	1/1	0.84	0.11	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3628	1/1	0.84	0.21	60,60,60,60	0
54	MG	1A	3741	1/1	0.84	0.10	48,48,48,48	0
54	MG	1a	1805	1/1	0.84	0.14	52,52,52,52	0
54	MG	2A	3640	1/1	0.84	0.15	52,52,52,52	0
54	MG	1A	3635	1/1	0.84	0.10	62,62,62,62	0
54	MG	1A	3964	1/1	0.84	0.38	36,36,36,36	0
54	MG	2A	3281	1/1	0.84	0.21	59,59,59,59	0
54	MG	1a	1649	1/1	0.84	0.25	41,41,41,41	0
54	MG	2A	3659	1/1	0.84	0.22	49,49,49,49	0
54	MG	2A	3475	1/1	0.84	0.17	30,30,30,30	0
54	MG	1A	3831	1/1	0.84	0.10	19,19,19,19	0
54	MG	1B	207	1/1	0.84	0.14	41,41,41,41	0
54	MG	1a	1824	1/1	0.84	0.24	55,55,55,55	0
54	MG	1B	211	1/1	0.84	0.26	64,64,64,64	0
54	MG	2a	1745	1/1	0.84	0.24	67,67,67,67	0
54	MG	2A	3680	1/1	0.84	0.11	50,50,50,50	0
54	MG	1A	3205	1/1	0.84	0.10	42,42,42,42	0
54	MG	1A	3679	1/1	0.84	0.14	52,52,52,52	0
54	MG	2A	3533	1/1	0.84	0.15	51,51,51,51	0
54	MG	1a	1812	1/1	0.85	0.10	59,59,59,59	0
54	MG	2A	3435	1/1	0.85	0.13	60,60,60,60	0
54	MG	1a	1715	1/1	0.85	0.20	58,58,58,58	0
54	MG	1A	3548	1/1	0.85	0.11	34,34,34,34	0
54	MG	2A	3214	1/1	0.85	0.17	56,56,56,56	0
54	MG	1A	3551	1/1	0.85	0.11	43,43,43,43	0
54	MG	2A	3707	1/1	0.85	0.20	61,61,61,61	0
54	MG	1a	1747	1/1	0.85	0.38	56,56,56,56	0
54	MG	2A	3469	1/1	0.85	0.32	61,61,61,61	0
54	MG	2A	3470	1/1	0.85	0.16	43,43,43,43	0
54	MG	2B	3004	1/1	0.85	0.16	58,58,58,58	0
54	MG	1a	1749	1/1	0.85	0.12	46,46,46,46	0
54	MG	2A	3477	1/1	0.85	0.15	59,59,59,59	0
54	MG	1A	3158	1/1	0.85	0.12	41,41,41,41	0
54	MG	1a	1837	1/1	0.85	0.10	44,44,44,44	0
54	MG	1A	3440	1/1	0.85	0.12	18,18,18,18	0
54	MG	1U	201	1/1	0.85	0.19	38,38,38,38	0
54	MG	1A	3751	1/1	0.85	0.20	55,55,55,55	0
54	MG	1A	3927	1/1	0.85	0.12	42,42,42,42	0
54	MG	2A	3520	1/1	0.85	0.17	54,54,54,54	0
54	MG	1A	3452	1/1	0.85	0.14	21,21,21,21	0
54	MG	2A	3285	1/1	0.85	0.13	65,65,65,65	0
54	MG	1A	3330	1/1	0.85	0.14	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3303	1/1	0.85	0.10	40,40,40,40	0
54	MG	2A	3314	1/1	0.85	0.12	30,30,30,30	0
54	MG	2A	3552	1/1	0.85	0.16	63,63,63,63	0
54	MG	1A	3403	1/1	0.85	0.10	50,50,50,50	0
54	MG	2A	3558	1/1	0.85	0.20	58,58,58,58	0
54	MG	2A	3563	1/1	0.85	0.13	60,60,60,60	0
54	MG	2a	1656	1/1	0.85	0.18	63,63,63,63	0
54	MG	2a	1658	1/1	0.85	0.29	60,60,60,60	0
54	MG	1A	3939	1/1	0.85	0.26	55,55,55,55	0
54	MG	1A	3940	1/1	0.85	0.42	67,67,67,67	0
54	MG	1A	3337	1/1	0.85	0.12	55,55,55,55	0
54	MG	2A	3339	1/1	0.85	0.15	71,71,71,71	0
54	MG	2a	1681	1/1	0.85	0.18	57,57,57,57	0
54	MG	1a	1779	1/1	0.85	0.18	58,58,58,58	0
54	MG	2A	3078	1/1	0.85	0.13	63,63,63,63	0
54	MG	1a	1782	1/1	0.85	0.23	61,61,61,61	0
54	MG	1A	3805	1/1	0.85	0.11	54,54,54,54	0
54	MG	1A	3486	1/1	0.85	0.09	21,21,21,21	0
54	MG	1A	3820	1/1	0.85	0.13	50,50,50,50	0
54	MG	2a	1704	1/1	0.85	0.27	63,63,63,63	0
54	MG	2a	1717	1/1	0.85	0.17	60,60,60,60	0
54	MG	2A	3629	1/1	0.85	0.13	51,51,51,51	0
54	MG	2a	1721	1/1	0.85	0.35	76,76,76,76	0
54	MG	1A	3823	1/1	0.85	0.20	29,29,29,29	0
54	MG	1A	3271	1/1	0.85	0.13	49,49,49,49	0
54	MG	2A	3406	1/1	0.85	0.13	54,54,54,54	0
54	MG	1A	3670	1/1	0.85	0.13	25,25,25,25	0
54	MG	2a	1737	1/1	0.85	0.28	60,60,60,60	0
54	MG	1A	3419	1/1	0.85	0.14	47,47,47,47	0
54	MG	2A	3179	1/1	0.85	0.30	65,65,65,65	0
54	MG	1A	3849	1/1	0.85	0.12	58,58,58,58	0
54	MG	2p	3001	1/1	0.85	0.37	61,61,61,61	0
54	MG	1A	3371	1/1	0.85	0.21	49,49,49,49	0
54	MG	2A	3428	1/1	0.85	0.26	53,53,53,53	0
54	MG	2A	3663	1/1	0.85	0.14	61,61,61,61	0
54	MG	1B	206	1/1	0.86	0.09	45,45,45,45	0
54	MG	1A	3784	1/1	0.86	0.12	42,42,42,42	0
54	MG	1a	1774	1/1	0.86	0.12	53,53,53,53	0
54	MG	1A	3203	1/1	0.86	0.25	55,55,55,55	0
54	MG	2A	3708	1/1	0.86	0.13	58,58,58,58	0
54	MG	2A	3476	1/1	0.86	0.14	54,54,54,54	0
54	MG	1B	224	1/1	0.86	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1g	3002	1/1	0.86	0.12	60,60,60,60	0
54	MG	2A	3492	1/1	0.86	0.14	66,66,66,66	0
54	MG	1B	230	1/1	0.86	0.08	68,68,68,68	0
54	MG	1A	3789	1/1	0.86	0.14	31,31,31,31	0
54	MG	1y	3001	1/1	0.86	0.12	61,61,61,61	0
54	MG	2A	3286	1/1	0.86	0.10	47,47,47,47	0
54	MG	2A	3507	1/1	0.86	0.19	54,54,54,54	0
54	MG	2B	3017	1/1	0.86	0.12	80,80,80,80	0
54	MG	1y	3002	1/1	0.86	0.11	62,62,62,62	0
54	MG	2A	3291	1/1	0.86	0.10	47,47,47,47	0
54	MG	1E	301	1/1	0.86	0.12	35,35,35,35	0
54	MG	2A	3004	1/1	0.86	0.14	44,44,44,44	0
54	MG	2A	3536	1/1	0.86	0.19	57,57,57,57	0
54	MG	2A	3049	1/1	0.86	0.23	53,53,53,53	0
54	MG	2A	3330	1/1	0.86	0.23	69,69,69,69	0
54	MG	2A	3063	1/1	0.86	0.14	58,58,58,58	0
54	MG	2A	3071	1/1	0.86	0.15	46,46,46,46	0
54	MG	2a	1627	1/1	0.86	0.26	61,61,61,61	0
54	MG	1A	3938	1/1	0.86	0.17	64,64,64,64	0
54	MG	2a	1633	1/1	0.86	0.26	68,68,68,68	0
54	MG	2A	3081	1/1	0.86	0.22	55,55,55,55	0
54	MG	2A	3097	1/1	0.86	0.33	67,67,67,67	0
54	MG	2A	3564	1/1	0.86	0.17	57,57,57,57	0
54	MG	1A	3190	1/1	0.86	0.21	45,45,45,45	0
54	MG	2A	3380	1/1	0.86	0.13	56,56,56,56	0
54	MG	2A	3382	1/1	0.86	0.14	43,43,43,43	0
54	MG	2A	3581	1/1	0.86	0.18	39,39,39,39	0
54	MG	1a	1710	1/1	0.86	0.16	63,63,63,63	0
54	MG	2a	1676	1/1	0.86	0.24	68,68,68,68	0
54	MG	2A	3124	1/1	0.86	0.10	54,54,54,54	0
54	MG	1A	3732	1/1	0.86	0.17	41,41,41,41	0
54	MG	2a	1684	1/1	0.86	0.16	60,60,60,60	0
54	MG	1a	1718	1/1	0.86	0.14	56,56,56,56	0
54	MG	2a	1688	1/1	0.86	0.20	54,54,54,54	0
54	MG	1a	1719	1/1	0.86	0.17	48,48,48,48	0
54	MG	1A	3278	1/1	0.86	0.10	38,38,38,38	0
54	MG	2A	3623	1/1	0.86	0.12	43,43,43,43	0
54	MG	2A	3627	1/1	0.86	0.17	53,53,53,53	0
54	MG	2A	3404	1/1	0.86	0.19	56,56,56,56	0
54	MG	1A	3521	1/1	0.86	0.14	42,42,42,42	0
54	MG	2A	3630	1/1	0.86	0.20	52,52,52,52	0
54	MG	2A	3173	1/1	0.86	0.18	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3175	1/1	0.86	0.21	55,55,55,55	0
54	MG	1A	3907	1/1	0.86	0.15	52,52,52,52	0
54	MG	1A	3949	1/1	0.86	0.19	68,68,68,68	0
54	MG	1a	1606	1/1	0.86	0.16	58,58,58,58	0
54	MG	1A	3589	1/1	0.86	0.13	54,54,54,54	0
54	MG	1A	3916	1/1	0.86	0.12	29,29,29,29	0
54	MG	1A	3961	1/1	0.86	0.13	38,38,38,38	0
54	MG	1A	3339	1/1	0.86	0.19	48,48,48,48	0
54	MG	1a	1640	1/1	0.86	0.23	59,59,59,59	0
54	MG	2A	3664	1/1	0.86	0.17	57,57,57,57	0
54	MG	1A	3702	1/1	0.86	0.10	27,27,27,27	0
54	MG	2A	3461	1/1	0.86	0.16	55,55,55,55	0
54	MG	1B	203	1/1	0.86	0.09	57,57,57,57	0
54	MG	2A	3691	1/1	0.87	0.10	64,64,64,64	0
54	MG	2A	3702	1/1	0.87	0.11	46,46,46,46	0
54	MG	1a	1856	1/1	0.87	0.20	67,67,67,67	0
54	MG	2A	3233	1/1	0.87	0.29	58,58,58,58	0
54	MG	1b	3001	1/1	0.87	0.23	76,76,76,76	0
54	MG	1d	306	1/1	0.87	0.15	56,56,56,56	0
54	MG	2A	3248	1/1	0.87	0.13	55,55,55,55	0
54	MG	1a	1763	1/1	0.87	0.25	64,64,64,64	0
54	MG	1A	3563	1/1	0.87	0.11	30,30,30,30	0
54	MG	1A	3882	1/1	0.87	0.11	60,60,60,60	0
54	MG	1A	3297	1/1	0.87	0.13	37,37,37,37	0
54	MG	1a	1644	1/1	0.87	0.17	60,60,60,60	0
54	MG	1A	3415	1/1	0.87	0.12	47,47,47,47	0
54	MG	1a	1654	1/1	0.87	0.15	56,56,56,56	0
54	MG	1a	1659	1/1	0.87	0.23	64,64,64,64	0
54	MG	2D	308	1/1	0.87	0.09	27,27,27,27	0
54	MG	1A	4007	1/1	0.87	0.12	23,23,23,23	0
54	MG	1A	3479	1/1	0.87	0.13	20,20,20,20	0
54	MG	2A	3308	1/1	0.87	0.21	48,48,48,48	0
54	MG	2A	3019	1/1	0.87	0.17	56,56,56,56	0
54	MG	1A	3450	1/1	0.87	0.17	27,27,27,27	0
54	MG	2A	3328	1/1	0.87	0.18	56,56,56,56	0
54	MG	1A	3801	1/1	0.87	0.06	34,34,34,34	0
54	MG	1a	1791	1/1	0.87	0.25	60,60,60,60	0
54	MG	2a	1618	1/1	0.87	0.31	66,66,66,66	0
54	MG	2a	1625	1/1	0.87	0.17	67,67,67,67	0
54	MG	1a	1792	1/1	0.87	0.16	57,57,57,57	0
54	MG	1A	3913	1/1	0.87	0.17	61,61,61,61	0
54	MG	2A	3083	1/1	0.87	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3350	1/1	0.87	0.10	31,31,31,31	0
54	MG	2a	1638	1/1	0.87	0.23	60,60,60,60	0
54	MG	2A	3096	1/1	0.87	0.16	60,60,60,60	0
54	MG	2a	1642	1/1	0.87	0.18	58,58,58,58	0
54	MG	2a	1645	1/1	0.87	0.24	62,62,62,62	0
54	MG	1a	1797	1/1	0.87	0.12	66,66,66,66	0
54	MG	2A	3106	1/1	0.87	0.11	46,46,46,46	0
54	MG	1a	1799	1/1	0.87	0.18	58,58,58,58	0
54	MG	2a	1662	1/1	0.87	0.26	67,67,67,67	0
54	MG	2A	3114	1/1	0.87	0.17	56,56,56,56	0
54	MG	1A	3522	1/1	0.87	0.09	38,38,38,38	0
54	MG	1A	3813	1/1	0.87	0.19	56,56,56,56	0
54	MG	2a	1673	1/1	0.87	0.17	56,56,56,56	0
54	MG	1A	3737	1/1	0.87	0.14	53,53,53,53	0
54	MG	2A	3612	1/1	0.87	0.10	40,40,40,40	0
54	MG	2a	1678	1/1	0.87	0.12	57,57,57,57	0
54	MG	2a	1679	1/1	0.87	0.12	53,53,53,53	0
54	MG	2a	1680	1/1	0.87	0.10	58,58,58,58	0
54	MG	2A	3146	1/1	0.87	0.22	52,52,52,52	0
54	MG	2A	3149	1/1	0.87	0.23	68,68,68,68	0
54	MG	1A	3524	1/1	0.87	0.10	46,46,46,46	0
54	MG	2A	3405	1/1	0.87	0.17	66,66,66,66	0
54	MG	2A	3164	1/1	0.87	0.17	69,69,69,69	0
54	MG	1A	3603	1/1	0.87	0.22	60,60,60,60	0
54	MG	2A	3632	1/1	0.87	0.14	49,49,49,49	0
54	MG	1A	3544	1/1	0.87	0.33	34,34,34,34	0
54	MG	1H	8001	1/1	0.87	0.23	67,67,67,67	0
54	MG	1A	3428	1/1	0.87	0.28	52,52,52,52	0
54	MG	2a	1709	1/1	0.87	0.34	48,48,48,48	0
54	MG	1A	3833	1/1	0.87	0.10	30,30,30,30	0
54	MG	1A	3835	1/1	0.87	0.08	50,50,50,50	0
54	MG	1Z	8001	1/1	0.87	0.15	60,60,60,60	0
54	MG	2A	3431	1/1	0.87	0.19	53,53,53,53	0
54	MG	1a	1738	1/1	0.87	0.11	62,62,62,62	0
54	MG	2A	3444	1/1	0.87	0.17	60,60,60,60	0
54	MG	10	104	1/1	0.87	0.11	51,51,51,51	0
54	MG	1A	3753	1/1	0.87	0.13	35,35,35,35	0
54	MG	1A	3487	1/1	0.87	0.19	51,51,51,51	0
54	MG	1A	3858	1/1	0.87	0.10	28,28,28,28	0
54	MG	2a	1749	1/1	0.87	0.28	64,64,64,64	0
54	MG	1A	3868	1/1	0.87	0.14	23,23,23,23	0
54	MG	1A	3870	1/1	0.87	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MPD	1a	1854	8/8	0.87	0.12	46,63,67,69	0
57	MPD	2A	3710	8/8	0.87	0.23	43,49,51,57	0
54	MG	2A	3468	1/1	0.87	0.13	61,61,61,61	0
54	MG	1a	1628	1/1	0.87	0.20	49,49,49,49	0
54	MG	2A	3687	1/1	0.87	0.25	64,64,64,64	0
54	MG	2A	3205	1/1	0.88	0.26	60,60,60,60	0
54	MG	1a	1601	1/1	0.88	0.16	56,56,56,56	0
54	MG	1A	3637	1/1	0.88	0.12	47,47,47,47	0
54	MG	2A	3457	1/1	0.88	0.13	54,54,54,54	0
54	MG	1A	3189	1/1	0.88	0.21	41,41,41,41	0
54	MG	1a	1612	1/1	0.88	0.18	72,72,72,72	0
54	MG	2A	3226	1/1	0.88	0.14	53,53,53,53	0
54	MG	2A	3231	1/1	0.88	0.13	42,42,42,42	0
54	MG	1a	1756	1/1	0.88	0.25	58,58,58,58	0
54	MG	1A	3030	1/1	0.88	0.25	54,54,54,54	0
54	MG	2A	3471	1/1	0.88	0.14	61,61,61,61	0
54	MG	1A	3148	1/1	0.88	0.10	30,30,30,30	0
54	MG	1A	3966	1/1	0.88	0.17	36,36,36,36	0
54	MG	1A	3903	1/1	0.88	0.31	63,63,63,63	0
54	MG	2B	3013	1/1	0.88	0.10	80,80,80,80	0
54	MG	2A	3484	1/1	0.88	0.38	65,65,65,65	0
54	MG	1A	3437	1/1	0.88	0.16	41,41,41,41	0
54	MG	1n	502	1/1	0.88	0.13	51,51,51,51	0
54	MG	2B	3018	1/1	0.88	0.14	76,76,76,76	0
54	MG	2A	3269	1/1	0.88	0.17	32,32,32,32	0
54	MG	2D	306	1/1	0.88	0.10	56,56,56,56	0
54	MG	2D	307	1/1	0.88	0.25	43,43,43,43	0
54	MG	1A	3493	1/1	0.88	0.15	56,56,56,56	0
54	MG	1a	1648	1/1	0.88	0.12	72,72,72,72	0
54	MG	1A	3573	1/1	0.88	0.32	52,52,52,52	0
54	MG	2T	3003	1/1	0.88	0.09	61,61,61,61	0
54	MG	1a	1776	1/1	0.88	0.43	69,69,69,69	0
54	MG	2A	3509	1/1	0.88	0.24	60,60,60,60	0
54	MG	1A	3498	1/1	0.88	0.10	32,32,32,32	0
54	MG	2A	3037	1/1	0.88	0.23	56,56,56,56	0
54	MG	2A	3523	1/1	0.88	0.24	49,49,49,49	0
54	MG	2a	1605	1/1	0.88	0.09	57,57,57,57	0
54	MG	2A	3526	1/1	0.88	0.26	53,53,53,53	0
54	MG	2A	3532	1/1	0.88	0.20	52,52,52,52	0
54	MG	2a	1620	1/1	0.88	0.17	56,56,56,56	0
54	MG	2a	1623	1/1	0.88	0.30	64,64,64,64	0
54	MG	2A	3041	1/1	0.88	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3039	1/1	0.88	0.16	56,56,56,56	0
54	MG	1A	3445	1/1	0.88	0.10	21,21,21,21	0
54	MG	2A	3544	1/1	0.88	0.09	56,56,56,56	0
54	MG	1B	227	1/1	0.88	0.09	52,52,52,52	0
54	MG	1a	1669	1/1	0.88	0.11	51,51,51,51	0
54	MG	1A	3825	1/1	0.88	0.10	45,45,45,45	0
54	MG	1a	1676	1/1	0.88	0.20	46,46,46,46	0
54	MG	1A	3504	1/1	0.88	0.07	16,16,16,16	0
54	MG	1D	309	1/1	0.88	0.17	52,52,52,52	0
54	MG	2A	3103	1/1	0.88	0.23	66,66,66,66	0
54	MG	1a	1684	1/1	0.88	0.14	49,49,49,49	0
54	MG	1A	3159	1/1	0.88	0.16	38,38,38,38	0
54	MG	2A	3568	1/1	0.88	0.24	50,50,50,50	0
54	MG	2A	3111	1/1	0.88	0.14	66,66,66,66	0
54	MG	2a	1670	1/1	0.88	0.23	59,59,59,59	0
54	MG	2A	3371	1/1	0.88	0.15	26,26,26,26	0
54	MG	2A	3379	1/1	0.88	0.14	40,40,40,40	0
54	MG	1a	1691	1/1	0.88	0.17	56,56,56,56	0
54	MG	1F	302	1/1	0.88	0.09	32,32,32,32	0
54	MG	2A	3594	1/1	0.88	0.28	60,60,60,60	0
54	MG	2A	3597	1/1	0.88	0.37	61,61,61,61	0
54	MG	2A	3600	1/1	0.88	0.25	54,54,54,54	0
54	MG	2A	3384	1/1	0.88	0.23	38,38,38,38	0
54	MG	1A	3161	1/1	0.88	0.07	34,34,34,34	0
54	MG	2A	3126	1/1	0.88	0.09	42,42,42,42	0
54	MG	1A	3752	1/1	0.88	0.11	55,55,55,55	0
54	MG	1a	1809	1/1	0.88	0.22	66,66,66,66	0
54	MG	1A	3611	1/1	0.88	0.10	41,41,41,41	0
54	MG	2a	1698	1/1	0.88	0.24	50,50,50,50	0
54	MG	1a	1707	1/1	0.88	0.11	58,58,58,58	0
54	MG	2A	3399	1/1	0.88	0.13	42,42,42,42	0
54	MG	1A	3838	1/1	0.88	0.18	60,60,60,60	0
54	MG	1a	1818	1/1	0.88	0.21	62,62,62,62	0
54	MG	1a	1712	1/1	0.88	0.16	51,51,51,51	0
54	MG	2A	3408	1/1	0.88	0.13	54,54,54,54	0
54	MG	2A	3409	1/1	0.88	0.09	51,51,51,51	0
54	MG	1A	3757	1/1	0.88	0.11	48,48,48,48	0
54	MG	1A	3854	1/1	0.88	0.09	19,19,19,19	0
54	MG	2A	3417	1/1	0.88	0.14	37,37,37,37	0
54	MG	1W	3001	1/1	0.88	0.21	46,46,46,46	0
54	MG	2a	1734	1/1	0.88	0.27	55,55,55,55	0
54	MG	2A	3649	1/1	0.88	0.17	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3652	1/1	0.88	0.18	44,44,44,44	0
54	MG	2a	1741	1/1	0.88	0.27	55,55,55,55	0
54	MG	2A	3421	1/1	0.88	0.14	62,62,62,62	0
54	MG	1a	1833	1/1	0.88	0.23	60,60,60,60	0
54	MG	2a	1746	1/1	0.88	0.18	60,60,60,60	0
54	MG	2a	1747	1/1	0.88	0.27	61,61,61,61	0
54	MG	1A	3857	1/1	0.88	0.10	26,26,26,26	0
54	MG	1A	3347	1/1	0.88	0.10	36,36,36,36	0
54	MG	1A	3948	1/1	0.88	0.11	60,60,60,60	0
54	MG	1l	102	1/1	0.88	0.08	47,47,47,47	0
54	MG	1a	1748	1/1	0.88	0.19	57,57,57,57	0
54	MG	2A	3674	1/1	0.88	0.15	63,63,63,63	0
54	MG	1A	3055	1/1	0.88	0.11	45,45,45,45	0
54	MG	2A	3449	1/1	0.88	0.14	58,58,58,58	0
54	MG	2A	3677	1/1	0.89	0.11	50,50,50,50	0
54	MG	2A	3472	1/1	0.89	0.09	52,52,52,52	0
54	MG	2A	3068	1/1	0.89	0.13	59,59,59,59	0
54	MG	1T	202	1/1	0.89	0.08	48,48,48,48	0
54	MG	2A	3072	1/1	0.89	0.12	49,49,49,49	0
54	MG	2A	3482	1/1	0.89	0.14	51,51,51,51	0
54	MG	2A	3703	1/1	0.89	0.09	81,81,81,81	0
54	MG	2A	3287	1/1	0.89	0.13	42,42,42,42	0
54	MG	1a	1692	1/1	0.89	0.19	46,46,46,46	0
54	MG	1A	3777	1/1	0.89	0.08	19,19,19,19	0
54	MG	2A	3082	1/1	0.89	0.11	62,62,62,62	0
54	MG	2A	3501	1/1	0.89	0.14	43,43,43,43	0
54	MG	1A	3780	1/1	0.89	0.13	45,45,45,45	0
54	MG	2A	3094	1/1	0.89	0.12	49,49,49,49	0
54	MG	1A	3430	1/1	0.89	0.12	38,38,38,38	0
54	MG	1a	1703	1/1	0.89	0.17	60,60,60,60	0
54	MG	2B	3010	1/1	0.89	0.21	68,68,68,68	0
54	MG	2B	3011	1/1	0.89	0.10	65,65,65,65	0
54	MG	1A	3861	1/1	0.89	0.11	22,22,22,22	0
54	MG	2A	3510	1/1	0.89	0.24	64,64,64,64	0
54	MG	1A	3867	1/1	0.89	0.16	47,47,47,47	0
54	MG	1A	3785	1/1	0.89	0.17	28,28,28,28	0
54	MG	1A	3518	1/1	0.89	0.14	51,51,51,51	0
54	MG	2A	3525	1/1	0.89	0.13	28,28,28,28	0
54	MG	1A	3873	1/1	0.89	0.20	57,57,57,57	0
54	MG	2A	3528	1/1	0.89	0.14	32,32,32,32	0
54	MG	2A	3343	1/1	0.89	0.23	50,50,50,50	0
54	MG	2E	302	1/1	0.89	0.19	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2G	3001	1/1	0.89	0.14	71,71,71,71	0
54	MG	2G	3002	1/1	0.89	0.14	65,65,65,65	0
54	MG	1A	3719	1/1	0.89	0.18	56,56,56,56	0
54	MG	2A	3122	1/1	0.89	0.19	66,66,66,66	0
54	MG	2A	3360	1/1	0.89	0.18	48,48,48,48	0
54	MG	2W	8002	1/1	0.89	0.13	59,59,59,59	0
54	MG	2A	3542	1/1	0.89	0.15	45,45,45,45	0
54	MG	2A	3543	1/1	0.89	0.19	49,49,49,49	0
54	MG	2A	3361	1/1	0.89	0.11	33,33,33,33	0
54	MG	2A	3364	1/1	0.89	0.22	58,58,58,58	0
54	MG	1A	3214	1/1	0.89	0.16	30,30,30,30	0
54	MG	1a	1720	1/1	0.89	0.10	60,60,60,60	0
54	MG	2a	1607	1/1	0.89	0.39	64,64,64,64	0
54	MG	2a	1611	1/1	0.89	0.11	62,62,62,62	0
54	MG	2A	3137	1/1	0.89	0.21	52,52,52,52	0
54	MG	2A	3553	1/1	0.89	0.28	56,56,56,56	0
54	MG	2A	3554	1/1	0.89	0.12	49,49,49,49	0
54	MG	1a	1730	1/1	0.89	0.13	43,43,43,43	0
54	MG	1A	3983	1/1	0.89	0.11	36,36,36,36	0
54	MG	1A	3296	1/1	0.89	0.12	19,19,19,19	0
54	MG	1a	1623	1/1	0.89	0.11	47,47,47,47	0
54	MG	1a	1739	1/1	0.89	0.11	61,61,61,61	0
54	MG	2a	1634	1/1	0.89	0.21	55,55,55,55	0
54	MG	2A	3166	1/1	0.89	0.14	51,51,51,51	0
54	MG	1a	1740	1/1	0.89	0.16	59,59,59,59	0
54	MG	2A	3572	1/1	0.89	0.07	21,21,21,21	0
54	MG	1a	1743	1/1	0.89	0.19	62,62,62,62	0
54	MG	2A	3397	1/1	0.89	0.14	55,55,55,55	0
54	MG	2a	1650	1/1	0.89	0.08	58,58,58,58	0
54	MG	2a	1651	1/1	0.89	0.24	58,58,58,58	0
54	MG	2A	3582	1/1	0.89	0.17	47,47,47,47	0
54	MG	1A	3799	1/1	0.89	0.12	46,46,46,46	0
54	MG	2A	3587	1/1	0.89	0.22	44,44,44,44	0
54	MG	1a	1631	1/1	0.89	0.20	64,64,64,64	0
54	MG	2A	3403	1/1	0.89	0.15	57,57,57,57	0
54	MG	2a	1668	1/1	0.89	0.14	45,45,45,45	0
54	MG	2A	3595	1/1	0.89	0.22	53,53,53,53	0
54	MG	2A	3596	1/1	0.89	0.27	50,50,50,50	0
54	MG	1A	3249	1/1	0.89	0.14	34,34,34,34	0
54	MG	1a	1636	1/1	0.89	0.17	60,60,60,60	0
54	MG	2A	3178	1/1	0.89	0.20	53,53,53,53	0
54	MG	1A	3804	1/1	0.89	0.10	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3362	1/1	0.89	0.10	36,36,36,36	0
54	MG	1B	215	1/1	0.89	0.12	61,61,61,61	0
54	MG	1d	303	1/1	0.89	0.28	68,68,68,68	0
54	MG	2A	3621	1/1	0.89	0.11	28,28,28,28	0
54	MG	2a	1682	1/1	0.89	0.14	60,60,60,60	0
54	MG	1B	219	1/1	0.89	0.09	46,46,46,46	0
54	MG	2A	3626	1/1	0.89	0.11	70,70,70,70	0
54	MG	2A	3200	1/1	0.89	0.08	45,45,45,45	0
54	MG	1A	3314	1/1	0.89	0.10	46,46,46,46	0
54	MG	1a	1760	1/1	0.89	0.25	52,52,52,52	0
54	MG	2A	3207	1/1	0.89	0.13	55,55,55,55	0
54	MG	1a	1650	1/1	0.89	0.24	62,62,62,62	0
54	MG	1A	3744	1/1	0.89	0.19	54,54,54,54	0
54	MG	1A	3182	1/1	0.89	0.09	43,43,43,43	0
54	MG	1A	3626	1/1	0.89	0.15	51,51,51,51	0
54	MG	2a	1706	1/1	0.89	0.13	63,63,63,63	0
54	MG	2a	1708	1/1	0.89	0.31	52,52,52,52	0
54	MG	1A	3749	1/1	0.89	0.09	36,36,36,36	0
54	MG	2a	1714	1/1	0.89	0.20	48,48,48,48	0
54	MG	1A	3500	1/1	0.89	0.10	44,44,44,44	0
54	MG	1A	3118	1/1	0.89	0.26	49,49,49,49	0
54	MG	2a	1720	1/1	0.89	0.22	50,50,50,50	0
54	MG	1A	3644	1/1	0.89	0.09	58,58,58,58	0
54	MG	2A	3651	1/1	0.89	0.20	58,58,58,58	0
54	MG	1a	1679	1/1	0.89	0.29	60,60,60,60	0
54	MG	2A	3654	1/1	0.89	0.18	57,57,57,57	0
54	MG	2A	3655	1/1	0.89	0.17	42,42,42,42	0
54	MG	2A	3244	1/1	0.89	0.38	44,44,44,44	0
54	MG	2A	3460	1/1	0.89	0.19	53,53,53,53	0
54	MG	2a	1738	1/1	0.89	0.32	52,52,52,52	0
54	MG	2A	3660	1/1	0.89	0.17	61,61,61,61	0
54	MG	2A	3661	1/1	0.89	0.10	47,47,47,47	0
54	MG	1A	3756	1/1	0.89	0.15	57,57,57,57	0
54	MG	2A	3465	1/1	0.89	0.15	56,56,56,56	0
54	MG	2A	3028	1/1	0.89	0.15	68,68,68,68	0
54	MG	2A	3666	1/1	0.89	0.23	51,51,51,51	0
54	MG	2e	3001	1/1	0.89	0.24	58,58,58,58	0
54	MG	2A	3669	1/1	0.89	0.18	59,59,59,59	0
54	MG	2A	3671	1/1	0.89	0.14	56,56,56,56	0
54	MG	2r	8001	1/1	0.89	0.22	65,65,65,65	0
57	MPD	1T	204	8/8	0.89	0.20	57,64,66,66	0
54	MG	1A	3570	1/1	0.89	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1683	1/1	0.89	0.16	59,59,59,59	0
54	MG	2A	3265	1/1	0.89	0.15	57,57,57,57	0
54	MG	1A	3759	1/1	0.89	0.24	43,43,43,43	0
54	MG	1A	3391	1/1	0.89	0.13	37,37,37,37	0
54	MG	1A	3678	1/1	0.90	0.12	40,40,40,40	0
54	MG	1G	3003	1/1	0.90	0.10	57,57,57,57	0
54	MG	1A	3355	1/1	0.90	0.08	33,33,33,33	0
54	MG	2A	3113	1/1	0.90	0.21	59,59,59,59	0
54	MG	1A	3688	1/1	0.90	0.13	34,34,34,34	0
54	MG	1A	3696	1/1	0.90	0.13	52,52,52,52	0
54	MG	2A	3546	1/1	0.90	0.18	41,41,41,41	0
54	MG	2D	305	1/1	0.90	0.22	53,53,53,53	0
54	MG	1A	3698	1/1	0.90	0.14	58,58,58,58	0
54	MG	1A	3187	1/1	0.90	0.13	49,49,49,49	0
54	MG	1A	3703	1/1	0.90	0.23	47,47,47,47	0
54	MG	1A	3302	1/1	0.90	0.14	27,27,27,27	0
54	MG	1A	3564	1/1	0.90	0.08	39,39,39,39	0
54	MG	1a	1819	1/1	0.90	0.27	51,51,51,51	0
54	MG	1a	1713	1/1	0.90	0.13	53,53,53,53	0
54	MG	1A	3727	1/1	0.90	0.15	22,22,22,22	0
54	MG	2A	3151	1/1	0.90	0.20	66,66,66,66	0
54	MG	2A	3162	1/1	0.90	0.16	53,53,53,53	0
54	MG	1a	1825	1/1	0.90	0.15	54,54,54,54	0
54	MG	1A	3162	1/1	0.90	0.12	41,41,41,41	0
54	MG	1A	3568	1/1	0.90	0.16	48,48,48,48	0
54	MG	19	503	1/1	0.90	0.08	50,50,50,50	0
54	MG	2a	1602	1/1	0.90	0.15	52,52,52,52	0
54	MG	2A	3401	1/1	0.90	0.08	54,54,54,54	0
54	MG	1A	3495	1/1	0.90	0.10	18,18,18,18	0
54	MG	1A	3572	1/1	0.90	0.17	46,46,46,46	0
54	MG	1a	1733	1/1	0.90	0.17	55,55,55,55	0
54	MG	2a	1612	1/1	0.90	0.09	50,50,50,50	0
54	MG	1a	1842	1/1	0.90	0.09	51,51,51,51	0
54	MG	2A	3590	1/1	0.90	0.14	58,58,58,58	0
54	MG	2A	3592	1/1	0.90	0.11	47,47,47,47	0
54	MG	1A	3316	1/1	0.90	0.10	38,38,38,38	0
54	MG	1A	3954	1/1	0.90	0.08	36,36,36,36	0
54	MG	2A	3411	1/1	0.90	0.07	55,55,55,55	0
54	MG	2a	1629	1/1	0.90	0.18	60,60,60,60	0
54	MG	1A	3380	1/1	0.90	0.09	29,29,29,29	0
54	MG	2A	3598	1/1	0.90	0.12	53,53,53,53	0
54	MG	1a	1847	1/1	0.90	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2a	1636	1/1	0.90	0.19	69,69,69,69	0
54	MG	2A	3601	1/1	0.90	0.28	57,57,57,57	0
54	MG	1a	1848	1/1	0.90	0.28	53,53,53,53	0
54	MG	1a	1621	1/1	0.90	0.20	46,46,46,46	0
54	MG	1A	3383	1/1	0.90	0.09	24,24,24,24	0
54	MG	2A	3423	1/1	0.90	0.10	45,45,45,45	0
54	MG	2a	1646	1/1	0.90	0.24	63,63,63,63	0
54	MG	2A	3614	1/1	0.90	0.20	58,58,58,58	0
54	MG	1a	1624	1/1	0.90	0.10	60,60,60,60	0
54	MG	2A	3203	1/1	0.90	0.10	51,51,51,51	0
54	MG	1A	3168	1/1	0.90	0.07	46,46,46,46	0
54	MG	1A	3503	1/1	0.90	0.20	58,58,58,58	0
54	MG	1A	3392	1/1	0.90	0.13	23,23,23,23	0
54	MG	2A	3433	1/1	0.90	0.20	57,57,57,57	0
54	MG	1e	3001	1/1	0.90	0.28	56,56,56,56	0
54	MG	1A	3173	1/1	0.90	0.14	43,43,43,43	0
54	MG	1A	3160	1/1	0.90	0.16	41,41,41,41	0
54	MG	2A	3220	1/1	0.90	0.18	58,58,58,58	0
54	MG	1B	202	1/1	0.90	0.15	36,36,36,36	0
54	MG	2A	3230	1/1	0.90	0.09	55,55,55,55	0
54	MG	1A	3279	1/1	0.90	0.13	61,61,61,61	0
54	MG	2A	3458	1/1	0.90	0.18	34,34,34,34	0
54	MG	1B	204	1/1	0.90	0.19	52,52,52,52	0
54	MG	1A	3872	1/1	0.90	0.15	50,50,50,50	0
54	MG	2A	3462	1/1	0.90	0.14	53,53,53,53	0
54	MG	1A	3621	1/1	0.90	0.15	52,52,52,52	0
54	MG	1A	3408	1/1	0.90	0.16	50,50,50,50	0
54	MG	1a	1657	1/1	0.90	0.19	59,59,59,59	0
54	MG	1A	3523	1/1	0.90	0.19	48,48,48,48	0
54	MG	2A	3657	1/1	0.90	0.15	43,43,43,43	0
54	MG	2A	3017	1/1	0.90	0.22	41,41,41,41	0
54	MG	2a	1695	1/1	0.90	0.23	62,62,62,62	0
54	MG	2A	3258	1/1	0.90	0.09	36,36,36,36	0
54	MG	1A	3036	1/1	0.90	0.10	38,38,38,38	0
54	MG	1A	3894	1/1	0.90	0.13	80,80,80,80	0
54	MG	2A	3032	1/1	0.90	0.20	54,54,54,54	0
54	MG	2A	3036	1/1	0.90	0.17	57,57,57,57	0
54	MG	2A	3275	1/1	0.90	0.14	62,62,62,62	0
54	MG	2A	3481	1/1	0.90	0.12	46,46,46,46	0
54	MG	1a	1668	1/1	0.90	0.40	74,74,74,74	0
54	MG	2A	3283	1/1	0.90	0.11	50,50,50,50	0
54	MG	1B	225	1/1	0.90	0.08	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	1777	1/1	0.90	0.48	61,61,61,61	0
54	MG	1A	3899	1/1	0.90	0.11	51,51,51,51	0
54	MG	1A	3639	1/1	0.90	0.13	34,34,34,34	0
54	MG	2a	1722	1/1	0.90	0.29	49,49,49,49	0
54	MG	1a	1677	1/1	0.90	0.20	64,64,64,64	0
54	MG	2A	3678	1/1	0.90	0.16	51,51,51,51	0
54	MG	1a	1678	1/1	0.90	0.22	53,53,53,53	0
54	MG	2a	1730	1/1	0.90	0.17	49,49,49,49	0
54	MG	2A	3684	1/1	0.90	0.10	65,65,65,65	0
54	MG	2A	3505	1/1	0.90	0.18	55,55,55,55	0
54	MG	1A	3527	1/1	0.90	0.09	51,51,51,51	0
54	MG	1A	3534	1/1	0.90	0.17	60,60,60,60	0
54	MG	2a	1740	1/1	0.90	0.42	59,59,59,59	0
54	MG	2A	3694	1/1	0.90	0.13	69,69,69,69	0
54	MG	2A	3696	1/1	0.90	0.09	52,52,52,52	0
54	MG	2a	1743	1/1	0.90	0.25	63,63,63,63	0
54	MG	2A	3508	1/1	0.90	0.30	57,57,57,57	0
54	MG	1D	310	1/1	0.90	0.08	62,62,62,62	0
54	MG	2A	3706	1/1	0.90	0.15	48,48,48,48	0
54	MG	2A	3320	1/1	0.90	0.19	59,59,59,59	0
54	MG	2A	3323	1/1	0.90	0.15	34,34,34,34	0
54	MG	1a	1793	1/1	0.90	0.22	63,63,63,63	0
54	MG	1A	3654	1/1	0.90	0.14	42,42,42,42	0
54	MG	2A	3524	1/1	0.90	0.13	26,26,26,26	0
57	MPD	1A	3988	8/8	0.90	0.20	48,52,54,59	0
54	MG	1a	1795	1/1	0.90	0.20	49,49,49,49	0
54	MG	1A	3668	1/1	0.90	0.19	63,63,63,63	0
54	MG	2A	3098	1/1	0.90	0.24	53,53,53,53	0
54	MG	1A	3481	1/1	0.90	0.08	48,48,48,48	0
54	MG	2B	3009	1/1	0.90	0.11	62,62,62,62	0
54	MG	2A	3342	1/1	0.90	0.21	51,51,51,51	0
54	MG	2A	3340	1/1	0.91	0.17	55,55,55,55	0
54	MG	1A	3774	1/1	0.91	0.08	12,12,12,12	0
54	MG	1A	3880	1/1	0.91	0.08	37,37,37,37	0
54	MG	2A	3346	1/1	0.91	0.16	52,52,52,52	0
54	MG	2A	3347	1/1	0.91	0.28	56,56,56,56	0
54	MG	1A	3011	1/1	0.91	0.10	47,47,47,47	0
54	MG	2A	3354	1/1	0.91	0.12	49,49,49,49	0
54	MG	1A	3883	1/1	0.91	0.15	47,47,47,47	0
54	MG	1A	3574	1/1	0.91	0.10	26,26,26,26	0
54	MG	1A	3889	1/1	0.91	0.10	36,36,36,36	0
54	MG	2A	3549	1/1	0.91	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3783	1/1	0.91	0.09	48,48,48,48	0
54	MG	1A	3687	1/1	0.91	0.09	44,44,44,44	0
54	MG	1A	3332	1/1	0.91	0.14	60,60,60,60	0
54	MG	2A	3376	1/1	0.91	0.10	47,47,47,47	0
54	MG	1A	3690	1/1	0.91	0.13	46,46,46,46	0
54	MG	1A	3057	1/1	0.91	0.15	27,27,27,27	0
54	MG	2A	3562	1/1	0.91	0.14	63,63,63,63	0
54	MG	2X	101	1/1	0.91	0.09	59,59,59,59	0
54	MG	2A	3381	1/1	0.91	0.19	53,53,53,53	0
54	MG	1a	1696	1/1	0.91	0.13	70,70,70,70	0
54	MG	2A	3566	1/1	0.91	0.10	35,35,35,35	0
54	MG	1a	1811	1/1	0.91	0.17	42,42,42,42	0
54	MG	1A	3793	1/1	0.91	0.14	41,41,41,41	0
54	MG	2A	3143	1/1	0.91	0.13	41,41,41,41	0
54	MG	2A	3570	1/1	0.91	0.16	44,44,44,44	0
54	MG	1a	1813	1/1	0.91	0.16	60,60,60,60	0
54	MG	1A	3583	1/1	0.91	0.19	20,20,20,20	0
54	MG	2A	3580	1/1	0.91	0.14	36,36,36,36	0
54	MG	1P	202	1/1	0.91	0.08	66,66,66,66	0
54	MG	1A	3402	1/1	0.91	0.10	50,50,50,50	0
54	MG	1A	3058	1/1	0.91	0.07	34,34,34,34	0
54	MG	1A	3919	1/1	0.91	0.16	45,45,45,45	0
54	MG	2A	3588	1/1	0.91	0.11	48,48,48,48	0
54	MG	1A	3716	1/1	0.91	0.13	47,47,47,47	0
54	MG	1A	3718	1/1	0.91	0.10	26,26,26,26	0
54	MG	1A	3283	1/1	0.91	0.09	32,32,32,32	0
54	MG	2a	1632	1/1	0.91	0.19	59,59,59,59	0
54	MG	1A	3291	1/1	0.91	0.14	45,45,45,45	0
54	MG	1A	3815	1/1	0.91	0.07	33,33,33,33	0
54	MG	1a	1836	1/1	0.91	0.09	62,62,62,62	0
54	MG	1A	3724	1/1	0.91	0.11	27,27,27,27	0
54	MG	1A	3818	1/1	0.91	0.13	31,31,31,31	0
54	MG	2a	1639	1/1	0.91	0.24	54,54,54,54	0
54	MG	2A	3599	1/1	0.91	0.12	45,45,45,45	0
54	MG	1a	1721	1/1	0.91	0.12	42,42,42,42	0
54	MG	2A	3189	1/1	0.91	0.30	66,66,66,66	0
54	MG	1a	1726	1/1	0.91	0.25	62,62,62,62	0
54	MG	1A	3357	1/1	0.91	0.09	20,20,20,20	0
54	MG	1A	3612	1/1	0.91	0.07	22,22,22,22	0
54	MG	2A	3611	1/1	0.91	0.15	56,56,56,56	0
54	MG	1a	1604	1/1	0.91	0.12	62,62,62,62	0
54	MG	1A	3208	1/1	0.91	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3829	1/1	0.91	0.13	54,54,54,54	0
54	MG	1a	1853	1/1	0.91	0.15	47,47,47,47	0
54	MG	1A	3538	1/1	0.91	0.10	55,55,55,55	0
54	MG	2A	3430	1/1	0.91	0.18	41,41,41,41	0
54	MG	1A	3739	1/1	0.91	0.13	51,51,51,51	0
54	MG	2A	3432	1/1	0.91	0.14	57,57,57,57	0
54	MG	2A	3213	1/1	0.91	0.17	67,67,67,67	0
54	MG	1a	1742	1/1	0.91	0.26	62,62,62,62	0
54	MG	1A	3416	1/1	0.91	0.13	48,48,48,48	0
54	MG	1A	3951	1/1	0.91	0.08	50,50,50,50	0
54	MG	1A	3010	1/1	0.91	0.10	38,38,38,38	0
54	MG	1A	3235	1/1	0.91	0.10	39,39,39,39	0
54	MG	2A	3453	1/1	0.91	0.16	64,64,64,64	0
54	MG	2A	3225	1/1	0.91	0.14	56,56,56,56	0
54	MG	2a	1683	1/1	0.91	0.14	57,57,57,57	0
54	MG	1A	3145	1/1	0.91	0.17	43,43,43,43	0
54	MG	1a	1633	1/1	0.91	0.09	37,37,37,37	0
54	MG	1A	3841	1/1	0.91	0.09	29,29,29,29	0
54	MG	2A	3232	1/1	0.91	0.12	44,44,44,44	0
54	MG	1A	3844	1/1	0.91	0.11	46,46,46,46	0
54	MG	2a	1694	1/1	0.91	0.21	60,60,60,60	0
54	MG	1A	3252	1/1	0.91	0.10	52,52,52,52	0
54	MG	1t	3001	1/1	0.91	0.16	52,52,52,52	0
54	MG	1a	1757	1/1	0.91	0.12	77,77,77,77	0
54	MG	1A	3850	1/1	0.91	0.13	48,48,48,48	0
54	MG	2a	1702	1/1	0.91	0.16	73,73,73,73	0
54	MG	1A	3991	1/1	0.91	0.17	43,43,43,43	0
54	MG	1A	3647	1/1	0.91	0.08	38,38,38,38	0
54	MG	1A	4023	1/1	0.91	0.21	36,36,36,36	0
54	MG	1A	3093	1/1	0.91	0.09	38,38,38,38	0
54	MG	2A	3473	1/1	0.91	0.11	60,60,60,60	0
54	MG	2a	1712	1/1	0.91	0.17	37,37,37,37	0
54	MG	1a	1652	1/1	0.91	0.32	61,61,61,61	0
54	MG	2a	1715	1/1	0.91	0.34	60,60,60,60	0
54	MG	2A	3667	1/1	0.91	0.11	49,49,49,49	0
54	MG	1a	1769	1/1	0.91	0.25	56,56,56,56	0
54	MG	1a	1771	1/1	0.91	0.17	46,46,46,46	0
54	MG	2A	3479	1/1	0.91	0.12	41,41,41,41	0
54	MG	2A	3480	1/1	0.91	0.33	37,37,37,37	0
54	MG	1a	1653	1/1	0.91	0.12	60,60,60,60	0
54	MG	1A	3387	1/1	0.91	0.10	54,54,54,54	0
54	MG	2A	3483	1/1	0.91	0.08	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	2A	3044	1/1	0.91	0.20	46,46,46,46	0
54	MG	2A	3486	1/1	0.91	0.17	56,56,56,56	0
54	MG	2A	3488	1/1	0.91	0.09	62,62,62,62	0
54	MG	2A	3047	1/1	0.91	0.20	56,56,56,56	0
54	MG	1A	3662	1/1	0.91	0.12	62,62,62,62	0
54	MG	2A	3056	1/1	0.91	0.10	46,46,46,46	0
54	MG	1a	1658	1/1	0.91	0.17	46,46,46,46	0
54	MG	1A	3502	1/1	0.91	0.21	54,54,54,54	0
54	MG	2A	3294	1/1	0.91	0.07	41,41,41,41	0
54	MG	2A	3301	1/1	0.91	0.13	56,56,56,56	0
54	MG	1A	3389	1/1	0.91	0.10	27,27,27,27	0
54	MG	1A	3760	1/1	0.91	0.29	61,61,61,61	0
54	MG	1A	3675	1/1	0.91	0.12	54,54,54,54	0
54	MG	2A	3079	1/1	0.91	0.15	47,47,47,47	0
54	MG	2A	3723	1/1	0.91	0.16	37,37,37,37	0
54	MG	1A	3765	1/1	0.91	0.08	39,39,39,39	0
54	MG	1a	1788	1/1	0.91	0.17	54,54,54,54	0
54	MG	2A	3519	1/1	0.91	0.12	54,54,54,54	0
54	MG	1a	1671	1/1	0.91	0.21	60,60,60,60	0
54	MG	2A	3087	1/1	0.91	0.13	52,52,52,52	0
54	MG	2A	3088	1/1	0.91	0.19	56,56,56,56	0
54	MG	2A	3092	1/1	0.91	0.12	46,46,46,46	0
54	MG	1a	1673	1/1	0.91	0.09	55,55,55,55	0
54	MG	1B	221	1/1	0.91	0.12	34,34,34,34	0
54	MG	1A	3881	1/1	0.92	0.19	43,43,43,43	0
54	MG	1A	3766	1/1	0.92	0.11	47,47,47,47	0
54	MG	2A	3463	1/1	0.92	0.17	62,62,62,62	0
54	MG	1D	313	1/1	0.92	0.13	43,43,43,43	0
54	MG	2A	3204	1/1	0.92	0.09	47,47,47,47	0
54	MG	2A	3688	1/1	0.92	0.14	56,56,56,56	0
54	MG	1A	3470	1/1	0.92	0.12	36,36,36,36	0
54	MG	1F	301	1/1	0.92	0.25	41,41,41,41	0
54	MG	1a	1844	1/1	0.92	0.16	58,58,58,58	0
54	MG	2A	3697	1/1	0.92	0.10	53,53,53,53	0
54	MG	1A	3885	1/1	0.92	0.08	53,53,53,53	0
54	MG	1F	309	1/1	0.92	0.12	43,43,43,43	0
54	MG	1A	3400	1/1	0.92	0.09	35,35,35,35	0
54	MG	1a	1714	1/1	0.92	0.15	56,56,56,56	0
54	MG	1A	3660	1/1	0.92	0.10	51,51,51,51	0
54	MG	2A	3714	1/1	0.92	0.20	45,45,45,45	0
54	MG	1a	1717	1/1	0.92	0.18	53,53,53,53	0
54	MG	1a	1855	1/1	0.92	0.07	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	3478	1/1	0.92	0.08	36,36,36,36	0
54	MG	2A	3228	1/1	0.92	0.09	58,58,58,58	0
54	MG	1A	3781	1/1	0.92	0.07	40,40,40,40	0
54	MG	1A	3340	1/1	0.92	0.09	28,28,28,28	0
54	MG	1A	3663	1/1	0.92	0.10	43,43,43,43	0
54	MG	1A	3341	1/1	0.92	0.08	36,36,36,36	0
54	MG	1A	3482	1/1	0.92	0.12	17,17,17,17	0
54	MG	2A	3485	1/1	0.92	0.11	45,45,45,45	0
54	MG	2A	3238	1/1	0.92	0.15	44,44,44,44	0
54	MG	1a	1729	1/1	0.92	0.18	60,60,60,60	0
54	MG	1e	3002	1/1	0.92	0.08	53,53,53,53	0
54	MG	2A	3245	1/1	0.92	0.30	60,60,60,60	0
54	MG	1A	3346	1/1	0.92	0.09	48,48,48,48	0
54	MG	2A	3499	1/1	0.92	0.10	30,30,30,30	0
54	MG	1A	3791	1/1	0.92	0.12	59,59,59,59	0
54	MG	1V	201	1/1	0.92	0.12	50,50,50,50	0
54	MG	1A	3910	1/1	0.92	0.09	59,59,59,59	0
54	MG	1i	3001	1/1	0.92	0.12	53,53,53,53	0
54	MG	1A	3021	1/1	0.92	0.09	38,38,38,38	0
54	MG	10	103	1/1	0.92	0.07	43,43,43,43	0
54	MG	2F	301	1/1	0.92	0.09	39,39,39,39	0
54	MG	2A	3272	1/1	0.92	0.09	38,38,38,38	0
54	MG	1A	3156	1/1	0.92	0.16	49,49,49,49	0
54	MG	1A	3917	1/1	0.92	0.11	51,51,51,51	0
54	MG	2A	3513	1/1	0.92	0.26	50,50,50,50	0
54	MG	2N	8001	1/1	0.92	0.08	70,70,70,70	0
54	MG	1A	3414	1/1	0.92	0.09	49,49,49,49	0
54	MG	2W	8001	1/1	0.92	0.14	42,42,42,42	0
54	MG	1y	3003	1/1	0.92	0.09	74,74,74,74	0
54	MG	1A	3798	1/1	0.92	0.12	35,35,35,35	0
54	MG	17	102	1/1	0.92	0.10	40,40,40,40	0
54	MG	1A	3123	1/1	0.92	0.07	32,32,32,32	0
54	MG	1A	3928	1/1	0.92	0.11	27,27,27,27	0
54	MG	1A	3496	1/1	0.92	0.10	47,47,47,47	0
54	MG	2A	3030	1/1	0.92	0.11	53,53,53,53	0
54	MG	1A	3497	1/1	0.92	0.09	46,46,46,46	0
54	MG	2a	1604	1/1	0.92	0.10	58,58,58,58	0
54	MG	1A	3065	1/1	0.92	0.22	26,26,26,26	0
54	MG	1A	3807	1/1	0.92	0.13	40,40,40,40	0
54	MG	2a	1608	1/1	0.92	0.15	62,62,62,62	0
54	MG	2A	3040	1/1	0.92	0.14	58,58,58,58	0
54	MG	2A	3315	1/1	0.92	0.23	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	3317	1/1	0.92	0.07	33,33,33,33	0
54	MG	1a	1614	1/1	0.92	0.08	56,56,56,56	0
54	MG	2A	3319	1/1	0.92	0.11	39,39,39,39	0
54	MG	2A	3042	1/1	0.92	0.19	49,49,49,49	0
54	MG	2a	1624	1/1	0.92	0.19	65,65,65,65	0
54	MG	2A	3321	1/1	0.92	0.09	43,43,43,43	0
54	MG	2a	1626	1/1	0.92	0.24	53,53,53,53	0
54	MG	1a	1758	1/1	0.92	0.21	52,52,52,52	0
54	MG	2A	3324	1/1	0.92	0.10	30,30,30,30	0
54	MG	2A	3045	1/1	0.92	0.09	40,40,40,40	0
54	MG	2A	3046	1/1	0.92	0.22	59,59,59,59	0
54	MG	1A	3810	1/1	0.92	0.08	37,37,37,37	0
54	MG	2A	3334	1/1	0.92	0.18	35,35,35,35	0
54	MG	1A	3099	1/1	0.92	0.11	30,30,30,30	0
54	MG	2A	3054	1/1	0.92	0.10	63,63,63,63	0
54	MG	1a	1761	1/1	0.92	0.09	57,57,57,57	0
54	MG	2A	3057	1/1	0.92	0.06	39,39,39,39	0
54	MG	2A	3060	1/1	0.92	0.21	48,48,48,48	0
54	MG	1A	3421	1/1	0.92	0.08	30,30,30,30	0
54	MG	1A	3704	1/1	0.92	0.14	50,50,50,50	0
54	MG	1A	3943	1/1	0.92	0.09	52,52,52,52	0
54	MG	1A	3100	1/1	0.92	0.11	39,39,39,39	0
54	MG	1A	3819	1/1	0.92	0.07	39,39,39,39	0
54	MG	2A	3575	1/1	0.92	0.12	41,41,41,41	0
54	MG	1a	1770	1/1	0.92	0.19	54,54,54,54	0
54	MG	2A	3356	1/1	0.92	0.15	40,40,40,40	0
54	MG	2A	3080	1/1	0.92	0.26	57,57,57,57	0
54	MG	2a	1663	1/1	0.92	0.19	48,48,48,48	0
54	MG	1A	3584	1/1	0.92	0.10	51,51,51,51	0
54	MG	2A	3583	1/1	0.92	0.13	42,42,42,42	0
54	MG	1A	3313	1/1	0.92	0.08	46,46,46,46	0
54	MG	2A	3368	1/1	0.92	0.07	30,30,30,30	0
54	MG	2a	1671	1/1	0.92	0.25	47,47,47,47	0
54	MG	1A	3590	1/1	0.92	0.09	32,32,32,32	0
54	MG	1a	1639	1/1	0.92	0.18	49,49,49,49	0
54	MG	2A	3375	1/1	0.92	0.19	64,64,64,64	0
54	MG	1A	3953	1/1	0.92	0.09	51,51,51,51	0
54	MG	1a	1643	1/1	0.92	0.17	52,52,52,52	0
54	MG	1A	3591	1/1	0.92	0.10	36,36,36,36	0
54	MG	2A	3095	1/1	0.92	0.10	58,58,58,58	0
54	MG	1A	3253	1/1	0.92	0.20	59,59,59,59	0
54	MG	1A	3599	1/1	0.92	0.12	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3381	1/1	0.92	0.09	40,40,40,40	0
54	MG	2A	3102	1/1	0.92	0.13	42,42,42,42	0
54	MG	2a	1686	1/1	0.92	0.21	52,52,52,52	0
54	MG	1A	3734	1/1	0.92	0.13	26,26,26,26	0
54	MG	1A	3836	1/1	0.92	0.15	51,51,51,51	0
54	MG	2A	3392	1/1	0.92	0.16	56,56,56,56	0
54	MG	2a	1692	1/1	0.92	0.26	48,48,48,48	0
54	MG	1A	3976	1/1	0.92	0.08	38,38,38,38	0
54	MG	1A	3981	1/1	0.92	0.12	51,51,51,51	0
54	MG	1A	3144	1/1	0.92	0.18	51,51,51,51	0
54	MG	2a	1696	1/1	0.92	0.14	59,59,59,59	0
54	MG	2a	1697	1/1	0.92	0.20	59,59,59,59	0
54	MG	2A	3613	1/1	0.92	0.21	57,57,57,57	0
54	MG	1A	3986	1/1	0.92	0.12	61,61,61,61	0
54	MG	1A	3513	1/1	0.92	0.09	53,53,53,53	0
54	MG	1A	3515	1/1	0.92	0.15	30,30,30,30	0
54	MG	1a	1667	1/1	0.92	0.13	50,50,50,50	0
54	MG	2A	3625	1/1	0.92	0.06	16,16,16,16	0
54	MG	2a	1705	1/1	0.92	0.22	55,55,55,55	0
54	MG	1A	4009	1/1	0.92	0.24	42,42,42,42	0
54	MG	2A	3136	1/1	0.92	0.20	51,51,51,51	0
54	MG	1A	4015	1/1	0.92	0.13	39,39,39,39	0
54	MG	1a	1804	1/1	0.92	0.24	59,59,59,59	0
54	MG	1A	4017	1/1	0.92	0.13	34,34,34,34	0
54	MG	1a	1806	1/1	0.92	0.11	53,53,53,53	0
54	MG	2A	3147	1/1	0.92	0.26	44,44,44,44	0
54	MG	2A	3416	1/1	0.92	0.14	54,54,54,54	0
54	MG	1A	3742	1/1	0.92	0.09	32,32,32,32	0
54	MG	2A	3644	1/1	0.92	0.11	48,48,48,48	0
54	MG	2A	3418	1/1	0.92	0.09	54,54,54,54	0
54	MG	1A	3615	1/1	0.92	0.12	50,50,50,50	0
54	MG	1A	3257	1/1	0.92	0.11	42,42,42,42	0
54	MG	2a	1727	1/1	0.92	0.17	61,61,61,61	0
54	MG	2A	3422	1/1	0.92	0.07	55,55,55,55	0
54	MG	2A	3160	1/1	0.92	0.11	63,63,63,63	0
54	MG	1A	3261	1/1	0.92	0.23	36,36,36,36	0
54	MG	1A	3197	1/1	0.92	0.10	41,41,41,41	0
54	MG	1A	3630	1/1	0.92	0.11	54,54,54,54	0
54	MG	1A	3631	1/1	0.92	0.13	48,48,48,48	0
54	MG	1a	1816	1/1	0.92	0.13	52,52,52,52	0
54	MG	2A	3658	1/1	0.92	0.09	34,34,34,34	0
54	MG	1A	3865	1/1	0.92	0.33	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	3632	1/1	0.92	0.16	63,63,63,63	0
54	MG	1A	3272	1/1	0.92	0.13	38,38,38,38	0
54	MG	1A	3456	1/1	0.92	0.10	27,27,27,27	0
54	MG	2A	3436	1/1	0.92	0.11	56,56,56,56	0
54	MG	2a	1748	1/1	0.92	0.26	52,52,52,52	0
54	MG	2A	3440	1/1	0.92	0.11	49,49,49,49	0
54	MG	1A	3526	1/1	0.92	0.08	40,40,40,40	0
54	MG	2A	3445	1/1	0.92	0.15	41,41,41,41	0
54	MG	1A	3642	1/1	0.92	0.08	51,51,51,51	0
54	MG	2q	201	1/1	0.92	0.15	64,64,64,64	0
54	MG	2A	3670	1/1	0.92	0.13	49,49,49,49	0
54	MG	2A	3182	1/1	0.92	0.11	53,53,53,53	0
54	MG	1a	1694	1/1	0.92	0.15	32,32,32,32	0
54	MG	2A	3191	1/1	0.92	0.18	57,57,57,57	0
54	MG	1A	3102	1/1	0.92	0.10	53,53,53,53	0
54	MG	1a	1697	1/1	0.92	0.16	51,51,51,51	0
54	MG	1a	1834	1/1	0.92	0.34	58,58,58,58	0
54	MG	1A	3528	1/1	0.92	0.13	43,43,43,43	0
54	MG	1a	1629	1/1	0.93	0.12	45,45,45,45	0
54	MG	1A	3697	1/1	0.93	0.20	50,50,50,50	0
54	MG	2A	3112	1/1	0.93	0.20	44,44,44,44	0
54	MG	1a	1784	1/1	0.93	0.13	59,59,59,59	0
54	MG	1a	1786	1/1	0.93	0.27	57,57,57,57	0
54	MG	1A	3167	1/1	0.93	0.30	28,28,28,28	0
54	MG	1a	1789	1/1	0.93	0.15	69,69,69,69	0
54	MG	2A	3665	1/1	0.93	0.19	56,56,56,56	0
54	MG	1A	3816	1/1	0.93	0.09	35,35,35,35	0
54	MG	2A	3125	1/1	0.93	0.11	38,38,38,38	0
54	MG	2A	3668	1/1	0.93	0.12	48,48,48,48	0
54	MG	1A	3335	1/1	0.93	0.10	22,22,22,22	0
54	MG	1A	3405	1/1	0.93	0.06	17,17,17,17	0
54	MG	1A	3580	1/1	0.93	0.08	22,22,22,22	0
54	MG	1A	3406	1/1	0.93	0.21	52,52,52,52	0
54	MG	1A	3821	1/1	0.93	0.09	26,26,26,26	0
54	MG	2A	3144	1/1	0.93	0.17	54,54,54,54	0
54	MG	1A	3717	1/1	0.93	0.10	52,52,52,52	0
54	MG	2A	3427	1/1	0.93	0.16	57,57,57,57	0
54	MG	1a	1647	1/1	0.93	0.24	52,52,52,52	0
54	MG	2A	3148	1/1	0.93	0.09	57,57,57,57	0
54	MG	2A	3679	1/1	0.93	0.12	57,57,57,57	0
54	MG	1a	1800	1/1	0.93	0.11	43,43,43,43	0
54	MG	2A	3683	1/1	0.93	0.10	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	3198	1/1	0.93	0.17	42,42,42,42	0
54	MG	1A	3958	1/1	0.93	0.12	53,53,53,53	0
54	MG	2A	3157	1/1	0.93	0.11	42,42,42,42	0
54	MG	1A	3265	1/1	0.93	0.13	46,46,46,46	0
54	MG	2A	3161	1/1	0.93	0.08	46,46,46,46	0
54	MG	1a	1651	1/1	0.93	0.12	59,59,59,59	0
54	MG	2A	3695	1/1	0.93	0.09	36,36,36,36	0
54	MG	2A	3441	1/1	0.93	0.12	47,47,47,47	0
54	MG	1A	3413	1/1	0.93	0.25	57,57,57,57	0
54	MG	1A	3722	1/1	0.93	0.20	39,39,39,39	0
54	MG	1A	3266	1/1	0.93	0.20	40,40,40,40	0
54	MG	1A	3074	1/1	0.93	0.12	45,45,45,45	0
54	MG	1A	3979	1/1	0.93	0.06	47,47,47,47	0
54	MG	1A	3729	1/1	0.93	0.16	31,31,31,31	0
54	MG	1a	1661	1/1	0.93	0.19	49,49,49,49	0
54	MG	2A	3717	1/1	0.93	0.08	61,61,61,61	0
54	MG	2A	3455	1/1	0.93	0.10	48,48,48,48	0
54	MG	2A	3456	1/1	0.93	0.08	31,31,31,31	0
54	MG	1A	3154	1/1	0.93	0.11	41,41,41,41	0
54	MG	1A	3600	1/1	0.93	0.10	27,27,27,27	0
54	MG	1A	3839	1/1	0.93	0.12	32,32,32,32	0
54	MG	2A	3180	1/1	0.93	0.14	63,63,63,63	0
54	MG	1A	4005	1/1	0.93	0.11	32,32,32,32	0
54	MG	2A	3184	1/1	0.93	0.24	68,68,68,68	0
54	MG	1A	3013	1/1	0.93	0.18	50,50,50,50	0
54	MG	1a	1820	1/1	0.93	0.13	56,56,56,56	0
54	MG	1a	1670	1/1	0.93	0.07	50,50,50,50	0
54	MG	2B	3012	1/1	0.93	0.11	50,50,50,50	0
54	MG	2A	3194	1/1	0.93	0.14	60,60,60,60	0
54	MG	1A	3354	1/1	0.93	0.06	20,20,20,20	0
54	MG	1a	1672	1/1	0.93	0.09	51,51,51,51	0
54	MG	1A	4013	1/1	0.93	0.26	29,29,29,29	0
54	MG	1a	1829	1/1	0.93	0.18	42,42,42,42	0
54	MG	1A	3848	1/1	0.93	0.10	48,48,48,48	0
54	MG	1A	3738	1/1	0.93	0.08	24,24,24,24	0
54	MG	1A	3606	1/1	0.93	0.15	42,42,42,42	0
54	MG	1B	201	1/1	0.93	0.28	34,34,34,34	0
54	MG	1A	3851	1/1	0.93	0.07	41,41,41,41	0
54	MG	2A	3211	1/1	0.93	0.14	46,46,46,46	0
54	MG	1A	3043	1/1	0.93	0.26	52,52,52,52	0
54	MG	1A	3514	1/1	0.93	0.19	47,47,47,47	0
54	MG	1a	1682	1/1	0.93	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3743	1/1	0.93	0.08	62,62,62,62	0
54	MG	2A	3218	1/1	0.93	0.23	57,57,57,57	0
54	MG	1A	3280	1/1	0.93	0.14	44,44,44,44	0
54	MG	2O	201	1/1	0.93	0.08	48,48,48,48	0
54	MG	2P	201	1/1	0.93	0.15	52,52,52,52	0
54	MG	1A	3617	1/1	0.93	0.09	38,38,38,38	0
54	MG	2A	3487	1/1	0.93	0.15	46,46,46,46	0
54	MG	1a	1687	1/1	0.93	0.19	54,54,54,54	0
54	MG	1a	1688	1/1	0.93	0.21	53,53,53,53	0
54	MG	1A	3866	1/1	0.93	0.07	35,35,35,35	0
54	MG	2A	3229	1/1	0.93	0.27	49,49,49,49	0
54	MG	2A	3494	1/1	0.93	0.08	50,50,50,50	0
54	MG	2A	3496	1/1	0.93	0.12	40,40,40,40	0
54	MG	1A	3220	1/1	0.93	0.18	31,31,31,31	0
54	MG	1A	3619	1/1	0.93	0.22	25,25,25,25	0
54	MG	1B	222	1/1	0.93	0.15	57,57,57,57	0
54	MG	1A	3869	1/1	0.93	0.13	56,56,56,56	0
54	MG	2A	3235	1/1	0.93	0.22	54,54,54,54	0
54	MG	1A	3520	1/1	0.93	0.07	38,38,38,38	0
54	MG	1A	3284	1/1	0.93	0.14	32,32,32,32	0
54	MG	2A	3239	1/1	0.93	0.16	50,50,50,50	0
54	MG	1d	305	1/1	0.93	0.14	56,56,56,56	0
54	MG	2a	1615	1/1	0.93	0.10	60,60,60,60	0
54	MG	2a	1616	1/1	0.93	0.32	60,60,60,60	0
54	MG	2a	1617	1/1	0.93	0.09	43,43,43,43	0
54	MG	1A	3368	1/1	0.93	0.12	16,16,16,16	0
54	MG	2A	3511	1/1	0.93	0.12	43,43,43,43	0
54	MG	1A	3874	1/1	0.93	0.11	43,43,43,43	0
54	MG	1A	3754	1/1	0.93	0.27	37,37,37,37	0
54	MG	1a	1705	1/1	0.93	0.11	59,59,59,59	0
54	MG	1A	3877	1/1	0.93	0.10	57,57,57,57	0
54	MG	1D	311	1/1	0.93	0.08	66,66,66,66	0
54	MG	2A	3260	1/1	0.93	0.14	53,53,53,53	0
54	MG	1A	3230	1/1	0.93	0.23	46,46,46,46	0
54	MG	2a	1631	1/1	0.93	0.17	52,52,52,52	0
54	MG	2A	3262	1/1	0.93	0.21	62,62,62,62	0
54	MG	2A	3527	1/1	0.93	0.14	38,38,38,38	0
54	MG	1g	3003	1/1	0.93	0.11	45,45,45,45	0
54	MG	2a	1635	1/1	0.93	0.23	71,71,71,71	0
54	MG	2A	3531	1/1	0.93	0.11	54,54,54,54	0
54	MG	1A	3233	1/1	0.93	0.17	48,48,48,48	0
54	MG	1E	305	1/1	0.93	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3273	1/1	0.93	0.16	51,51,51,51	0
54	MG	2a	1640	1/1	0.93	0.23	53,53,53,53	0
54	MG	1E	306	1/1	0.93	0.12	31,31,31,31	0
54	MG	2A	3538	1/1	0.93	0.07	35,35,35,35	0
54	MG	2a	1644	1/1	0.93	0.24	55,55,55,55	0
54	MG	2A	3539	1/1	0.93	0.15	41,41,41,41	0
54	MG	2A	3541	1/1	0.93	0.07	47,47,47,47	0
54	MG	2a	1649	1/1	0.93	0.07	49,49,49,49	0
54	MG	1A	3448	1/1	0.93	0.09	24,24,24,24	0
54	MG	2A	3277	1/1	0.93	0.12	38,38,38,38	0
54	MG	2A	3279	1/1	0.93	0.10	63,63,63,63	0
54	MG	1o	3001	1/1	0.93	0.15	44,44,44,44	0
54	MG	1A	3140	1/1	0.93	0.19	29,29,29,29	0
54	MG	2a	1660	1/1	0.93	0.15	55,55,55,55	0
54	MG	2A	3547	1/1	0.93	0.07	38,38,38,38	0
54	MG	1F	307	1/1	0.93	0.10	31,31,31,31	0
54	MG	1A	3884	1/1	0.93	0.07	48,48,48,48	0
54	MG	2a	1666	1/1	0.93	0.32	57,57,57,57	0
54	MG	1A	3241	1/1	0.93	0.06	43,43,43,43	0
54	MG	1A	3641	1/1	0.93	0.12	29,29,29,29	0
54	MG	2A	3001	1/1	0.93	0.15	46,46,46,46	0
54	MG	1A	3303	1/1	0.93	0.13	55,55,55,55	0
54	MG	2A	3297	1/1	0.93	0.18	51,51,51,51	0
54	MG	2A	3016	1/1	0.93	0.19	37,37,37,37	0
54	MG	2a	1675	1/1	0.93	0.17	56,56,56,56	0
54	MG	1A	3385	1/1	0.93	0.07	51,51,51,51	0
54	MG	2A	3307	1/1	0.93	0.12	51,51,51,51	0
54	MG	1N	202	1/1	0.93	0.10	56,56,56,56	0
54	MG	2A	3020	1/1	0.93	0.07	57,57,57,57	0
54	MG	2A	3021	1/1	0.93	0.08	47,47,47,47	0
54	MG	1N	203	1/1	0.93	0.08	53,53,53,53	0
54	MG	1a	1736	1/1	0.93	0.16	57,57,57,57	0
54	MG	1O	8001	1/1	0.93	0.08	43,43,43,43	0
54	MG	1A	3543	1/1	0.93	0.19	44,44,44,44	0
54	MG	1A	3901	1/1	0.93	0.11	37,37,37,37	0
54	MG	2A	3576	1/1	0.93	0.10	62,62,62,62	0
54	MG	2A	3577	1/1	0.93	0.25	68,68,68,68	0
54	MG	1A	3778	1/1	0.93	0.10	35,35,35,35	0
54	MG	2a	1691	1/1	0.93	0.17	56,56,56,56	0
54	MG	1A	3461	1/1	0.93	0.10	45,45,45,45	0
54	MG	1A	3650	1/1	0.93	0.07	38,38,38,38	0
54	MG	1a	1744	1/1	0.93	0.11	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	3651	1/1	0.93	0.11	30,30,30,30	0
54	MG	2A	3585	1/1	0.93	0.13	57,57,57,57	0
54	MG	1A	3546	1/1	0.93	0.16	52,52,52,52	0
54	MG	1A	3309	1/1	0.93	0.08	34,34,34,34	0
54	MG	2A	3048	1/1	0.93	0.26	61,61,61,61	0
54	MG	1a	1750	1/1	0.93	0.12	59,59,59,59	0
54	MG	2A	3052	1/1	0.93	0.07	40,40,40,40	0
54	MG	2A	3591	1/1	0.93	0.12	51,51,51,51	0
54	MG	2A	3341	1/1	0.93	0.10	33,33,33,33	0
54	MG	2A	3053	1/1	0.93	0.12	47,47,47,47	0
54	MG	1A	3911	1/1	0.93	0.11	46,46,46,46	0
54	MG	2a	1707	1/1	0.93	0.15	47,47,47,47	0
54	MG	2A	3055	1/1	0.93	0.11	38,38,38,38	0
54	MG	1A	3242	1/1	0.93	0.16	53,53,53,53	0
54	MG	2A	3348	1/1	0.93	0.14	42,42,42,42	0
54	MG	2A	3349	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3557	1/1	0.93	0.08	35,35,35,35	0
54	MG	2A	3058	1/1	0.93	0.10	51,51,51,51	0
54	MG	10	106	1/1	0.93	0.17	41,41,41,41	0
54	MG	2A	3061	1/1	0.93	0.15	51,51,51,51	0
54	MG	2A	3609	1/1	0.93	0.13	45,45,45,45	0
54	MG	2A	3357	1/1	0.93	0.14	41,41,41,41	0
54	MG	2a	1724	1/1	0.93	0.20	41,41,41,41	0
54	MG	1A	3559	1/1	0.93	0.12	55,55,55,55	0
54	MG	11	103	1/1	0.93	0.09	42,42,42,42	0
54	MG	2A	3363	1/1	0.93	0.19	61,61,61,61	0
54	MG	1A	3918	1/1	0.93	0.11	38,38,38,38	0
54	MG	1A	3142	1/1	0.93	0.11	50,50,50,50	0
54	MG	2A	3074	1/1	0.93	0.11	39,39,39,39	0
54	MG	1A	3120	1/1	0.93	0.11	44,44,44,44	0
54	MG	1A	3924	1/1	0.93	0.12	45,45,45,45	0
54	MG	1a	1762	1/1	0.93	0.38	56,56,56,56	0
54	MG	2A	3377	1/1	0.93	0.11	43,43,43,43	0
54	MG	1A	3395	1/1	0.93	0.09	13,13,13,13	0
54	MG	1A	3797	1/1	0.93	0.12	34,34,34,34	0
54	MG	1A	3483	1/1	0.93	0.09	49,49,49,49	0
54	MG	2a	1744	1/1	0.93	0.20	50,50,50,50	0
54	MG	2A	3631	1/1	0.93	0.14	60,60,60,60	0
54	MG	2A	3084	1/1	0.93	0.08	52,52,52,52	0
54	MG	1a	1609	1/1	0.93	0.09	51,51,51,51	0
54	MG	1A	3680	1/1	0.93	0.13	25,25,25,25	0
54	MG	1A	3936	1/1	0.93	0.15	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3569	1/1	0.93	0.18	34,34,34,34	0
54	MG	2A	3645	1/1	0.93	0.11	40,40,40,40	0
54	MG	1a	1618	1/1	0.93	0.09	51,51,51,51	0
54	MG	1A	3325	1/1	0.93	0.08	53,53,53,53	0
54	MG	1a	1622	1/1	0.93	0.21	51,51,51,51	0
54	MG	2t	3001	1/1	0.93	0.19	45,45,45,45	0
54	MG	1A	3070	1/1	0.93	0.07	42,42,42,42	0
54	MG	2A	3100	1/1	0.93	0.14	48,48,48,48	0
54	MG	2A	3101	1/1	0.93	0.15	50,50,50,50	0
54	MG	2A	3400	1/1	0.93	0.12	36,36,36,36	0
54	MG	1A	3692	1/1	0.93	0.08	34,34,34,34	0
54	MG	1a	1626	1/1	0.93	0.28	59,59,59,59	0
58	ARG	1B	228	12/12	0.93	0.09	26,40,53,54	0
54	MG	1A	3193	1/1	0.93	0.08	44,44,44,44	0
59	ZN	2n	501	1/1	0.93	0.08	101,101,101,101	0
54	MG	1A	3480	1/1	0.94	0.10	36,36,36,36	0
54	MG	1A	4027	1/1	0.94	0.20	37,37,37,37	0
54	MG	1A	3731	1/1	0.94	0.14	40,40,40,40	0
54	MG	1a	1831	1/1	0.94	0.14	54,54,54,54	0
54	MG	1a	1832	1/1	0.94	0.07	42,42,42,42	0
54	MG	2A	3682	1/1	0.94	0.12	51,51,51,51	0
54	MG	2A	3188	1/1	0.94	0.16	51,51,51,51	0
54	MG	1A	3853	1/1	0.94	0.08	15,15,15,15	0
54	MG	2A	3452	1/1	0.94	0.16	38,38,38,38	0
54	MG	2A	3686	1/1	0.94	0.08	42,42,42,42	0
54	MG	1A	3324	1/1	0.94	0.13	39,39,39,39	0
54	MG	1A	3587	1/1	0.94	0.08	26,26,26,26	0
54	MG	2A	3689	1/1	0.94	0.11	59,59,59,59	0
54	MG	1A	3153	1/1	0.94	0.14	42,42,42,42	0
54	MG	2A	3693	1/1	0.94	0.09	50,50,50,50	0
54	MG	1A	3860	1/1	0.94	0.10	43,43,43,43	0
54	MG	2A	3196	1/1	0.94	0.14	50,50,50,50	0
54	MG	1a	1839	1/1	0.94	0.14	59,59,59,59	0
54	MG	1B	208	1/1	0.94	0.24	51,51,51,51	0
54	MG	2A	3698	1/1	0.94	0.08	40,40,40,40	0
54	MG	1a	1841	1/1	0.94	0.17	57,57,57,57	0
54	MG	1A	3184	1/1	0.94	0.16	50,50,50,50	0
54	MG	2A	3704	1/1	0.94	0.10	33,33,33,33	0
54	MG	1A	3484	1/1	0.94	0.07	35,35,35,35	0
54	MG	1A	3328	1/1	0.94	0.06	13,13,13,13	0
54	MG	1A	3393	1/1	0.94	0.06	18,18,18,18	0
54	MG	1A	3394	1/1	0.94	0.10	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3716	1/1	0.94	0.18	51,51,51,51	0
54	MG	2A	3208	1/1	0.94	0.17	43,43,43,43	0
54	MG	2A	3719	1/1	0.94	0.08	48,48,48,48	0
54	MG	2A	3721	1/1	0.94	0.06	42,42,42,42	0
54	MG	1A	3490	1/1	0.94	0.08	50,50,50,50	0
54	MG	2A	3725	1/1	0.94	0.10	37,37,37,37	0
54	MG	1A	3276	1/1	0.94	0.09	26,26,26,26	0
54	MG	1A	3871	1/1	0.94	0.20	50,50,50,50	0
54	MG	1a	1852	1/1	0.94	0.18	54,54,54,54	0
54	MG	1A	3397	1/1	0.94	0.13	49,49,49,49	0
54	MG	1A	3087	1/1	0.94	0.30	26,26,26,26	0
54	MG	1A	3059	1/1	0.94	0.14	42,42,42,42	0
54	MG	1A	3236	1/1	0.94	0.26	38,38,38,38	0
54	MG	2A	3222	1/1	0.94	0.05	46,46,46,46	0
54	MG	1d	301	1/1	0.94	0.07	68,68,68,68	0
54	MG	1A	3125	1/1	0.94	0.21	30,30,30,30	0
54	MG	1d	304	1/1	0.94	0.07	56,56,56,56	0
54	MG	1A	3097	1/1	0.94	0.27	23,23,23,23	0
54	MG	1A	3285	1/1	0.94	0.20	36,36,36,36	0
54	MG	1A	3620	1/1	0.94	0.10	44,44,44,44	0
54	MG	1A	3342	1/1	0.94	0.11	48,48,48,48	0
54	MG	1A	3343	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3628	1/1	0.94	0.09	47,47,47,47	0
54	MG	1a	1709	1/1	0.94	0.10	54,54,54,54	0
54	MG	1g	3001	1/1	0.94	0.29	52,52,52,52	0
54	MG	1F	305	1/1	0.94	0.18	34,34,34,34	0
54	MG	1A	3098	1/1	0.94	0.16	35,35,35,35	0
54	MG	1A	3293	1/1	0.94	0.10	18,18,18,18	0
54	MG	2E	303	1/1	0.94	0.14	44,44,44,44	0
54	MG	2A	3495	1/1	0.94	0.16	45,45,45,45	0
54	MG	2F	303	1/1	0.94	0.15	43,43,43,43	0
54	MG	1F	310	1/1	0.94	0.11	42,42,42,42	0
54	MG	2A	3498	1/1	0.94	0.14	30,30,30,30	0
54	MG	1A	3768	1/1	0.94	0.07	54,54,54,54	0
54	MG	1a	1716	1/1	0.94	0.14	39,39,39,39	0
54	MG	2A	3502	1/1	0.94	0.40	64,64,64,64	0
54	MG	1F	312	1/1	0.94	0.08	51,51,51,51	0
54	MG	2A	3253	1/1	0.94	0.14	25,25,25,25	0
54	MG	2T	3001	1/1	0.94	0.15	50,50,50,50	0
54	MG	1G	3001	1/1	0.94	0.08	52,52,52,52	0
54	MG	1A	3895	1/1	0.94	0.07	16,16,16,16	0
54	MG	1A	3898	1/1	0.94	0.08	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3770	1/1	0.94	0.12	27,27,27,27	0
54	MG	2A	3264	1/1	0.94	0.18	48,48,48,48	0
54	MG	1A	3900	1/1	0.94	0.08	40,40,40,40	0
54	MG	1a	1728	1/1	0.94	0.12	51,51,51,51	0
54	MG	2A	3002	1/1	0.94	0.07	53,53,53,53	0
54	MG	2a	1601	1/1	0.94	0.12	48,48,48,48	0
54	MG	1A	3773	1/1	0.94	0.10	64,64,64,64	0
54	MG	2A	3517	1/1	0.94	0.23	46,46,46,46	0
54	MG	2A	3010	1/1	0.94	0.08	54,54,54,54	0
54	MG	1A	3350	1/1	0.94	0.09	29,29,29,29	0
54	MG	2A	3521	1/1	0.94	0.27	51,51,51,51	0
54	MG	1A	3352	1/1	0.94	0.09	20,20,20,20	0
54	MG	1R	202	1/1	0.94	0.13	46,46,46,46	0
54	MG	1A	3353	1/1	0.94	0.09	18,18,18,18	0
54	MG	2a	1613	1/1	0.94	0.17	51,51,51,51	0
54	MG	1A	3779	1/1	0.94	0.10	48,48,48,48	0
54	MG	2A	3025	1/1	0.94	0.10	44,44,44,44	0
54	MG	1A	3295	1/1	0.94	0.09	19,19,19,19	0
54	MG	1T	203	1/1	0.94	0.10	52,52,52,52	0
54	MG	1A	3909	1/1	0.94	0.07	35,35,35,35	0
54	MG	1A	3063	1/1	0.94	0.10	32,32,32,32	0
54	MG	2a	1621	1/1	0.94	0.19	68,68,68,68	0
54	MG	2A	3292	1/1	0.94	0.20	47,47,47,47	0
54	MG	1A	3053	1/1	0.94	0.18	47,47,47,47	0
54	MG	2A	3296	1/1	0.94	0.07	36,36,36,36	0
54	MG	2A	3039	1/1	0.94	0.11	56,56,56,56	0
54	MG	1A	3643	1/1	0.94	0.10	56,56,56,56	0
54	MG	2A	3302	1/1	0.94	0.07	25,25,25,25	0
54	MG	1a	1746	1/1	0.94	0.17	60,60,60,60	0
54	MG	2A	3304	1/1	0.94	0.07	44,44,44,44	0
54	MG	10	102	1/1	0.94	0.06	36,36,36,36	0
54	MG	1A	3914	1/1	0.94	0.08	38,38,38,38	0
54	MG	1A	3423	1/1	0.94	0.12	51,51,51,51	0
54	MG	1A	3427	1/1	0.94	0.11	37,37,37,37	0
54	MG	1A	3361	1/1	0.94	0.13	27,27,27,27	0
54	MG	1A	3299	1/1	0.94	0.09	19,19,19,19	0
54	MG	1a	1753	1/1	0.94	0.18	66,66,66,66	0
54	MG	1A	3432	1/1	0.94	0.11	35,35,35,35	0
54	MG	1A	3363	1/1	0.94	0.10	28,28,28,28	0
54	MG	15	102	1/1	0.94	0.09	42,42,42,42	0
54	MG	1A	3659	1/1	0.94	0.15	52,52,52,52	0
54	MG	2a	1643	1/1	0.94	0.11	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	3325	1/1	0.94	0.11	40,40,40,40	0
54	MG	2A	3326	1/1	0.94	0.11	61,61,61,61	0
54	MG	1A	3531	1/1	0.94	0.20	40,40,40,40	0
54	MG	2a	1647	1/1	0.94	0.22	52,52,52,52	0
54	MG	2a	1648	1/1	0.94	0.25	60,60,60,60	0
54	MG	2A	3329	1/1	0.94	0.11	29,29,29,29	0
54	MG	1A	3929	1/1	0.94	0.13	38,38,38,38	0
54	MG	1a	1602	1/1	0.94	0.10	71,71,71,71	0
54	MG	2A	3059	1/1	0.94	0.09	42,42,42,42	0
54	MG	1A	3930	1/1	0.94	0.08	60,60,60,60	0
54	MG	2A	3337	1/1	0.94	0.07	38,38,38,38	0
54	MG	2A	3573	1/1	0.94	0.09	19,19,19,19	0
54	MG	1a	1605	1/1	0.94	0.20	56,56,56,56	0
54	MG	1A	3031	1/1	0.94	0.09	39,39,39,39	0
54	MG	1A	3535	1/1	0.94	0.09	38,38,38,38	0
54	MG	1A	3537	1/1	0.94	0.18	46,46,46,46	0
54	MG	1a	1610	1/1	0.94	0.06	44,44,44,44	0
54	MG	2A	3073	1/1	0.94	0.14	45,45,45,45	0
54	MG	1A	3802	1/1	0.94	0.07	47,47,47,47	0
54	MG	1A	3438	1/1	0.94	0.10	43,43,43,43	0
54	MG	1a	1616	1/1	0.94	0.12	60,60,60,60	0
54	MG	1A	3539	1/1	0.94	0.09	22,22,22,22	0
54	MG	1A	3366	1/1	0.94	0.13	16,16,16,16	0
54	MG	1a	1620	1/1	0.94	0.06	43,43,43,43	0
54	MG	1a	1775	1/1	0.94	0.20	59,59,59,59	0
54	MG	1A	3809	1/1	0.94	0.14	39,39,39,39	0
54	MG	1A	3441	1/1	0.94	0.13	34,34,34,34	0
54	MG	2A	3358	1/1	0.94	0.15	38,38,38,38	0
54	MG	2A	3593	1/1	0.94	0.08	53,53,53,53	0
54	MG	2A	3359	1/1	0.94	0.14	52,52,52,52	0
54	MG	1A	3812	1/1	0.94	0.14	35,35,35,35	0
54	MG	1A	3442	1/1	0.94	0.07	15,15,15,15	0
54	MG	1a	1780	1/1	0.94	0.15	60,60,60,60	0
54	MG	1a	1781	1/1	0.94	0.13	58,58,58,58	0
54	MG	2A	3367	1/1	0.94	0.15	47,47,47,47	0
54	MG	1A	3814	1/1	0.94	0.10	25,25,25,25	0
54	MG	1a	1627	1/1	0.94	0.22	54,54,54,54	0
54	MG	1A	3367	1/1	0.94	0.17	18,18,18,18	0
54	MG	2A	3373	1/1	0.94	0.17	55,55,55,55	0
54	MG	2A	3606	1/1	0.94	0.10	50,50,50,50	0
54	MG	2A	3607	1/1	0.94	0.22	62,62,62,62	0
54	MG	2A	3099	1/1	0.94	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1785	1/1	0.94	0.07	47,47,47,47	0
54	MG	1A	3037	1/1	0.94	0.17	39,39,39,39	0
54	MG	1A	3555	1/1	0.94	0.08	39,39,39,39	0
54	MG	1A	3260	1/1	0.94	0.07	38,38,38,38	0
54	MG	2a	1701	1/1	0.94	0.21	42,42,42,42	0
54	MG	2A	3105	1/1	0.94	0.15	46,46,46,46	0
54	MG	2A	3615	1/1	0.94	0.12	35,35,35,35	0
54	MG	2A	3617	1/1	0.94	0.14	46,46,46,46	0
54	MG	2A	3618	1/1	0.94	0.09	50,50,50,50	0
54	MG	1A	3695	1/1	0.94	0.09	49,49,49,49	0
54	MG	2A	3620	1/1	0.94	0.08	48,48,48,48	0
54	MG	1a	1635	1/1	0.94	0.10	34,34,34,34	0
54	MG	1A	3955	1/1	0.94	0.10	39,39,39,39	0
54	MG	1A	3372	1/1	0.94	0.13	47,47,47,47	0
54	MG	2a	1713	1/1	0.94	0.38	55,55,55,55	0
54	MG	1A	3375	1/1	0.94	0.07	16,16,16,16	0
54	MG	1A	3312	1/1	0.94	0.07	17,17,17,17	0
54	MG	2A	3391	1/1	0.94	0.12	49,49,49,49	0
54	MG	1a	1796	1/1	0.94	0.19	50,50,50,50	0
54	MG	2A	3118	1/1	0.94	0.18	54,54,54,54	0
54	MG	2A	3120	1/1	0.94	0.12	41,41,41,41	0
54	MG	2A	3121	1/1	0.94	0.08	53,53,53,53	0
54	MG	1A	3566	1/1	0.94	0.10	35,35,35,35	0
54	MG	2A	3634	1/1	0.94	0.14	42,42,42,42	0
54	MG	1a	1798	1/1	0.94	0.16	61,61,61,61	0
54	MG	2A	3636	1/1	0.94	0.18	47,47,47,47	0
54	MG	1A	3826	1/1	0.94	0.12	26,26,26,26	0
54	MG	2A	3402	1/1	0.94	0.08	43,43,43,43	0
54	MG	2a	1731	1/1	0.94	0.18	61,61,61,61	0
54	MG	1a	1646	1/1	0.94	0.21	48,48,48,48	0
54	MG	2A	3131	1/1	0.94	0.31	44,44,44,44	0
54	MG	2A	3133	1/1	0.94	0.16	47,47,47,47	0
54	MG	1a	1801	1/1	0.94	0.12	43,43,43,43	0
54	MG	2a	1739	1/1	0.94	0.13	51,51,51,51	0
54	MG	1A	3460	1/1	0.94	0.20	30,30,30,30	0
54	MG	1A	3050	1/1	0.94	0.10	27,27,27,27	0
54	MG	1A	3977	1/1	0.94	0.12	38,38,38,38	0
54	MG	1A	3710	1/1	0.94	0.14	38,38,38,38	0
54	MG	1A	3712	1/1	0.94	0.14	52,52,52,52	0
54	MG	2A	3414	1/1	0.94	0.12	46,46,46,46	0
54	MG	1A	3466	1/1	0.94	0.10	40,40,40,40	0
54	MG	1A	3468	1/1	0.94	0.09	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3209	1/1	0.94	0.11	52,52,52,52	0
54	MG	1a	1656	1/1	0.94	0.08	63,63,63,63	0
54	MG	1A	3998	1/1	0.94	0.21	32,32,32,32	0
54	MG	2f	3001	1/1	0.94	0.08	44,44,44,44	0
54	MG	1A	3472	1/1	0.94	0.07	20,20,20,20	0
54	MG	1A	3151	1/1	0.94	0.19	40,40,40,40	0
54	MG	1A	3474	1/1	0.94	0.17	44,44,44,44	0
54	MG	1A	3478	1/1	0.94	0.09	16,16,16,16	0
54	MG	1A	3578	1/1	0.94	0.12	23,23,23,23	0
56	EZP	2A	3709	25/25	0.94	0.11	38,42,50,58	0
54	MG	1a	1666	1/1	0.94	0.12	50,50,50,50	0
54	MG	1A	4016	1/1	0.94	0.12	41,41,41,41	0
54	MG	1A	3321	1/1	0.94	0.07	16,16,16,16	0
54	MG	1a	1823	1/1	0.94	0.13	48,48,48,48	0
54	MG	1A	4020	1/1	0.94	0.27	27,27,27,27	0
54	MG	1A	4021	1/1	0.94	0.21	35,35,35,35	0
54	MG	2A	3176	1/1	0.94	0.17	42,42,42,42	0
54	MG	1a	1826	1/1	0.94	0.12	58,58,58,58	0
54	MG	2A	3438	1/1	0.94	0.11	50,50,50,50	0
54	MG	1a	1849	1/1	0.95	0.12	47,47,47,47	0
54	MG	1a	1689	1/1	0.95	0.18	55,55,55,55	0
54	MG	1B	217	1/1	0.95	0.14	61,61,61,61	0
54	MG	1B	218	1/1	0.95	0.06	50,50,50,50	0
54	MG	2A	3199	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3852	1/1	0.95	0.17	30,30,30,30	0
54	MG	1A	3451	1/1	0.95	0.08	15,15,15,15	0
54	MG	1A	3560	1/1	0.95	0.08	40,40,40,40	0
54	MG	1a	1698	1/1	0.95	0.11	36,36,36,36	0
54	MG	1A	3714	1/1	0.95	0.11	37,37,37,37	0
54	MG	2A	3700	1/1	0.95	0.14	21,21,21,21	0
54	MG	2A	3206	1/1	0.95	0.08	45,45,45,45	0
54	MG	1A	3369	1/1	0.95	0.07	16,16,16,16	0
54	MG	1B	226	1/1	0.95	0.06	60,60,60,60	0
54	MG	2A	3705	1/1	0.95	0.44	45,45,45,45	0
54	MG	1A	3454	1/1	0.95	0.09	22,22,22,22	0
54	MG	1A	3370	1/1	0.95	0.06	21,21,21,21	0
54	MG	1A	3864	1/1	0.95	0.05	36,36,36,36	0
54	MG	1D	304	1/1	0.95	0.05	33,33,33,33	0
54	MG	2A	3715	1/1	0.95	0.28	37,37,37,37	0
54	MG	1A	3232	1/1	0.95	0.17	31,31,31,31	0
54	MG	2A	3217	1/1	0.95	0.07	43,43,43,43	0
54	MG	2A	3718	1/1	0.95	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3458	1/1	0.95	0.11	21,21,21,21	0
54	MG	1a	1711	1/1	0.95	0.22	58,58,58,58	0
54	MG	1A	3459	1/1	0.95	0.10	23,23,23,23	0
54	MG	1A	3174	1/1	0.95	0.14	34,34,34,34	0
54	MG	1A	3374	1/1	0.95	0.12	50,50,50,50	0
54	MG	1A	3464	1/1	0.95	0.10	56,56,56,56	0
54	MG	1l	3001	1/1	0.95	0.09	47,47,47,47	0
54	MG	1A	3465	1/1	0.95	0.10	33,33,33,33	0
54	MG	1A	3234	1/1	0.95	0.23	24,24,24,24	0
54	MG	2B	3006	1/1	0.95	0.18	57,57,57,57	0
54	MG	1A	3576	1/1	0.95	0.08	43,43,43,43	0
54	MG	1A	3733	1/1	0.95	0.09	42,42,42,42	0
54	MG	1A	3377	1/1	0.95	0.17	44,44,44,44	0
54	MG	1A	3735	1/1	0.95	0.08	32,32,32,32	0
54	MG	1a	1723	1/1	0.95	0.07	50,50,50,50	0
54	MG	1A	3469	1/1	0.95	0.08	29,29,29,29	0
54	MG	1A	3305	1/1	0.95	0.07	39,39,39,39	0
54	MG	2A	3491	1/1	0.95	0.13	46,46,46,46	0
54	MG	1A	3581	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	3471	1/1	0.95	0.05	31,31,31,31	0
54	MG	1A	3308	1/1	0.95	0.15	34,34,34,34	0
54	MG	2A	3247	1/1	0.95	0.06	50,50,50,50	0
54	MG	1a	1732	1/1	0.95	0.10	59,59,59,59	0
54	MG	1A	3014	1/1	0.95	0.10	44,44,44,44	0
54	MG	1A	3886	1/1	0.95	0.11	52,52,52,52	0
54	MG	1N	201	1/1	0.95	0.16	35,35,35,35	0
54	MG	1A	3310	1/1	0.95	0.11	38,38,38,38	0
54	MG	2A	3023	1/1	0.95	0.09	55,55,55,55	0
54	MG	2E	305	1/1	0.95	0.20	52,52,52,52	0
54	MG	1A	3384	1/1	0.95	0.12	14,14,14,14	0
54	MG	2F	302	1/1	0.95	0.11	49,49,49,49	0
54	MG	1A	3746	1/1	0.95	0.11	59,59,59,59	0
54	MG	2A	3263	1/1	0.95	0.13	32,32,32,32	0
54	MG	1a	1741	1/1	0.95	0.12	51,51,51,51	0
54	MG	1A	3311	1/1	0.95	0.07	35,35,35,35	0
54	MG	2A	3267	1/1	0.95	0.10	52,52,52,52	0
54	MG	2A	3033	1/1	0.95	0.20	46,46,46,46	0
54	MG	2A	3034	1/1	0.95	0.16	42,42,42,42	0
54	MG	2A	3035	1/1	0.95	0.05	29,29,29,29	0
54	MG	2Q	3001	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	3594	1/1	0.95	0.21	54,54,54,54	0
54	MG	1A	3595	1/1	0.95	0.13	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3518	1/1	0.95	0.12	41,41,41,41	0
54	MG	1a	1745	1/1	0.95	0.13	47,47,47,47	0
54	MG	1A	3178	1/1	0.95	0.12	29,29,29,29	0
54	MG	2A	3280	1/1	0.95	0.06	58,58,58,58	0
54	MG	1A	3106	1/1	0.95	0.17	40,40,40,40	0
54	MG	2A	3282	1/1	0.95	0.12	33,33,33,33	0
54	MG	1A	3902	1/1	0.95	0.12	52,52,52,52	0
54	MG	2A	3043	1/1	0.95	0.39	68,68,68,68	0
54	MG	1A	3110	1/1	0.95	0.07	37,37,37,37	0
54	MG	1U	202	1/1	0.95	0.09	48,48,48,48	0
54	MG	1A	3755	1/1	0.95	0.07	47,47,47,47	0
54	MG	1A	3112	1/1	0.95	0.23	34,34,34,34	0
54	MG	2a	1606	1/1	0.95	0.11	45,45,45,45	0
54	MG	1A	3317	1/1	0.95	0.13	56,56,56,56	0
54	MG	2A	3293	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3758	1/1	0.95	0.06	42,42,42,42	0
54	MG	1A	3605	1/1	0.95	0.12	44,44,44,44	0
54	MG	1A	3320	1/1	0.95	0.05	24,24,24,24	0
54	MG	1A	3763	1/1	0.95	0.11	46,46,46,46	0
54	MG	1A	3608	1/1	0.95	0.12	50,50,50,50	0
54	MG	1A	3251	1/1	0.95	0.13	23,23,23,23	0
54	MG	1A	3188	1/1	0.95	0.16	53,53,53,53	0
54	MG	2A	3305	1/1	0.95	0.10	26,26,26,26	0
54	MG	1A	3767	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3117	1/1	0.95	0.19	39,39,39,39	0
54	MG	2a	1622	1/1	0.95	0.18	56,56,56,56	0
54	MG	1A	3086	1/1	0.95	0.17	26,26,26,26	0
54	MG	1a	1764	1/1	0.95	0.12	61,61,61,61	0
54	MG	2A	3550	1/1	0.95	0.11	31,31,31,31	0
54	MG	1A	3401	1/1	0.95	0.08	45,45,45,45	0
54	MG	2A	3065	1/1	0.95	0.08	49,49,49,49	0
54	MG	2A	3067	1/1	0.95	0.13	45,45,45,45	0
54	MG	1A	3061	1/1	0.95	0.12	43,43,43,43	0
54	MG	2A	3069	1/1	0.95	0.06	40,40,40,40	0
54	MG	2A	3322	1/1	0.95	0.15	49,49,49,49	0
54	MG	2A	3560	1/1	0.95	0.11	43,43,43,43	0
54	MG	2A	3070	1/1	0.95	0.17	42,42,42,42	0
54	MG	1A	3925	1/1	0.95	0.21	49,49,49,49	0
54	MG	1A	3259	1/1	0.95	0.29	62,62,62,62	0
54	MG	1A	3001	1/1	0.95	0.08	27,27,27,27	0
54	MG	2A	3327	1/1	0.95	0.11	48,48,48,48	0
54	MG	1A	3333	1/1	0.95	0.06	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3075	1/1	0.95	0.35	42,42,42,42	0
54	MG	2A	3076	1/1	0.95	0.14	44,44,44,44	0
54	MG	2A	3077	1/1	0.95	0.07	32,32,32,32	0
54	MG	1a	1607	1/1	0.95	0.22	51,51,51,51	0
54	MG	1A	3334	1/1	0.95	0.11	25,25,25,25	0
54	MG	1A	3931	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3932	1/1	0.95	0.08	58,58,58,58	0
54	MG	2A	3578	1/1	0.95	0.07	47,47,47,47	0
54	MG	1a	1611	1/1	0.95	0.19	37,37,37,37	0
54	MG	1A	3933	1/1	0.95	0.09	41,41,41,41	0
54	MG	1a	1613	1/1	0.95	0.09	60,60,60,60	0
54	MG	1A	3194	1/1	0.95	0.26	54,54,54,54	0
54	MG	2a	1652	1/1	0.95	0.26	48,48,48,48	0
54	MG	2a	1653	1/1	0.95	0.20	53,53,53,53	0
54	MG	1A	3264	1/1	0.95	0.25	42,42,42,42	0
54	MG	2A	3344	1/1	0.95	0.13	37,37,37,37	0
54	MG	1A	3412	1/1	0.95	0.09	45,45,45,45	0
54	MG	1A	3633	1/1	0.95	0.19	51,51,51,51	0
54	MG	2a	1661	1/1	0.95	0.32	54,54,54,54	0
54	MG	1A	3095	1/1	0.95	0.07	49,49,49,49	0
54	MG	1A	3787	1/1	0.95	0.18	40,40,40,40	0
54	MG	1A	3028	1/1	0.95	0.05	30,30,30,30	0
54	MG	2A	3351	1/1	0.95	0.12	25,25,25,25	0
54	MG	2a	1667	1/1	0.95	0.31	56,56,56,56	0
54	MG	1A	3512	1/1	0.95	0.20	40,40,40,40	0
54	MG	1A	3268	1/1	0.95	0.09	46,46,46,46	0
54	MG	1a	1625	1/1	0.95	0.07	51,51,51,51	0
54	MG	1A	3127	1/1	0.95	0.08	49,49,49,49	0
54	MG	1A	3944	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3946	1/1	0.95	0.08	44,44,44,44	0
54	MG	1A	3204	1/1	0.95	0.22	27,27,27,27	0
54	MG	1A	3516	1/1	0.95	0.08	31,31,31,31	0
54	MG	1A	3517	1/1	0.95	0.09	48,48,48,48	0
54	MG	2A	3109	1/1	0.95	0.27	39,39,39,39	0
54	MG	2A	3365	1/1	0.95	0.20	32,32,32,32	0
54	MG	2A	3603	1/1	0.95	0.17	32,32,32,32	0
54	MG	2A	3366	1/1	0.95	0.08	31,31,31,31	0
54	MG	1A	3274	1/1	0.95	0.05	40,40,40,40	0
54	MG	1A	3519	1/1	0.95	0.06	38,38,38,38	0
54	MG	2A	3608	1/1	0.95	0.06	40,40,40,40	0
54	MG	2A	3369	1/1	0.95	0.24	51,51,51,51	0
54	MG	1A	3046	1/1	0.95	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
54	MG	1A	3348	1/1	0.95	0.13	41,41,41,41	0
54	MG	1A	3424	1/1	0.95	0.10	41,41,41,41	0
54	MG	2A	3116	1/1	0.95	0.26	53,53,53,53	0
54	MG	2A	3117	1/1	0.95	0.06	36,36,36,36	0
54	MG	1A	3425	1/1	0.95	0.12	35,35,35,35	0
54	MG	1a	1641	1/1	0.95	0.22	54,54,54,54	0
54	MG	1A	3808	1/1	0.95	0.18	41,41,41,41	0
54	MG	1A	3960	1/1	0.95	0.08	32,32,32,32	0
54	MG	2A	3123	1/1	0.95	0.19	49,49,49,49	0
54	MG	1A	3661	1/1	0.95	0.10	32,32,32,32	0
54	MG	2A	3622	1/1	0.95	0.12	18,18,18,18	0
54	MG	1A	3963	1/1	0.95	0.17	38,38,38,38	0
54	MG	1A	3426	1/1	0.95	0.08	14,14,14,14	0
54	MG	2A	3387	1/1	0.95	0.08	45,45,45,45	0
54	MG	2A	3128	1/1	0.95	0.26	45,45,45,45	0
54	MG	1A	3206	1/1	0.95	0.15	18,18,18,18	0
54	MG	2A	3132	1/1	0.95	0.14	43,43,43,43	0
54	MG	1A	3665	1/1	0.95	0.06	32,32,32,32	0
54	MG	1A	3974	1/1	0.95	0.19	45,45,45,45	0
54	MG	2A	3395	1/1	0.95	0.22	56,56,56,56	0
54	MG	1A	3667	1/1	0.95	0.07	40,40,40,40	0
54	MG	2a	1710	1/1	0.95	0.22	56,56,56,56	0
54	MG	2A	3139	1/1	0.95	0.09	58,58,58,58	0
54	MG	1A	3207	1/1	0.95	0.15	39,39,39,39	0
54	MG	1A	3132	1/1	0.95	0.10	40,40,40,40	0
54	MG	2A	3639	1/1	0.95	0.07	56,56,56,56	0
54	MG	2a	1716	1/1	0.95	0.37	57,57,57,57	0
54	MG	1A	3671	1/1	0.95	0.05	15,15,15,15	0
54	MG	2a	1718	1/1	0.95	0.08	63,63,63,63	0
54	MG	2A	3641	1/1	0.95	0.16	46,46,46,46	0
54	MG	2A	3642	1/1	0.95	0.18	57,57,57,57	0
54	MG	2A	3145	1/1	0.95	0.25	44,44,44,44	0
54	MG	1A	3673	1/1	0.95	0.08	28,28,28,28	0
54	MG	2a	1723	1/1	0.95	0.18	45,45,45,45	0
54	MG	1A	3529	1/1	0.95	0.09	47,47,47,47	0
54	MG	1A	3676	1/1	0.95	0.08	28,28,28,28	0
54	MG	1A	3677	1/1	0.95	0.10	43,43,43,43	0
54	MG	1A	3822	1/1	0.95	0.05	40,40,40,40	0
54	MG	1a	1664	1/1	0.95	0.17	51,51,51,51	0
54	MG	1A	3163	1/1	0.95	0.10	47,47,47,47	0
54	MG	2A	3653	1/1	0.95	0.11	48,48,48,48	0
54	MG	2a	1732	1/1	0.95	0.44	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3159	1/1	0.95	0.12	50,50,50,50	0
54	MG	1A	3211	1/1	0.95	0.09	37,37,37,37	0
54	MG	1A	4010	1/1	0.95	0.35	31,31,31,31	0
54	MG	1A	3435	1/1	0.95	0.11	37,37,37,37	0
54	MG	1A	3048	1/1	0.95	0.10	33,33,33,33	0
54	MG	1A	3830	1/1	0.95	0.09	41,41,41,41	0
54	MG	1A	3286	1/1	0.95	0.09	56,56,56,56	0
54	MG	2A	3168	1/1	0.95	0.09	54,54,54,54	0
54	MG	1A	3689	1/1	0.95	0.07	22,22,22,22	0
54	MG	1A	3217	1/1	0.95	0.31	30,30,30,30	0
54	MG	2A	3172	1/1	0.95	0.10	56,56,56,56	0
54	MG	1A	3292	1/1	0.95	0.14	56,56,56,56	0
54	MG	2A	3174	1/1	0.95	0.32	45,45,45,45	0
54	MG	1A	4025	1/1	0.95	0.12	30,30,30,30	0
54	MG	1A	3081	1/1	0.95	0.31	34,34,34,34	0
54	MG	1A	3444	1/1	0.95	0.09	24,24,24,24	0
54	MG	1A	3222	1/1	0.95	0.20	32,32,32,32	0
54	MG	1A	3446	1/1	0.95	0.10	20,20,20,20	0
54	MG	1A	3700	1/1	0.95	0.08	34,34,34,34	0
54	MG	1A	3552	1/1	0.95	0.11	45,45,45,45	0
54	MG	2A	3183	1/1	0.95	0.10	53,53,53,53	0
54	MG	2A	3437	1/1	0.95	0.06	58,58,58,58	0
56	EZP	1A	3987	25/25	0.95	0.10	16,28,47,60	0
54	MG	1A	3226	1/1	0.95	0.12	32,32,32,32	0
54	MG	2A	3439	1/1	0.95	0.26	64,64,64,64	0
54	MG	2A	3186	1/1	0.95	0.17	34,34,34,34	0
57	MPD	18	102	8/8	0.95	0.13	22,28,35,36	0
54	MG	1A	3141	1/1	0.95	0.08	38,38,38,38	0
54	MG	1a	1685	1/1	0.95	0.22	40,40,40,40	0
54	MG	1B	210	1/1	0.95	0.07	50,50,50,50	0
54	MG	2A	3446	1/1	0.95	0.08	30,30,30,30	0
54	MG	2A	3192	1/1	0.95	0.08	52,52,52,52	0
54	MG	1A	3705	1/1	0.95	0.13	48,48,48,48	0
54	MG	1A	3707	1/1	0.95	0.06	40,40,40,40	0
54	MG	1A	3613	1/1	0.96	0.06	50,50,50,50	0
54	MG	1A	3965	1/1	0.96	0.18	10,10,10,10	0
54	MG	1A	3845	1/1	0.96	0.12	37,37,37,37	0
54	MG	1A	3614	1/1	0.96	0.08	17,17,17,17	0
54	MG	1A	3970	1/1	0.96	0.40	40,40,40,40	0
54	MG	2A	3249	1/1	0.96	0.11	45,45,45,45	0
54	MG	2A	3712	1/1	0.96	0.11	41,41,41,41	0
54	MG	2A	3250	1/1	0.96	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	2A	3050	1/1	0.96	0.23	58,58,58,58	0
54	MG	2A	3051	1/1	0.96	0.11	38,38,38,38	0
54	MG	1a	1615	1/1	0.96	0.18	59,59,59,59	0
54	MG	2A	3257	1/1	0.96	0.12	43,43,43,43	0
54	MG	1A	3247	1/1	0.96	0.09	40,40,40,40	0
54	MG	2A	3720	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3376	1/1	0.96	0.06	29,29,29,29	0
54	MG	2A	3722	1/1	0.96	0.10	48,48,48,48	0
54	MG	1A	3004	1/1	0.96	0.10	43,43,43,43	0
54	MG	1A	3449	1/1	0.96	0.10	17,17,17,17	0
54	MG	1A	3980	1/1	0.96	0.10	48,48,48,48	0
54	MG	1A	3250	1/1	0.96	0.21	27,27,27,27	0
54	MG	1A	3982	1/1	0.96	0.06	49,49,49,49	0
54	MG	2A	3490	1/1	0.96	0.19	44,44,44,44	0
54	MG	2A	3266	1/1	0.96	0.11	40,40,40,40	0
54	MG	1A	3002	1/1	0.96	0.07	47,47,47,47	0
54	MG	2A	3268	1/1	0.96	0.07	29,29,29,29	0
54	MG	1A	3856	1/1	0.96	0.15	42,42,42,42	0
54	MG	1A	3622	1/1	0.96	0.07	51,51,51,51	0
54	MG	2A	3064	1/1	0.96	0.11	21,21,21,21	0
54	MG	2A	3497	1/1	0.96	0.13	43,43,43,43	0
54	MG	1A	3995	1/1	0.96	0.05	26,26,26,26	0
54	MG	2A	3066	1/1	0.96	0.19	51,51,51,51	0
54	MG	2A	3276	1/1	0.96	0.08	44,44,44,44	0
54	MG	1A	3624	1/1	0.96	0.14	45,45,45,45	0
54	MG	2A	3278	1/1	0.96	0.07	25,25,25,25	0
54	MG	1A	3999	1/1	0.96	0.22	32,32,32,32	0
54	MG	1A	4001	1/1	0.96	0.12	37,37,37,37	0
54	MG	2D	303	1/1	0.96	0.11	40,40,40,40	0
54	MG	1A	3054	1/1	0.96	0.11	21,21,21,21	0
54	MG	1A	3627	1/1	0.96	0.16	30,30,30,30	0
54	MG	1A	4008	1/1	0.96	0.13	28,28,28,28	0
54	MG	2A	3284	1/1	0.96	0.05	55,55,55,55	0
54	MG	1A	3862	1/1	0.96	0.12	33,33,33,33	0
54	MG	1A	3101	1/1	0.96	0.13	30,30,30,30	0
54	MG	1A	4012	1/1	0.96	0.31	25,25,25,25	0
54	MG	2E	306	1/1	0.96	0.18	44,44,44,44	0
54	MG	1A	3629	1/1	0.96	0.07	41,41,41,41	0
54	MG	2A	3289	1/1	0.96	0.08	47,47,47,47	0
54	MG	2A	3290	1/1	0.96	0.13	30,30,30,30	0
54	MG	1A	3530	1/1	0.96	0.08	44,44,44,44	0
54	MG	1A	3255	1/1	0.96	0.20	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3071	1/1	0.96	0.25	29,29,29,29	0
54	MG	2A	3522	1/1	0.96	0.17	47,47,47,47	0
54	MG	1A	4018	1/1	0.96	0.08	36,36,36,36	0
54	MG	2A	3295	1/1	0.96	0.09	55,55,55,55	0
54	MG	1A	3040	1/1	0.96	0.09	26,26,26,26	0
54	MG	2P	202	1/1	0.96	0.09	59,59,59,59	0
54	MG	1A	3634	1/1	0.96	0.08	59,59,59,59	0
54	MG	2Q	3002	1/1	0.96	0.06	55,55,55,55	0
54	MG	2R	201	1/1	0.96	0.09	35,35,35,35	0
54	MG	1A	4022	1/1	0.96	0.06	30,30,30,30	0
54	MG	2T	3002	1/1	0.96	0.16	61,61,61,61	0
54	MG	1A	3536	1/1	0.96	0.06	26,26,26,26	0
54	MG	2T	3004	1/1	0.96	0.05	44,44,44,44	0
54	MG	1A	3388	1/1	0.96	0.11	22,22,22,22	0
54	MG	1A	3322	1/1	0.96	0.09	21,21,21,21	0
54	MG	2A	3089	1/1	0.96	0.10	41,41,41,41	0
54	MG	1A	3640	1/1	0.96	0.06	45,45,45,45	0
54	MG	2A	3535	1/1	0.96	0.05	42,42,42,42	0
54	MG	2A	3093	1/1	0.96	0.08	58,58,58,58	0
54	MG	28	8001	1/1	0.96	0.08	46,46,46,46	0
54	MG	2A	3309	1/1	0.96	0.08	25,25,25,25	0
54	MG	2A	3310	1/1	0.96	0.09	29,29,29,29	0
54	MG	1A	3390	1/1	0.96	0.13	40,40,40,40	0
54	MG	1a	1655	1/1	0.96	0.04	57,57,57,57	0
54	MG	2A	3316	1/1	0.96	0.15	41,41,41,41	0
54	MG	1A	3258	1/1	0.96	0.12	32,32,32,32	0
54	MG	1A	3878	1/1	0.96	0.13	57,57,57,57	0
54	MG	1A	3761	1/1	0.96	0.06	32,32,32,32	0
54	MG	1A	3762	1/1	0.96	0.08	19,19,19,19	0
54	MG	1a	1660	1/1	0.96	0.18	46,46,46,46	0
54	MG	1A	3108	1/1	0.96	0.20	42,42,42,42	0
54	MG	1A	3326	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3078	1/1	0.96	0.12	47,47,47,47	0
54	MG	2A	3104	1/1	0.96	0.09	42,42,42,42	0
54	MG	1B	212	1/1	0.96	0.05	53,53,53,53	0
54	MG	1A	3550	1/1	0.96	0.12	53,53,53,53	0
54	MG	2A	3107	1/1	0.96	0.13	43,43,43,43	0
54	MG	2A	3557	1/1	0.96	0.08	22,22,22,22	0
54	MG	1B	216	1/1	0.96	0.07	33,33,33,33	0
54	MG	2A	3559	1/1	0.96	0.10	32,32,32,32	0
54	MG	1A	3080	1/1	0.96	0.20	37,37,37,37	0
54	MG	2A	3561	1/1	0.96	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3329	1/1	0.96	0.06	33,33,33,33	0
54	MG	1A	3201	1/1	0.96	0.13	39,39,39,39	0
54	MG	1A	3892	1/1	0.96	0.06	39,39,39,39	0
54	MG	2a	1628	1/1	0.96	0.10	31,31,31,31	0
54	MG	1A	3655	1/1	0.96	0.13	30,30,30,30	0
54	MG	1a	1821	1/1	0.96	0.11	44,44,44,44	0
54	MG	1B	223	1/1	0.96	0.06	46,46,46,46	0
54	MG	1A	3556	1/1	0.96	0.14	39,39,39,39	0
54	MG	1A	3775	1/1	0.96	0.09	34,34,34,34	0
54	MG	2A	3119	1/1	0.96	0.20	64,64,64,64	0
54	MG	1A	3331	1/1	0.96	0.06	12,12,12,12	0
54	MG	2A	3574	1/1	0.96	0.13	52,52,52,52	0
54	MG	1A	3202	1/1	0.96	0.33	32,32,32,32	0
54	MG	2A	3345	1/1	0.96	0.21	45,45,45,45	0
54	MG	1B	229	1/1	0.96	0.06	41,41,41,41	0
54	MG	1A	3115	1/1	0.96	0.10	22,22,22,22	0
54	MG	1A	3562	1/1	0.96	0.07	32,32,32,32	0
54	MG	1A	3664	1/1	0.96	0.09	30,30,30,30	0
54	MG	1D	305	1/1	0.96	0.16	39,39,39,39	0
54	MG	2A	3127	1/1	0.96	0.07	36,36,36,36	0
54	MG	1A	3904	1/1	0.96	0.06	60,60,60,60	0
54	MG	2A	3584	1/1	0.96	0.09	46,46,46,46	0
54	MG	2A	3130	1/1	0.96	0.17	64,64,64,64	0
54	MG	1A	3782	1/1	0.96	0.06	41,41,41,41	0
54	MG	1A	3475	1/1	0.96	0.06	42,42,42,42	0
54	MG	1A	3116	1/1	0.96	0.09	28,28,28,28	0
54	MG	1A	3056	1/1	0.96	0.07	52,52,52,52	0
54	MG	1A	3023	1/1	0.96	0.09	19,19,19,19	0
54	MG	1a	1690	1/1	0.96	0.14	45,45,45,45	0
54	MG	2a	1654	1/1	0.96	0.08	58,58,58,58	0
54	MG	2A	3362	1/1	0.96	0.09	34,34,34,34	0
54	MG	1A	3273	1/1	0.96	0.11	30,30,30,30	0
54	MG	1A	3672	1/1	0.96	0.09	40,40,40,40	0
54	MG	2a	1659	1/1	0.96	0.40	48,48,48,48	0
54	MG	1a	1693	1/1	0.96	0.08	42,42,42,42	0
54	MG	1A	3407	1/1	0.96	0.08	38,38,38,38	0
54	MG	1A	3084	1/1	0.96	0.08	33,33,33,33	0
54	MG	1F	306	1/1	0.96	0.07	31,31,31,31	0
54	MG	1A	3571	1/1	0.96	0.22	27,27,27,27	0
54	MG	2a	1665	1/1	0.96	0.36	55,55,55,55	0
54	MG	1a	1699	1/1	0.96	0.09	57,57,57,57	0
54	MG	1F	308	1/1	0.96	0.15	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3372	1/1	0.96	0.05	51,51,51,51	0
54	MG	1A	3122	1/1	0.96	0.08	32,32,32,32	0
54	MG	2A	3374	1/1	0.96	0.07	26,26,26,26	0
54	MG	2A	3152	1/1	0.96	0.08	58,58,58,58	0
54	MG	2A	3153	1/1	0.96	0.17	42,42,42,42	0
54	MG	2A	3154	1/1	0.96	0.19	41,41,41,41	0
54	MG	2A	3378	1/1	0.96	0.09	28,28,28,28	0
54	MG	2A	3156	1/1	0.96	0.06	41,41,41,41	0
54	MG	1A	3032	1/1	0.96	0.06	45,45,45,45	0
54	MG	2A	3158	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3047	1/1	0.96	0.16	38,38,38,38	0
54	MG	2A	3383	1/1	0.96	0.14	64,64,64,64	0
54	MG	1A	3091	1/1	0.96	0.05	41,41,41,41	0
54	MG	2A	3616	1/1	0.96	0.09	45,45,45,45	0
54	MG	1F	313	1/1	0.96	0.04	31,31,31,31	0
54	MG	1A	3684	1/1	0.96	0.09	46,46,46,46	0
54	MG	1a	1708	1/1	0.96	0.18	32,32,32,32	0
54	MG	1A	3489	1/1	0.96	0.09	21,21,21,21	0
54	MG	1A	3926	1/1	0.96	0.06	45,45,45,45	0
54	MG	1A	3281	1/1	0.96	0.10	36,36,36,36	0
54	MG	2a	1690	1/1	0.96	0.15	68,68,68,68	0
54	MG	1H	8002	1/1	0.96	0.06	37,37,37,37	0
54	MG	1A	3169	1/1	0.96	0.25	33,33,33,33	0
54	MG	1A	3092	1/1	0.96	0.06	32,32,32,32	0
54	MG	1A	3129	1/1	0.96	0.24	26,26,26,26	0
54	MG	1A	3582	1/1	0.96	0.16	41,41,41,41	0
54	MG	1O	8002	1/1	0.96	0.08	46,46,46,46	0
54	MG	1A	3223	1/1	0.96	0.21	28,28,28,28	0
54	MG	1Q	201	1/1	0.96	0.09	38,38,38,38	0
54	MG	1Q	203	1/1	0.96	0.07	36,36,36,36	0
54	MG	1h	3001	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3811	1/1	0.96	0.12	31,31,31,31	0
54	MG	1a	1722	1/1	0.96	0.20	56,56,56,56	0
54	MG	1A	3224	1/1	0.96	0.23	36,36,36,36	0
54	MG	2A	3637	1/1	0.96	0.08	30,30,30,30	0
54	MG	2A	3638	1/1	0.96	0.06	32,32,32,32	0
54	MG	2A	3407	1/1	0.96	0.09	50,50,50,50	0
54	MG	1a	1724	1/1	0.96	0.17	41,41,41,41	0
54	MG	1A	3175	1/1	0.96	0.23	35,35,35,35	0
54	MG	2A	3410	1/1	0.96	0.15	47,47,47,47	0
54	MG	2A	3187	1/1	0.96	0.09	44,44,44,44	0
54	MG	1A	3588	1/1	0.96	0.10	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3176	1/1	0.96	0.07	49,49,49,49	0
54	MG	2A	3190	1/1	0.96	0.13	47,47,47,47	0
54	MG	1A	3294	1/1	0.96	0.07	46,46,46,46	0
54	MG	1A	3130	1/1	0.96	0.24	25,25,25,25	0
54	MG	1A	3592	1/1	0.96	0.15	44,44,44,44	0
54	MG	1A	3060	1/1	0.96	0.07	28,28,28,28	0
54	MG	1W	3002	1/1	0.96	0.12	39,39,39,39	0
54	MG	1A	3025	1/1	0.96	0.20	29,29,29,29	0
54	MG	1A	3596	1/1	0.96	0.18	38,38,38,38	0
54	MG	2A	3005	1/1	0.96	0.08	41,41,41,41	0
54	MG	2A	3007	1/1	0.96	0.12	36,36,36,36	0
54	MG	1A	3713	1/1	0.96	0.07	49,49,49,49	0
54	MG	2A	3011	1/1	0.96	0.07	21,21,21,21	0
54	MG	2A	3013	1/1	0.96	0.17	33,33,33,33	0
54	MG	2A	3014	1/1	0.96	0.18	51,51,51,51	0
54	MG	2A	3015	1/1	0.96	0.14	43,43,43,43	0
54	MG	1A	3945	1/1	0.96	0.10	36,36,36,36	0
54	MG	1A	3183	1/1	0.96	0.19	45,45,45,45	0
54	MG	2A	3434	1/1	0.96	0.10	26,26,26,26	0
54	MG	1A	3598	1/1	0.96	0.12	51,51,51,51	0
54	MG	1A	3301	1/1	0.96	0.08	27,27,27,27	0
54	MG	2A	3212	1/1	0.96	0.09	60,60,60,60	0
54	MG	1A	3062	1/1	0.96	0.12	25,25,25,25	0
54	MG	2A	3022	1/1	0.96	0.10	39,39,39,39	0
54	MG	1A	3237	1/1	0.96	0.10	28,28,28,28	0
54	MG	1A	3304	1/1	0.96	0.09	26,26,26,26	0
54	MG	15	104	1/1	0.96	0.09	62,62,62,62	0
54	MG	2A	3029	1/1	0.96	0.15	55,55,55,55	0
54	MG	17	101	1/1	0.96	0.17	54,54,54,54	0
54	MG	2A	3447	1/1	0.96	0.13	55,55,55,55	0
54	MG	2A	3031	1/1	0.96	0.16	48,48,48,48	0
54	MG	2A	3221	1/1	0.96	0.16	57,57,57,57	0
54	MG	1A	3952	1/1	0.96	0.04	46,46,46,46	0
54	MG	2A	3223	1/1	0.96	0.45	43,43,43,43	0
54	MG	2a	1751	1/1	0.96	0.08	53,53,53,53	0
54	MG	2A	3224	1/1	0.96	0.25	35,35,35,35	0
54	MG	18	101	1/1	0.96	0.06	46,46,46,46	0
54	MG	19	502	1/1	0.96	0.26	50,50,50,50	0
54	MG	2A	3227	1/1	0.96	0.24	38,38,38,38	0
54	MG	1A	3604	1/1	0.96	0.05	29,29,29,29	0
54	MG	1A	3723	1/1	0.96	0.07	36,36,36,36	0
54	MG	2A	3459	1/1	0.96	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3239	1/1	0.96	0.12	33,33,33,33	0
54	MG	2A	3038	1/1	0.96	0.09	46,46,46,46	0
54	MG	2A	3692	1/1	0.96	0.08	63,63,63,63	0
54	MG	1A	3725	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3185	1/1	0.96	0.23	42,42,42,42	0
54	MG	1A	3959	1/1	0.96	0.21	47,47,47,47	0
54	MG	1A	3373	1/1	0.96	0.11	25,25,25,25	0
54	MG	1A	3443	1/1	0.96	0.07	25,25,25,25	0
54	MG	1A	3186	1/1	0.96	0.21	36,36,36,36	0
54	MG	2A	3699	1/1	0.96	0.10	61,61,61,61	0
54	MG	2A	3240	1/1	0.96	0.20	49,49,49,49	0
54	MG	2A	3241	1/1	0.96	0.14	47,47,47,47	0
54	MG	1A	3072	1/1	0.97	0.24	26,26,26,26	0
54	MG	1A	3646	1/1	0.97	0.08	37,37,37,37	0
54	MG	1A	3344	1/1	0.97	0.04	21,21,21,21	0
54	MG	1A	3648	1/1	0.97	0.14	32,32,32,32	0
54	MG	2A	3085	1/1	0.97	0.17	35,35,35,35	0
54	MG	1A	3790	1/1	0.97	0.07	39,39,39,39	0
54	MG	1a	1603	1/1	0.97	0.10	45,45,45,45	0
54	MG	1A	3433	1/1	0.97	0.05	32,32,32,32	0
54	MG	1A	3345	1/1	0.97	0.09	50,50,50,50	0
54	MG	1A	3532	1/1	0.97	0.07	17,17,17,17	0
54	MG	2A	3300	1/1	0.97	0.07	28,28,28,28	0
54	MG	2A	3512	1/1	0.97	0.10	51,51,51,51	0
54	MG	1A	3795	1/1	0.97	0.04	32,32,32,32	0
54	MG	2A	3514	1/1	0.97	0.19	36,36,36,36	0
54	MG	1A	3652	1/1	0.97	0.08	44,44,44,44	0
54	MG	1A	3653	1/1	0.97	0.16	41,41,41,41	0
54	MG	1a	1787	1/1	0.97	0.27	40,40,40,40	0
54	MG	1A	3533	1/1	0.97	0.06	35,35,35,35	0
54	MG	2A	3306	1/1	0.97	0.05	27,27,27,27	0
54	MG	2D	304	1/1	0.97	0.16	42,42,42,42	0
54	MG	1A	3146	1/1	0.97	0.33	34,34,34,34	0
54	MG	1A	3800	1/1	0.97	0.10	44,44,44,44	0
54	MG	1A	3656	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3436	1/1	0.97	0.07	41,41,41,41	0
54	MG	2E	301	1/1	0.97	0.06	43,43,43,43	0
54	MG	2A	3312	1/1	0.97	0.10	39,39,39,39	0
54	MG	1A	3803	1/1	0.97	0.14	34,34,34,34	0
54	MG	1A	3199	1/1	0.97	0.18	38,38,38,38	0
54	MG	1A	3269	1/1	0.97	0.12	12,12,12,12	0
54	MG	2A	3530	1/1	0.97	0.06	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3806	1/1	0.97	0.08	34,34,34,34	0
54	MG	1A	3962	1/1	0.97	0.06	55,55,55,55	0
54	MG	1A	3439	1/1	0.97	0.11	34,34,34,34	0
54	MG	1A	3200	1/1	0.97	0.14	32,32,32,32	0
54	MG	1A	3542	1/1	0.97	0.16	31,31,31,31	0
54	MG	1A	3015	1/1	0.97	0.25	29,29,29,29	0
54	MG	2A	3537	1/1	0.97	0.16	42,42,42,42	0
54	MG	1A	3967	1/1	0.97	0.12	19,19,19,19	0
54	MG	1A	3150	1/1	0.97	0.34	28,28,28,28	0
54	MG	1A	3075	1/1	0.97	0.17	32,32,32,32	0
54	MG	1A	3972	1/1	0.97	0.22	32,32,32,32	0
54	MG	1A	3669	1/1	0.97	0.10	25,25,25,25	0
54	MG	1a	1630	1/1	0.97	0.18	46,46,46,46	0
54	MG	1A	3547	1/1	0.97	0.12	29,29,29,29	0
54	MG	1a	1632	1/1	0.97	0.08	35,35,35,35	0
54	MG	1A	3275	1/1	0.97	0.08	29,29,29,29	0
54	MG	1A	3978	1/1	0.97	0.16	26,26,26,26	0
54	MG	2V	201	1/1	0.97	0.09	60,60,60,60	0
54	MG	1A	3109	1/1	0.97	0.23	31,31,31,31	0
54	MG	2A	3336	1/1	0.97	0.12	36,36,36,36	0
54	MG	1A	3358	1/1	0.97	0.06	21,21,21,21	0
54	MG	1a	1814	1/1	0.97	0.25	52,52,52,52	0
54	MG	1A	3447	1/1	0.97	0.07	34,34,34,34	0
54	MG	1a	1638	1/1	0.97	0.16	44,44,44,44	0
54	MG	1A	3553	1/1	0.97	0.07	18,18,18,18	0
54	MG	28	8002	1/1	0.97	0.08	45,45,45,45	0
54	MG	1A	3554	1/1	0.97	0.07	40,40,40,40	0
54	MG	1A	3359	1/1	0.97	0.07	15,15,15,15	0
54	MG	1A	3077	1/1	0.97	0.17	28,28,28,28	0
54	MG	1A	3111	1/1	0.97	0.18	31,31,31,31	0
54	MG	1a	1645	1/1	0.97	0.05	41,41,41,41	0
54	MG	1A	3996	1/1	0.97	0.18	27,27,27,27	0
54	MG	2A	3138	1/1	0.97	0.11	33,33,33,33	0
54	MG	1A	3682	1/1	0.97	0.06	38,38,38,38	0
54	MG	2A	3140	1/1	0.97	0.07	51,51,51,51	0
54	MG	2A	3141	1/1	0.97	0.11	39,39,39,39	0
54	MG	2A	3352	1/1	0.97	0.07	52,52,52,52	0
54	MG	2A	3353	1/1	0.97	0.06	62,62,62,62	0
54	MG	1A	3558	1/1	0.97	0.04	34,34,34,34	0
54	MG	2A	3571	1/1	0.97	0.17	42,42,42,42	0
54	MG	1A	4000	1/1	0.97	0.04	30,30,30,30	0
54	MG	1A	3827	1/1	0.97	0.07	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	4003	1/1	0.97	0.10	27,27,27,27	0
54	MG	2a	1619	1/1	0.97	0.18	47,47,47,47	0
54	MG	1A	3685	1/1	0.97	0.12	42,42,42,42	0
54	MG	1A	3686	1/1	0.97	0.12	32,32,32,32	0
54	MG	1A	3157	1/1	0.97	0.04	28,28,28,28	0
54	MG	1A	3038	1/1	0.97	0.12	40,40,40,40	0
54	MG	1A	3561	1/1	0.97	0.05	25,25,25,25	0
54	MG	1A	3834	1/1	0.97	0.08	31,31,31,31	0
54	MG	1A	3453	1/1	0.97	0.05	51,51,51,51	0
54	MG	1A	4014	1/1	0.97	0.16	28,28,28,28	0
54	MG	1A	3282	1/1	0.97	0.17	24,24,24,24	0
54	MG	2A	3155	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	3693	1/1	0.97	0.07	33,33,33,33	0
54	MG	1A	3694	1/1	0.97	0.06	40,40,40,40	0
54	MG	1A	3455	1/1	0.97	0.07	10,10,10,10	0
54	MG	1A	3840	1/1	0.97	0.07	33,33,33,33	0
54	MG	1A	3079	1/1	0.97	0.20	30,30,30,30	0
54	MG	1A	3210	1/1	0.97	0.15	32,32,32,32	0
54	MG	1A	3029	1/1	0.97	0.04	12,12,12,12	0
54	MG	2A	3163	1/1	0.97	0.10	53,53,53,53	0
54	MG	1A	4024	1/1	0.97	0.21	30,30,30,30	0
54	MG	1A	3699	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	4026	1/1	0.97	0.09	35,35,35,35	0
54	MG	1A	3213	1/1	0.97	0.07	33,33,33,33	0
54	MG	2A	3169	1/1	0.97	0.11	38,38,38,38	0
54	MG	1A	3701	1/1	0.97	0.09	29,29,29,29	0
54	MG	1A	3289	1/1	0.97	0.06	23,23,23,23	0
54	MG	1a	1675	1/1	0.97	0.16	42,42,42,42	0
54	MG	1A	3290	1/1	0.97	0.12	32,32,32,32	0
54	MG	1A	3463	1/1	0.97	0.10	19,19,19,19	0
54	MG	1B	205	1/1	0.97	0.05	40,40,40,40	0
54	MG	1A	3017	1/1	0.97	0.09	25,25,25,25	0
54	MG	1A	3855	1/1	0.97	0.06	25,25,25,25	0
54	MG	1A	3041	1/1	0.97	0.12	12,12,12,12	0
54	MG	1B	209	1/1	0.97	0.04	36,36,36,36	0
54	MG	1A	3708	1/1	0.97	0.04	37,37,37,37	0
54	MG	1A	3709	1/1	0.97	0.18	46,46,46,46	0
54	MG	2A	3394	1/1	0.97	0.18	60,60,60,60	0
54	MG	1A	3218	1/1	0.97	0.14	30,30,30,30	0
54	MG	2a	1657	1/1	0.97	0.11	44,44,44,44	0
54	MG	2A	3396	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3467	1/1	0.97	0.06	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3119	1/1	0.97	0.09	38,38,38,38	0
54	MG	1A	3221	1/1	0.97	0.23	24,24,24,24	0
54	MG	1A	3579	1/1	0.97	0.11	24,24,24,24	0
54	MG	1A	3165	1/1	0.97	0.16	28,28,28,28	0
54	MG	1A	3166	1/1	0.97	0.06	32,32,32,32	0
54	MG	1A	3042	1/1	0.97	0.13	8,8,8,8	0
54	MG	1A	3382	1/1	0.97	0.05	19,19,19,19	0
54	MG	1A	3225	1/1	0.97	0.16	32,32,32,32	0
54	MG	1A	3585	1/1	0.97	0.07	36,36,36,36	0
54	MG	2A	3624	1/1	0.97	0.06	37,37,37,37	0
54	MG	1A	3121	1/1	0.97	0.14	57,57,57,57	0
54	MG	1A	3476	1/1	0.97	0.08	14,14,14,14	0
54	MG	1A	3726	1/1	0.97	0.05	32,32,32,32	0
54	MG	1A	3227	1/1	0.97	0.18	25,25,25,25	0
54	MG	1A	3229	1/1	0.97	0.22	55,55,55,55	0
54	MG	1A	3085	1/1	0.97	0.07	36,36,36,36	0
54	MG	2A	3201	1/1	0.97	0.07	50,50,50,50	0
54	MG	1A	3879	1/1	0.97	0.07	33,33,33,33	0
54	MG	2A	3415	1/1	0.97	0.07	41,41,41,41	0
54	MG	1D	307	1/1	0.97	0.06	40,40,40,40	0
54	MG	1A	3307	1/1	0.97	0.11	31,31,31,31	0
54	MG	1A	3593	1/1	0.97	0.13	40,40,40,40	0
54	MG	1A	3231	1/1	0.97	0.17	34,34,34,34	0
54	MG	2A	3420	1/1	0.97	0.10	28,28,28,28	0
54	MG	2a	1685	1/1	0.97	0.26	52,52,52,52	0
54	MG	2A	3008	1/1	0.97	0.10	57,57,57,57	0
54	MG	1D	312	1/1	0.97	0.13	54,54,54,54	0
54	MG	2A	3210	1/1	0.97	0.07	45,45,45,45	0
54	MG	1A	3171	1/1	0.97	0.10	23,23,23,23	0
54	MG	2A	3012	1/1	0.97	0.07	43,43,43,43	0
54	MG	1A	3012	1/1	0.97	0.04	17,17,17,17	0
54	MG	1E	304	1/1	0.97	0.09	16,16,16,16	0
54	MG	1A	3006	1/1	0.97	0.07	17,17,17,17	0
54	MG	1A	3090	1/1	0.97	0.07	12,12,12,12	0
54	MG	1A	3126	1/1	0.97	0.21	33,33,33,33	0
54	MG	1A	3740	1/1	0.97	0.07	29,29,29,29	0
54	MG	1F	304	1/1	0.97	0.08	24,24,24,24	0
54	MG	1A	3488	1/1	0.97	0.09	56,56,56,56	0
54	MG	1A	3893	1/1	0.97	0.15	50,50,50,50	0
54	MG	1A	3033	1/1	0.97	0.07	34,34,34,34	0
54	MG	2A	3024	1/1	0.97	0.12	35,35,35,35	0
54	MG	1A	3315	1/1	0.97	0.05	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3492	1/1	0.97	0.08	17,17,17,17	0
54	MG	1A	3238	1/1	0.97	0.20	40,40,40,40	0
54	MG	1A	3034	1/1	0.97	0.08	33,33,33,33	0
54	MG	2A	3443	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3747	1/1	0.97	0.12	44,44,44,44	0
54	MG	1a	1727	1/1	0.97	0.17	43,43,43,43	0
54	MG	1A	3318	1/1	0.97	0.12	26,26,26,26	0
54	MG	1A	3610	1/1	0.97	0.06	27,27,27,27	0
54	MG	2a	1711	1/1	0.97	0.25	45,45,45,45	0
54	MG	2A	3448	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3750	1/1	0.97	0.10	27,27,27,27	0
54	MG	1A	3240	1/1	0.97	0.09	37,37,37,37	0
54	MG	2A	3234	1/1	0.97	0.10	52,52,52,52	0
54	MG	1A	3179	1/1	0.97	0.16	36,36,36,36	0
54	MG	1A	3180	1/1	0.97	0.17	37,37,37,37	0
54	MG	1a	1734	1/1	0.97	0.21	47,47,47,47	0
54	MG	1a	1735	1/1	0.97	0.13	51,51,51,51	0
54	MG	1A	3323	1/1	0.97	0.08	18,18,18,18	0
54	MG	1A	3245	1/1	0.97	0.05	27,27,27,27	0
54	MG	1A	3181	1/1	0.97	0.22	57,57,57,57	0
54	MG	1A	3064	1/1	0.97	0.19	29,29,29,29	0
54	MG	1A	3094	1/1	0.97	0.24	29,29,29,29	0
54	MG	1A	3506	1/1	0.97	0.08	33,33,33,33	0
54	MG	1P	203	1/1	0.97	0.03	29,29,29,29	0
54	MG	1A	3915	1/1	0.97	0.05	25,25,25,25	0
54	MG	1A	3507	1/1	0.97	0.04	29,29,29,29	0
54	MG	1A	3035	1/1	0.97	0.09	38,38,38,38	0
54	MG	1A	3623	1/1	0.97	0.06	32,32,32,32	0
54	MG	1A	3509	1/1	0.97	0.13	41,41,41,41	0
54	MG	2a	1733	1/1	0.97	0.34	52,52,52,52	0
54	MG	2A	3256	1/1	0.97	0.12	51,51,51,51	0
54	MG	2a	1735	1/1	0.97	0.24	45,45,45,45	0
54	MG	1T	201	1/1	0.97	0.05	54,54,54,54	0
54	MG	1A	3625	1/1	0.97	0.11	35,35,35,35	0
54	MG	2A	3690	1/1	0.97	0.06	67,67,67,67	0
54	MG	1A	3922	1/1	0.97	0.12	61,61,61,61	0
54	MG	1A	3923	1/1	0.97	0.13	50,50,50,50	0
54	MG	2A	3474	1/1	0.97	0.06	50,50,50,50	0
54	MG	1A	3510	1/1	0.97	0.04	34,34,34,34	0
54	MG	1A	3133	1/1	0.97	0.08	27,27,27,27	0
54	MG	1V	203	1/1	0.97	0.10	55,55,55,55	0
54	MG	1A	3134	1/1	0.97	0.14	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3137	1/1	0.97	0.06	29,29,29,29	0
54	MG	2A	3062	1/1	0.97	0.14	35,35,35,35	0
54	MG	1X	101	1/1	0.97	0.09	52,52,52,52	0
54	MG	1A	3769	1/1	0.97	0.10	19,19,19,19	0
54	MG	2A	3270	1/1	0.97	0.06	37,37,37,37	0
54	MG	10	101	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3417	1/1	0.97	0.07	20,20,20,20	0
54	MG	1A	3066	1/1	0.97	0.16	30,30,30,30	0
54	MG	1A	3420	1/1	0.97	0.06	50,50,50,50	0
54	MG	1A	3139	1/1	0.97	0.06	29,29,29,29	0
54	MG	1A	3067	1/1	0.97	0.06	38,38,38,38	0
54	MG	2A	3713	1/1	0.97	0.37	40,40,40,40	0
54	MG	1a	1765	1/1	0.97	0.09	46,46,46,46	0
54	MG	1A	3068	1/1	0.97	0.07	23,23,23,23	0
54	MG	1A	3192	1/1	0.97	0.18	35,35,35,35	0
54	MG	13	101	1/1	0.97	0.07	53,53,53,53	0
54	MG	1A	3052	1/1	0.97	0.07	36,36,36,36	0
54	MG	1A	3262	1/1	0.97	0.07	28,28,28,28	0
54	MG	15	103	1/1	0.97	0.05	41,41,41,41	0
54	MG	1A	3263	1/1	0.97	0.13	25,25,25,25	0
54	MG	1A	3008	1/1	0.97	0.06	33,33,33,33	0
54	MG	1A	3429	1/1	0.97	0.07	41,41,41,41	0
54	MG	2A	3724	1/1	0.97	0.12	32,32,32,32	0
59	ZN	2Y	501	1/1	0.97	0.04	79,79,79,79	0
54	MG	2A	3500	1/1	0.97	0.16	51,51,51,51	0
54	MG	2A	3464	1/1	0.98	0.17	34,34,34,34	0
54	MG	1A	3681	1/1	0.98	0.09	38,38,38,38	0
54	MG	1A	3351	1/1	0.98	0.05	18,18,18,18	0
54	MG	2A	3313	1/1	0.98	0.05	33,33,33,33	0
54	MG	1A	3683	1/1	0.98	0.04	25,25,25,25	0
54	MG	2A	3026	1/1	0.98	0.07	41,41,41,41	0
54	MG	2a	1609	1/1	0.98	0.07	46,46,46,46	0
54	MG	2a	1610	1/1	0.98	0.13	45,45,45,45	0
54	MG	2A	3165	1/1	0.98	0.25	64,64,64,64	0
54	MG	2A	3027	1/1	0.98	0.07	30,30,30,30	0
54	MG	1A	3049	1/1	0.98	0.14	38,38,38,38	0
54	MG	1E	302	1/1	0.98	0.31	39,39,39,39	0
54	MG	1A	3096	1/1	0.98	0.14	25,25,25,25	0
54	MG	1A	3254	1/1	0.98	0.14	30,30,30,30	0
54	MG	1A	3609	1/1	0.98	0.24	41,41,41,41	0
54	MG	1E	307	1/1	0.98	0.06	53,53,53,53	0
54	MG	1A	3212	1/1	0.98	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3540	1/1	0.98	0.06	25,25,25,25	0
54	MG	1F	303	1/1	0.98	0.12	35,35,35,35	0
54	MG	1A	3859	1/1	0.98	0.07	16,16,16,16	0
54	MG	1A	3356	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3771	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3772	1/1	0.98	0.21	24,24,24,24	0
54	MG	2A	3331	1/1	0.98	0.07	49,49,49,49	0
54	MG	2A	3643	1/1	0.98	0.14	34,34,34,34	0
54	MG	1A	3863	1/1	0.98	0.03	12,12,12,12	0
54	MG	2A	3181	1/1	0.98	0.09	47,47,47,47	0
54	MG	1a	1663	1/1	0.98	0.08	59,59,59,59	0
54	MG	1A	3691	1/1	0.98	0.07	17,17,17,17	0
54	MG	1A	3147	1/1	0.98	0.06	39,39,39,39	0
54	MG	2A	3185	1/1	0.98	0.07	45,45,45,45	0
54	MG	1A	3306	1/1	0.98	0.08	23,23,23,23	0
54	MG	1A	3776	1/1	0.98	0.05	26,26,26,26	0
54	MG	1A	3545	1/1	0.98	0.07	39,39,39,39	0
54	MG	1A	3020	1/1	0.98	0.14	33,33,33,33	0
54	MG	1A	3360	1/1	0.98	0.08	18,18,18,18	0
54	MG	1A	3215	1/1	0.98	0.04	35,35,35,35	0
54	MG	1G	3004	1/1	0.98	0.08	34,34,34,34	0
54	MG	1A	3549	1/1	0.98	0.05	38,38,38,38	0
54	MG	1A	3971	1/1	0.98	0.04	16,16,16,16	0
54	MG	1A	3216	1/1	0.98	0.30	29,29,29,29	0
54	MG	1A	3149	1/1	0.98	0.11	21,21,21,21	0
54	MG	1A	3975	1/1	0.98	0.06	39,39,39,39	0
54	MG	1A	3051	1/1	0.98	0.28	26,26,26,26	0
54	MG	1A	3876	1/1	0.98	0.04	27,27,27,27	0
54	MG	1P	201	1/1	0.98	0.14	27,27,27,27	0
54	MG	1A	3219	1/1	0.98	0.14	25,25,25,25	0
54	MG	1A	3009	1/1	0.98	0.10	34,34,34,34	0
54	MG	1A	3152	1/1	0.98	0.07	31,31,31,31	0
54	MG	1Q	202	1/1	0.98	0.05	29,29,29,29	0
54	MG	1A	3022	1/1	0.98	0.05	29,29,29,29	0
54	MG	1Q	204	1/1	0.98	0.09	31,31,31,31	0
54	MG	1R	201	1/1	0.98	0.13	31,31,31,31	0
54	MG	1A	3706	1/1	0.98	0.06	32,32,32,32	0
54	MG	2A	3209	1/1	0.98	0.22	43,43,43,43	0
54	MG	2A	3516	1/1	0.98	0.13	19,19,19,19	0
54	MG	1A	3083	1/1	0.98	0.04	40,40,40,40	0
54	MG	1A	3984	1/1	0.98	0.03	37,37,37,37	0
54	MG	1A	3985	1/1	0.98	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3792	1/1	0.98	0.04	12,12,12,12	0
54	MG	1A	3989	1/1	0.98	0.09	50,50,50,50	0
54	MG	2A	3681	1/1	0.98	0.07	69,69,69,69	0
54	MG	1A	3267	1/1	0.98	0.12	29,29,29,29	0
54	MG	1a	1695	1/1	0.98	0.12	37,37,37,37	0
54	MG	1A	3992	1/1	0.98	0.27	28,28,28,28	0
54	MG	1A	3993	1/1	0.98	0.09	26,26,26,26	0
54	MG	1V	202	1/1	0.98	0.04	47,47,47,47	0
54	MG	1A	3155	1/1	0.98	0.06	26,26,26,26	0
54	MG	1A	3494	1/1	0.98	0.11	38,38,38,38	0
54	MG	2A	3529	1/1	0.98	0.07	49,49,49,49	0
54	MG	1A	3997	1/1	0.98	0.12	23,23,23,23	0
54	MG	2a	1674	1/1	0.98	0.13	43,43,43,43	0
54	MG	1A	3711	1/1	0.98	0.08	30,30,30,30	0
54	MG	1A	3888	1/1	0.98	0.05	18,18,18,18	0
54	MG	1A	3319	1/1	0.98	0.06	15,15,15,15	0
54	MG	1A	3890	1/1	0.98	0.15	46,46,46,46	0
54	MG	1a	1706	1/1	0.98	0.07	28,28,28,28	0
54	MG	2A	3086	1/1	0.98	0.10	48,48,48,48	0
54	MG	1A	4002	1/1	0.98	0.24	29,29,29,29	0
54	MG	1A	3891	1/1	0.98	0.04	30,30,30,30	0
54	MG	1A	3016	1/1	0.98	0.30	17,17,17,17	0
54	MG	2A	3540	1/1	0.98	0.10	37,37,37,37	0
54	MG	2A	3701	1/1	0.98	0.05	47,47,47,47	0
54	MG	2A	3090	1/1	0.98	0.05	19,19,19,19	0
54	MG	2A	3091	1/1	0.98	0.05	61,61,61,61	0
54	MG	1A	4006	1/1	0.98	0.10	31,31,31,31	0
54	MG	1a	1838	1/1	0.98	0.08	55,55,55,55	0
54	MG	1l	101	1/1	0.98	0.04	44,44,44,44	0
54	MG	2A	3390	1/1	0.98	0.04	31,31,31,31	0
54	MG	2A	3237	1/1	0.98	0.15	34,34,34,34	0
54	MG	1A	3103	1/1	0.98	0.22	25,25,25,25	0
54	MG	1A	3715	1/1	0.98	0.04	19,19,19,19	0
54	MG	1A	3128	1/1	0.98	0.05	32,32,32,32	0
54	MG	13	102	1/1	0.98	0.07	27,27,27,27	0
54	MG	1A	3896	1/1	0.98	0.06	22,22,22,22	0
54	MG	2A	3243	1/1	0.98	0.14	18,18,18,18	0
54	MG	1A	3636	1/1	0.98	0.12	17,17,17,17	0
54	MG	1A	3565	1/1	0.98	0.14	36,36,36,36	0
54	MG	2A	3556	1/1	0.98	0.21	35,35,35,35	0
54	MG	1A	3104	1/1	0.98	0.23	23,23,23,23	0
54	MG	1A	3720	1/1	0.98	0.04	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3024	1/1	0.98	0.08	29,29,29,29	0
54	MG	1A	3007	1/1	0.98	0.06	26,26,26,26	0
54	MG	1A	3044	1/1	0.98	0.08	23,23,23,23	0
54	MG	1A	4019	1/1	0.98	0.06	29,29,29,29	0
54	MG	1a	1725	1/1	0.98	0.07	46,46,46,46	0
54	MG	2A	3254	1/1	0.98	0.15	51,51,51,51	0
54	MG	2A	3565	1/1	0.98	0.09	48,48,48,48	0
54	MG	2A	3255	1/1	0.98	0.04	24,24,24,24	0
54	MG	1A	3277	1/1	0.98	0.08	28,28,28,28	0
54	MG	1A	3195	1/1	0.98	0.21	33,33,33,33	0
54	MG	1A	3645	1/1	0.98	0.07	35,35,35,35	0
54	MG	1A	3505	1/1	0.98	0.03	27,27,27,27	0
54	MG	1A	3196	1/1	0.98	0.16	40,40,40,40	0
54	MG	1A	3088	1/1	0.98	0.05	32,32,32,32	0
54	MG	1A	3386	1/1	0.98	0.06	19,19,19,19	0
54	MG	1A	3912	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3164	1/1	0.98	0.12	22,22,22,22	0
54	MG	1A	3089	1/1	0.98	0.09	26,26,26,26	0
54	MG	2B	3016	1/1	0.98	0.07	52,52,52,52	0
54	MG	1A	3511	1/1	0.98	0.04	32,32,32,32	0
54	MG	1A	3135	1/1	0.98	0.05	29,29,29,29	0
54	MG	2B	3019	1/1	0.98	0.04	65,65,65,65	0
54	MG	1A	3045	1/1	0.98	0.08	35,35,35,35	0
54	MG	2D	302	1/1	0.98	0.41	38,38,38,38	0
54	MG	2a	1728	1/1	0.98	0.10	53,53,53,53	0
54	MG	1A	3113	1/1	0.98	0.08	18,18,18,18	0
54	MG	2A	3271	1/1	0.98	0.06	23,23,23,23	0
54	MG	1A	3336	1/1	0.98	0.09	33,33,33,33	0
54	MG	1A	3658	1/1	0.98	0.03	24,24,24,24	0
54	MG	1A	3824	1/1	0.98	0.07	17,17,17,17	0
54	MG	1A	3114	1/1	0.98	0.07	22,22,22,22	0
54	MG	1a	1619	1/1	0.98	0.04	54,54,54,54	0
54	MG	2A	3129	1/1	0.98	0.06	52,52,52,52	0
54	MG	1A	3338	1/1	0.98	0.05	28,28,28,28	0
54	MG	2E	304	1/1	0.98	0.05	29,29,29,29	0
54	MG	1A	3288	1/1	0.98	0.08	16,16,16,16	0
54	MG	1B	214	1/1	0.98	0.04	35,35,35,35	0
54	MG	1A	3586	1/1	0.98	0.05	23,23,23,23	0
54	MG	2A	3134	1/1	0.98	0.04	36,36,36,36	0
54	MG	1A	3396	1/1	0.98	0.07	21,21,21,21	0
54	MG	1A	3026	1/1	0.98	0.20	28,28,28,28	0
54	MG	1A	3243	1/1	0.98	0.07	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3399	1/1	0.98	0.07	33,33,33,33	0
54	MG	1A	3244	1/1	0.98	0.15	27,27,27,27	0
54	MG	1A	3172	1/1	0.98	0.45	31,31,31,31	0
54	MG	1A	3525	1/1	0.98	0.16	37,37,37,37	0
54	MG	1A	3462	1/1	0.98	0.16	48,48,48,48	0
54	MG	2A	3006	1/1	0.98	0.20	43,43,43,43	0
54	MG	1A	3246	1/1	0.98	0.07	58,58,58,58	0
54	MG	1A	3027	1/1	0.98	0.08	34,34,34,34	0
54	MG	2A	3604	1/1	0.98	0.06	31,31,31,31	0
54	MG	2A	3009	1/1	0.98	0.05	30,30,30,30	0
54	MG	1A	3248	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3076	1/1	0.98	0.10	27,27,27,27	0
55	K	1A	3287	1/1	0.98	0.03	27,27,27,27	0
54	MG	1A	3842	1/1	0.98	0.04	42,42,42,42	0
54	MG	2A	3298	1/1	0.98	0.09	27,27,27,27	0
54	MG	2A	3299	1/1	0.98	0.10	28,28,28,28	0
54	MG	1D	301	1/1	0.98	0.08	25,25,25,25	0
54	MG	1A	3143	1/1	0.98	0.03	26,26,26,26	0
54	MG	1D	303	1/1	0.98	0.17	44,44,44,44	0
54	MG	1A	3349	1/1	0.98	0.08	40,40,40,40	0
54	MG	1A	3846	1/1	0.98	0.07	27,27,27,27	0
54	MG	2A	3018	1/1	0.98	0.05	40,40,40,40	0
54	MG	1a	1642	1/1	0.98	0.16	39,39,39,39	0
54	MG	1A	3847	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3019	1/1	0.98	0.20	33,33,33,33	0
59	ZN	24	501	1/1	0.98	0.08	108,108,108,108	0
54	MG	1A	3409	1/1	0.98	0.11	50,50,50,50	0
60	SF4	1d	302	8/8	0.98	0.06	48,59,66,72	0
60	SF4	2d	501	8/8	0.98	0.04	61,71,81,92	0
54	MG	1A	3300	1/1	0.99	0.03	23,23,23,23	0
54	MG	1A	3005	1/1	0.99	0.09	15,15,15,15	0
54	MG	1A	3994	1/1	0.99	0.09	26,26,26,26	0
54	MG	2A	3259	1/1	0.99	0.05	32,32,32,32	0
54	MG	2A	3311	1/1	0.99	0.06	43,43,43,43	0
54	MG	1A	3920	1/1	0.99	0.09	21,21,21,21	0
54	MG	1A	3431	1/1	0.99	0.04	34,34,34,34	0
54	MG	2A	3110	1/1	0.99	0.21	40,40,40,40	0
54	MG	1A	3073	1/1	0.99	0.13	30,30,30,30	0
54	MG	1A	3736	1/1	0.99	0.04	41,41,41,41	0
54	MG	1A	3607	1/1	0.99	0.04	50,50,50,50	0
54	MG	1a	1850	1/1	0.99	0.03	45,45,45,45	0
54	MG	2A	3424	1/1	0.99	0.03	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3069	1/1	0.99	0.03	23,23,23,23	0
54	MG	1B	213	1/1	0.99	0.05	38,38,38,38	0
54	MG	1A	3828	1/1	0.99	0.06	13,13,13,13	0
54	MG	1A	3228	1/1	0.99	0.13	18,18,18,18	0
54	MG	1A	3657	1/1	0.99	0.09	31,31,31,31	0
54	MG	1A	4004	1/1	0.99	0.11	25,25,25,25	0
54	MG	1A	3105	1/1	0.99	0.13	33,33,33,33	0
54	MG	1A	3491	1/1	0.99	0.02	36,36,36,36	0
54	MG	1B	220	1/1	0.99	0.04	20,20,20,20	0
54	MG	2A	3650	1/1	0.99	0.04	36,36,36,36	0
54	MG	1A	3897	1/1	0.99	0.09	23,23,23,23	0
54	MG	1A	3418	1/1	0.99	0.06	22,22,22,22	0
54	MG	1a	1815	1/1	0.99	0.04	44,44,44,44	0
54	MG	1A	3270	1/1	0.99	0.11	11,11,11,11	0
54	MG	1A	3018	1/1	0.99	0.17	24,24,24,24	0
54	MG	1A	4011	1/1	0.99	0.13	29,29,29,29	0
54	MG	1A	3638	1/1	0.99	0.06	38,38,38,38	0
54	MG	2a	1750	1/1	0.99	0.05	59,59,59,59	0
54	MG	1A	3107	1/1	0.99	0.13	27,27,27,27	0
54	MG	2A	3442	1/1	0.99	0.08	27,27,27,27	0
54	MG	1A	3973	1/1	0.99	0.04	42,42,42,42	0
54	MG	1A	3616	1/1	0.99	0.08	16,16,16,16	0
54	MG	1A	3666	1/1	0.99	0.06	20,20,20,20	0
54	MG	2A	3135	1/1	0.99	0.14	67,67,67,67	0
54	MG	1A	3136	1/1	0.99	0.06	24,24,24,24	0
54	MG	1A	3003	1/1	0.99	0.04	31,31,31,31	0
54	MG	1A	3298	1/1	0.99	0.05	14,14,14,14	0
55	K	2A	3246	1/1	0.99	0.02	30,30,30,30	0
54	MG	1a	1827	1/1	0.99	0.06	33,33,33,33	0
54	MG	1A	3843	1/1	0.99	0.11	30,30,30,30	0
54	MG	1D	306	1/1	0.99	0.05	11,11,11,11	0
54	MG	1A	3378	1/1	0.99	0.02	20,20,20,20	0
54	MG	1D	308	1/1	0.99	0.07	31,31,31,31	0
54	MG	1A	3170	1/1	0.99	0.11	28,28,28,28	0
54	MG	1A	3410	1/1	0.99	0.07	18,18,18,18	0
54	MG	1A	3365	1/1	0.99	0.06	13,13,13,13	0
54	MG	1A	3728	1/1	0.99	0.04	38,38,38,38	0
54	MG	1A	3674	1/1	0.99	0.05	35,35,35,35	0
54	MG	2A	3003	1/1	0.99	0.04	37,37,37,37	0
59	ZN	1Y	501	1/1	0.99	0.03	46,46,46,46	0
59	ZN	14	501	1/1	0.99	0.03	80,80,80,80	0
59	ZN	15	101	1/1	0.99	0.04	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	ZN	16	501	1/1	0.99	0.10	46,46,46,46	0
59	ZN	19	501	1/1	0.99	0.08	39,39,39,39	0
59	ZN	1n	501	1/1	0.99	0.03	60,60,60,60	0
54	MG	1A	3788	1/1	0.99	0.06	23,23,23,23	0
54	MG	1A	3601	1/1	0.99	0.06	31,31,31,31	0
59	ZN	26	501	1/1	0.99	0.04	59,59,59,59	0
59	ZN	29	501	1/1	0.99	0.03	62,62,62,62	0
54	MG	1E	303	1/1	0.99	0.05	32,32,32,32	0
54	MG	1A	3990	1/1	0.99	0.04	20,20,20,20	0
54	MG	1A	3541	1/1	0.99	0.08	19,19,19,19	0
59	ZN	25	501	1/1	1.00	0.04	44,44,44,44	0
54	MG	2A	3333	1/1	1.00	0.02	28,28,28,28	0
54	MG	1A	3956	1/1	1.00	0.04	24,24,24,24	0
54	MG	1A	3477	1/1	1.00	0.06	16,16,16,16	0
54	MG	1X	102	1/1	1.00	0.08	31,31,31,31	0
54	MG	1A	3968	1/1	1.00	0.03	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.