



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 11:03 am BST

PDB ID : 4Y4O
Title : Crystal structure of the Thermus thermophilus 70S ribosome with rRNA modifications and bound to protein Y (YfiA) at 2.3Å resolution
Authors : Polikanov, Y.S.; Melnikov, S.V.; Soll, D.; Steitz, T.A.
Deposited on : 2015-02-10
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

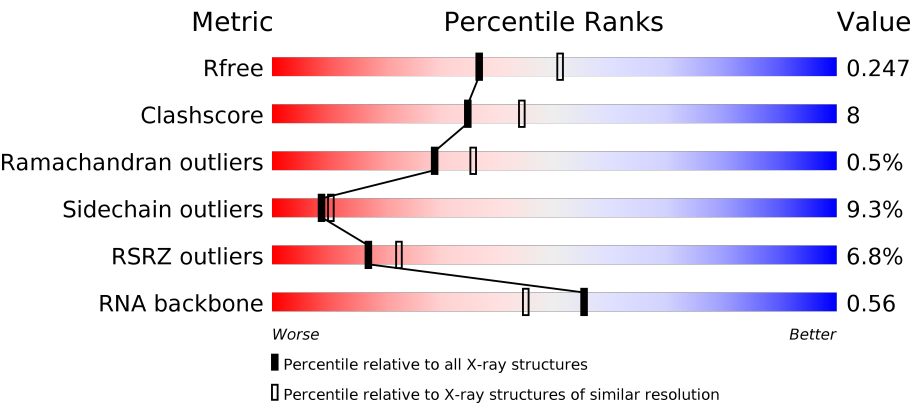
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>66%25%7% ..</div></div>
1	2A	2915	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>58%31%8% ..</div></div>
2	1B	121	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>71%23%5% .</div></div>
2	2B	121	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>60%34%5% ..</div></div>






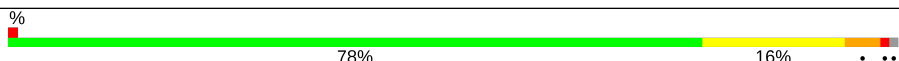
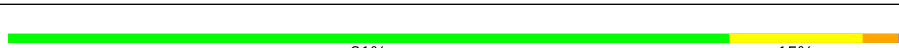
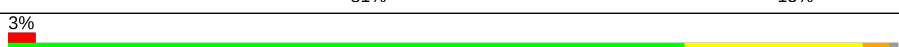
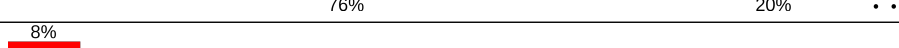
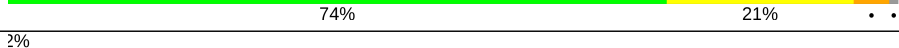


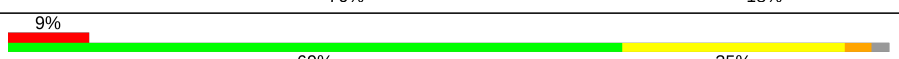
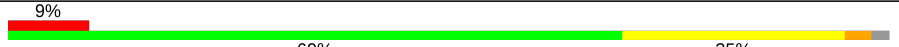

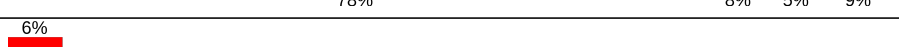







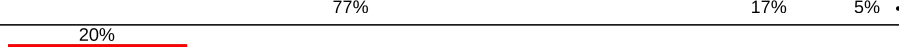

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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118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



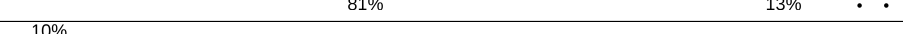


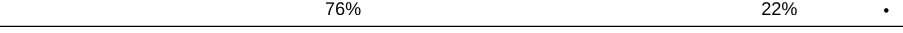

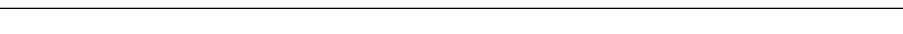





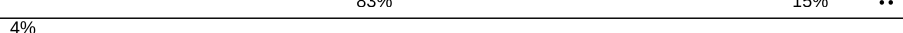


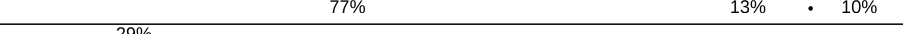




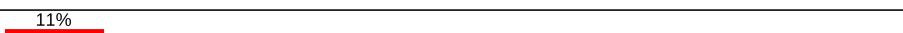


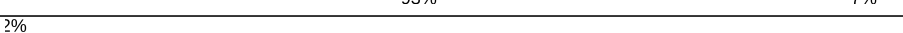
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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25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

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3612	-	-	-	X
54	MG	1A	4003	-	-	-	X
54	MG	1a	1744	-	-	-	X
54	MG	2A	3081	-	-	-	X
54	MG	2A	3174	-	-	-	X
54	MG	2A	3187	-	-	-	X
54	MG	2A	3234	-	-	-	X
54	MG	2A	3408	-	-	-	X
54	MG	2A	3431	-	-	-	X
54	MG	2A	3478	-	-	-	X
54	MG	2A	3535	-	-	-	X
54	MG	2A	3633	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 298502 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2E	5	Total	Mg	0	0
			5	5		
54	17	2	Total	Mg	0	0
			2	2		
54	1T	3	Total	Mg	0	0
			3	3		
54	1N	3	Total	Mg	0	0
			3	3		
54	20	2	Total	Mg	0	0
			2	2		
54	18	1	Total	Mg	0	0
			1	1		
54	1o	1	Total	Mg	0	0
			1	1		
54	2W	2	Total	Mg	0	0
			2	2		
54	2I	1	Total	Mg	0	0
			1	1		
54	13	2	Total	Mg	0	0
			2	2		
54	1f	1	Total	Mg	0	0
			1	1		
54	1P	2	Total	Mg	0	0
			2	2		
54	2B	19	Total	Mg	0	0
			19	19		
54	1q	2	Total	Mg	0	0
			2	2		
54	2a	193	Total	Mg	0	0
			193	193		
54	1E	6	Total	Mg	0	0
			6	6		
54	1b	1	Total	Mg	0	0
			1	1		
54	2l	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2F	3	Total 3	Mg 3	0	0
54	28	2	Total 2	Mg 2	0	0
54	2e	1	Total 1	Mg 1	0	0
54	1W	2	Total 2	Mg 2	0	0
54	1A	1075	Total 1075	Mg 1075	0	0
54	1t	1	Total 1	Mg 1	0	0
54	1n	2	Total 2	Mg 2	0	0
54	2P	2	Total 2	Mg 2	0	0
54	1X	1	Total 1	Mg 1	0	0
54	1y	4	Total 4	Mg 4	0	0
54	2T	3	Total 3	Mg 3	0	0
54	1D	14	Total 14	Mg 14	0	0
54	2N	1	Total 1	Mg 1	0	0
54	1e	4	Total 4	Mg 4	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2f	1	Total 1	Mg 1	0	0
54	1V	3	Total 3	Mg 3	0	0
54	2X	1	Total 1	Mg 1	0	0
54	1a	280	Total 280	Mg 280	0	0
54	2Q	2	Total 2	Mg 2	0	0
54	15	2	Total 2	Mg 2	0	0

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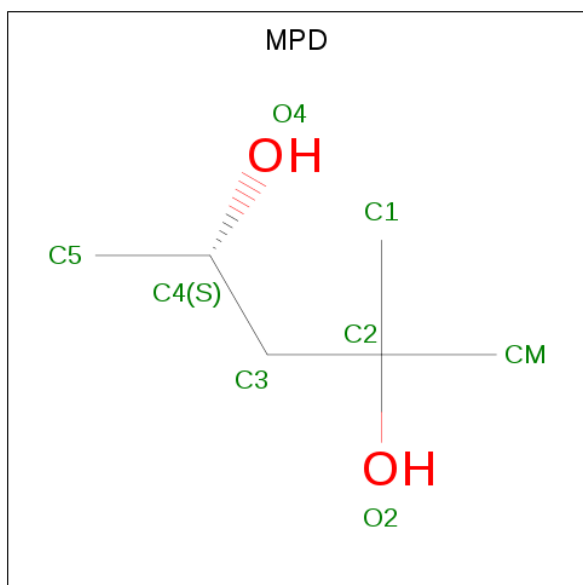
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2j	1	Total 1	Mg 1	0	0
54	1R	3	Total 3	Mg 3	0	0
54	26	1	Total 1	Mg 1	0	0
54	1G	4	Total 4	Mg 4	0	0
54	2O	2	Total 2	Mg 2	0	0
54	11	4	Total 4	Mg 4	0	0
54	1d	5	Total 5	Mg 5	0	0
54	2r	1	Total 1	Mg 1	0	0
54	1H	2	Total 2	Mg 2	0	0
54	21	1	Total 1	Mg 1	0	0
54	1i	1	Total 1	Mg 1	0	0
54	2R	1	Total 1	Mg 1	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	2D	9	Total 9	Mg 9	0	0
54	14	1	Total 1	Mg 1	0	0
54	1U	2	Total 2	Mg 2	0	0
54	1O	1	Total 1	Mg 1	0	0
54	1r	1	Total 1	Mg 1	0	0
54	19	2	Total 2	Mg 2	0	0
54	1l	2	Total 2	Mg 2	0	0
54	2V	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1F	10	Total	Mg	0	0
			10	10		
54	10	5	Total	Mg	0	0
			5	5		
54	1g	3	Total	Mg	0	0
			3	3		
54	2t	1	Total	Mg	0	0
			1	1		
54	1Q	4	Total	Mg	0	0
			4	4		
54	2A	761	Total	Mg	0	0
			761	761		
54	1h	2	Total	Mg	0	0
			2	2		
54	1B	30	Total	Mg	0	0
			30	30		
54	27	1	Total	Mg	0	0
			1	1		

- Molecule 55 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



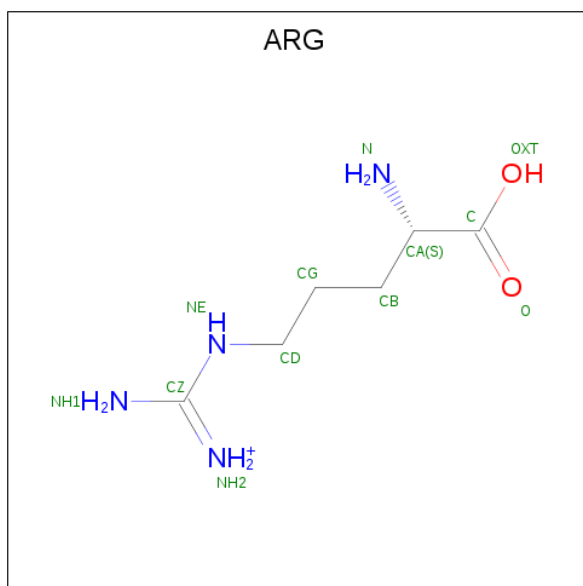
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
55	1A	1	Total	C	O	0	0
			8	6	2		
55	1T	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
55	18	1	Total	C	O	0	0
			8	6	2		
55	1a	1	Total	C	O	0	0
			8	6	2		
55	2A	1	Total	C	O	0	0
			8	6	2		
55	2A	1	Total	C	O	0	0
			8	6	2		
55	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 56 is ARGinine (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	1B	1	Total	C	N	O	0	0
			12	6	4	2		
56	1F	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

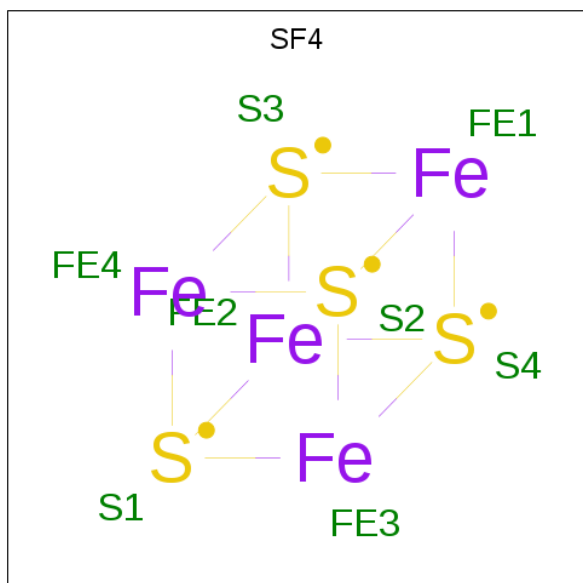
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		
57	14	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1n	1	Total	Zn	0	0
			1	1		
57	15	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	19	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	25	1	Total	Zn	0	0
			1	1		
57	24	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		
57	2Y	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	4154	Total	O	0	0
			4154	4154		
59	1B	109	Total	O	0	0
			109	109		
59	1D	119	Total	O	0	0
			119	119		
59	1E	81	Total	O	0	0
			81	81		
59	1F	66	Total	O	0	0
			66	66		
59	1G	20	Total	O	0	0
			20	20		
59	1H	16	Total	O	0	0
			16	16		
59	1I	9	Total	O	0	0
			9	9		
59	1N	55	Total	O	0	0
			55	55		
59	1O	29	Total	O	0	0
			29	29		
59	1P	56	Total	O	0	0
			56	56		
59	1Q	46	Total	O	0	0
			46	46		
59	1R	37	Total	O	0	0
			37	37		
59	1S	11	Total	O	0	0
			11	11		
59	1T	39	Total	O	0	0
			39	39		
59	1U	49	Total	O	0	0
			49	49		
59	1V	34	Total	O	0	0
			34	34		
59	1W	27	Total	O	0	0
			27	27		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1X	27	Total 27	O 27	0	0
59	1Y	20	Total 20	O 20	0	0
59	1Z	13	Total 13	O 13	0	0
59	10	25	Total 25	O 25	0	0
59	11	25	Total 25	O 25	0	0
59	12	15	Total 15	O 15	0	0
59	13	25	Total 25	O 25	0	0
59	14	4	Total 4	O 4	0	0
59	15	25	Total 25	O 25	0	0
59	16	22	Total 22	O 22	0	0
59	17	19	Total 19	O 19	0	0
59	18	31	Total 31	O 31	0	0
59	19	9	Total 9	O 9	0	0
59	1a	599	Total 599	O 599	0	0
59	1b	1	Total 1	O 1	0	0
59	1c	1	Total 1	O 1	0	0
59	1d	8	Total 8	O 8	0	0
59	1e	5	Total 5	O 5	0	0
59	1f	3	Total 3	O 3	0	0
59	1h	1	Total 1	O 1	0	0
59	1i	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1j	1	Total 1	O 1	0	0
59	1k	1	Total 1	O 1	0	0
59	1l	5	Total 5	O 5	0	0
59	1m	2	Total 2	O 2	0	0
59	1o	7	Total 7	O 7	0	0
59	1p	3	Total 3	O 3	0	0
59	1t	1	Total 1	O 1	0	0
59	1y	7	Total 7	O 7	0	0
59	2A	2665	Total 2665	O 2665	0	0
59	2B	69	Total 69	O 69	0	0
59	2D	59	Total 59	O 59	0	0
59	2E	33	Total 33	O 33	0	0
59	2F	26	Total 26	O 26	0	0
59	2G	9	Total 9	O 9	0	0
59	2H	4	Total 4	O 4	0	0
59	2I	4	Total 4	O 4	0	0
59	2N	6	Total 6	O 6	0	0
59	2O	23	Total 23	O 23	0	0
59	2P	30	Total 30	O 30	0	0
59	2Q	28	Total 28	O 28	0	0
59	2R	21	Total 21	O 21	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2S	7	Total 7	O 7	0	0
59	2T	11	Total 11	O 11	0	0
59	2U	20	Total 20	O 20	0	0
59	2V	6	Total 6	O 6	0	0
59	2W	20	Total 20	O 20	0	0
59	2X	10	Total 10	O 10	0	0
59	2Y	4	Total 4	O 4	0	0
59	2Z	16	Total 16	O 16	0	0
59	20	13	Total 13	O 13	0	0
59	21	22	Total 22	O 22	0	0
59	22	4	Total 4	O 4	0	0
59	23	3	Total 3	O 3	0	0
59	24	2	Total 2	O 2	0	0
59	25	10	Total 10	O 10	0	0
59	26	5	Total 5	O 5	0	0
59	27	9	Total 9	O 9	0	0
59	28	16	Total 16	O 16	0	0
59	29	3	Total 3	O 3	0	0
59	2a	459	Total 459	O 459	0	0
59	2d	6	Total 6	O 6	0	0
59	2e	2	Total 2	O 2	0	0

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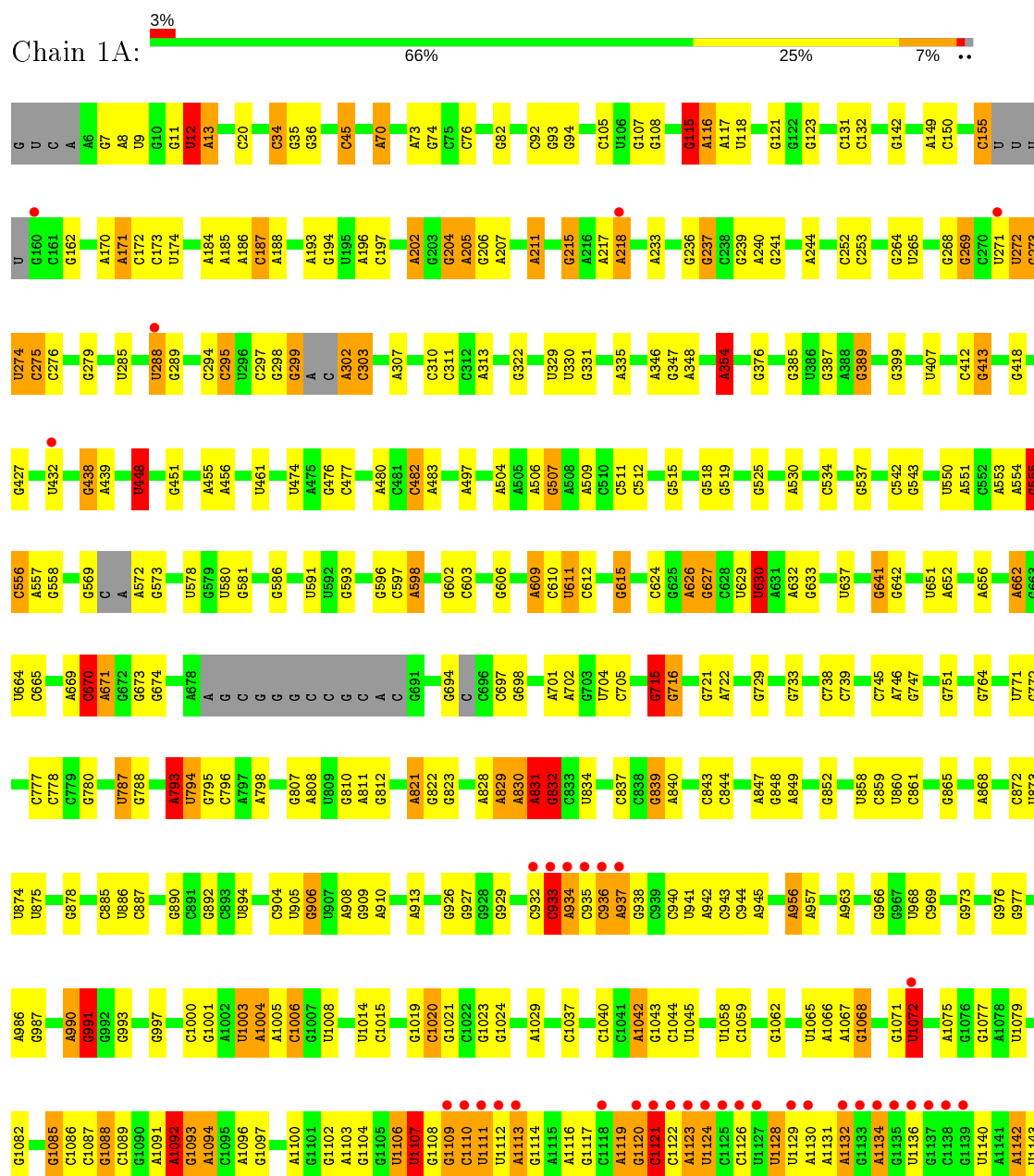
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2f	1	Total	O	0	0
			1	1		
59	2j	2	Total	O	0	0
			2	2		
59	2l	5	Total	O	0	0
			5	5		
59	2m	2	Total	O	0	0
			2	2		
59	2o	2	Total	O	0	0
			2	2		
59	2p	3	Total	O	0	0
			3	3		
59	2q	1	Total	O	0	0
			1	1		
59	2r	5	Total	O	0	0
			5	5		
59	2t	2	Total	O	0	0
			2	2		
59	2y	5	Total	O	0	0
			5	5		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

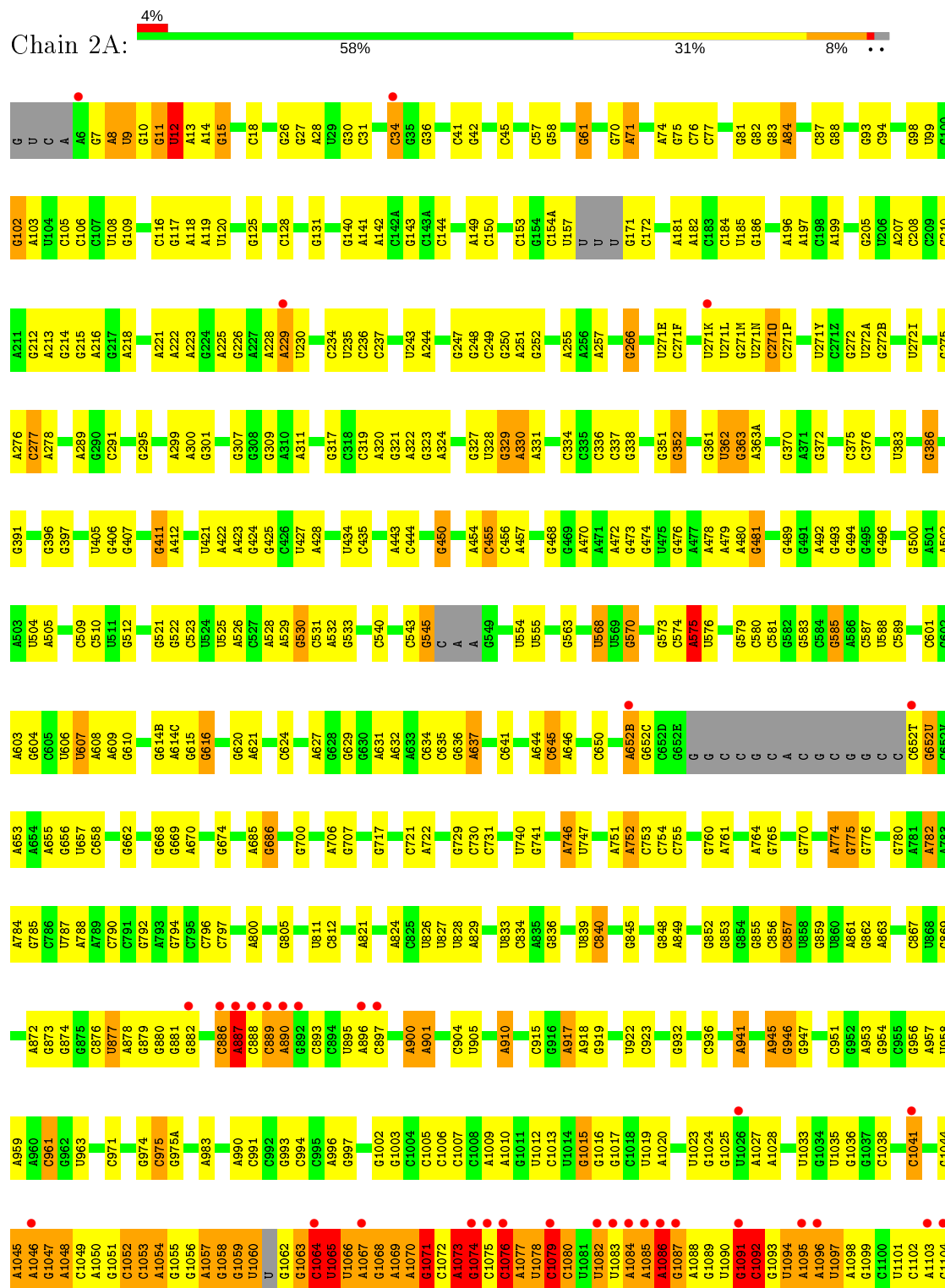
• Molecule 1: 23S Ribosomal RNA



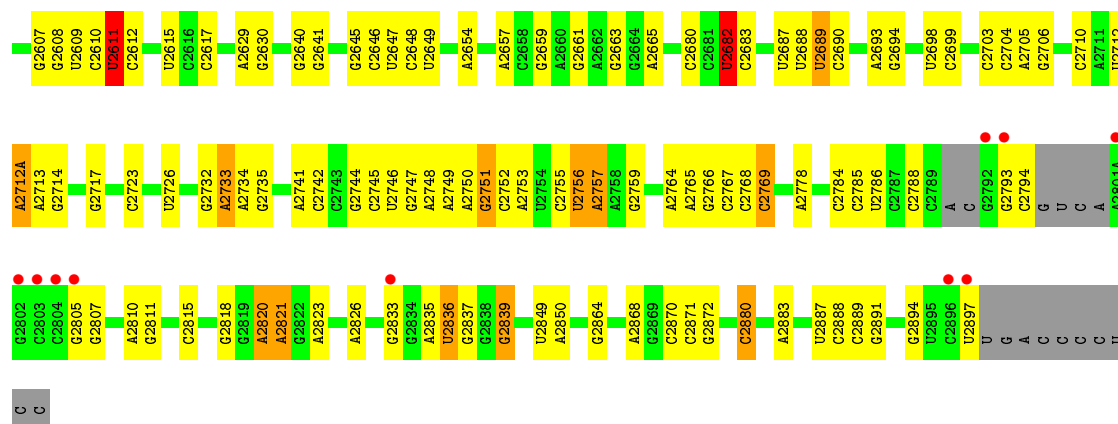
C2702	A2576	A2323	G2307	G2143	U2056	A1911	G1784	A1654	C1539	A1405	C1263	U1147
U2710	A2577	U2324	G2208	U2144	G2057	A1918	G1787	A1655	C1552	A1411	G1273	C1148
C2711	A2578	C2325	G2209	G2145	C2058	G1918	U1788	A1656	C1553	G1416	G1285	C1149
U2714	A2584	G2327	U2211	A2148	C2065	G1921	A1793	A1660	A1554	G1417	U1286	C1150
C2715	C2585	C2328	G2212	G2149	G2077	A1922	G1794	G1674	C1555	U1418	A1288	U1151
U2724	A2588	A2332	G2213	C2150	G2078	G1928	G1795	U1675	A1556	A1424	A1289	G1152
A2725	A2589	A2331	G2214	C2151	A2079	G1935	A1804	A1679	A1557	A1425	C1155	C1156
A2726	A2590	G2337	U2220	G2152	A2080	A1936	A1807	A1680	G1558	A1426	U1296	A1157
G2727	A2593	C2338	G2227	U2154	A2081	C1936	U1808	G1681	G1559	G1427	G1296	G1158
G2594	C2594	A2339	G2228	G2155	A2082	G1951	U1809	U1686	U1560	G1428	C1297	U1159
G2595	C2595	A2340	A2229	A2156	G2083	G1952	U1810	A1687	C1561	C1429	G1298	G1160
U2596	C2454	G2341	A2237	A2157	A2084	U1953	U1811	U1688	U1566	A1430	A1299	G1161
U2597	C2455	G2342	G2238	C2158	C2085	U1954	U1812	A1689	G1567	C1431	C1302	C1162
G2745	C2459	G2346	A2239	C2159	C2086	A1954	G1813	G1694	C1432	C1433	G1305	A1174
A2746	A2460	A2347	A2240	C2160	C2087	G1955	A1814	C1695	G1571	G1434	G1306	A1175
U2605	G2470	A2348	G2246	C2161	G2091	A1958	A1815	A1699	G1576	U1435	G1312	C1180
C2613	G2471	G2357	G2250	C2162	G2092	A1959	A1816	G1700	C1577	U1436	U1312	G1181
A2761	C2473	A2358	G2251	U2166	G2094	A1961	A1817	A1701	C1578	A1441	A1314	U1186
G2615	U2474	C2359	U2255	C2167	C2095	U1977	A1822	C1707	U	U1451	A1315	G1184
U2616	C2475	G2361	U2256	C2168	U2096	U1985	G1823	G1708	A	U1452	G1317	C1185
G2620	C2476	C2362	U2257	C2169	U2097	U1985	U1824	C1709	C	C1453	U1318	U1187
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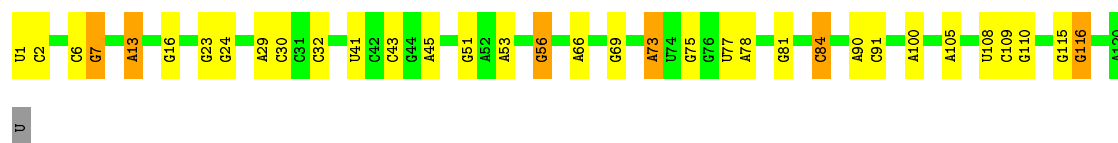
• Molecule 1: 23S Ribosomal RNA



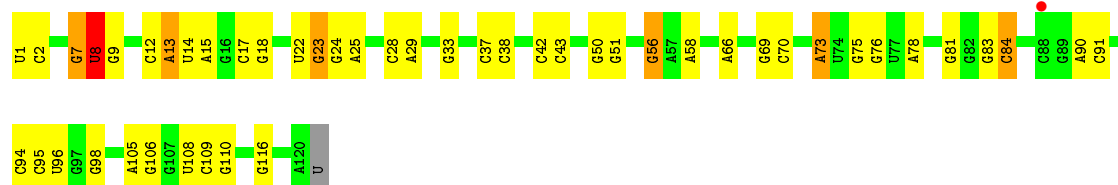
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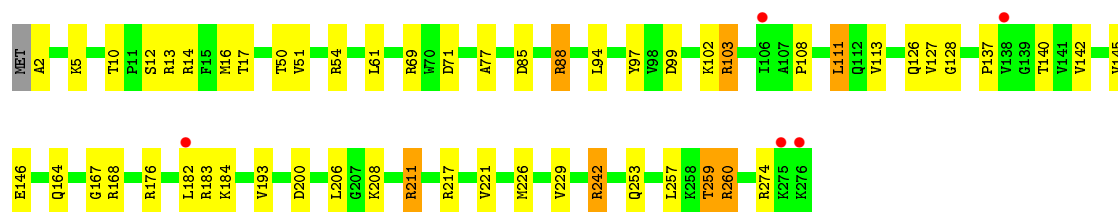
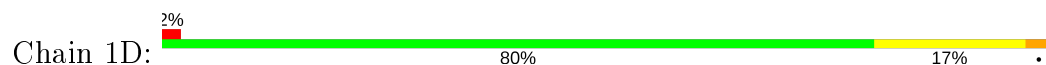
- Molecule 2: 5S Ribosomal RNA



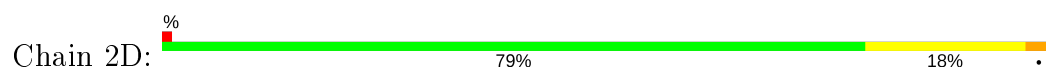
- Molecule 2: 5S Ribosomal RNA



- Molecule 3: 50S ribosomal protein L2

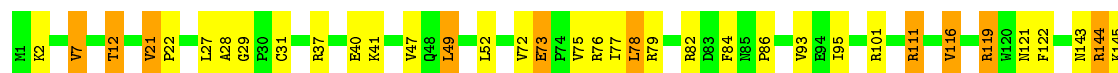


- Molecule 3: 50S ribosomal protein L2

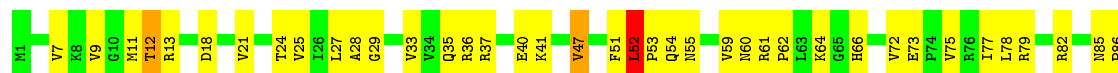




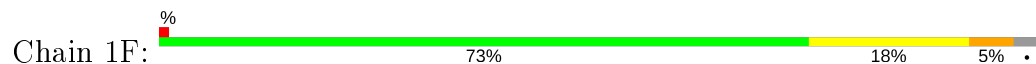
- Molecule 4: 50S ribosomal protein L3



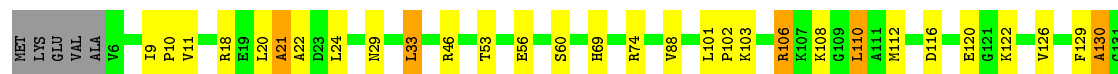
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

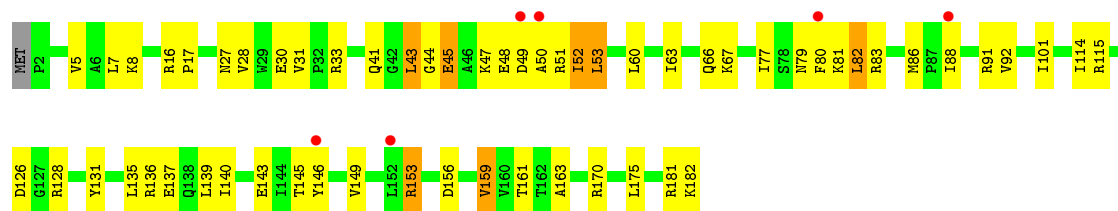


- Molecule 5: 50S ribosomal protein L4



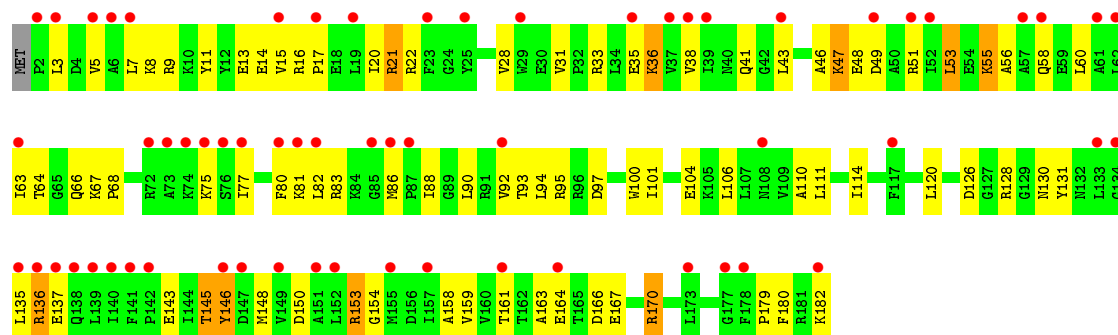
- Molecule 6: 50S ribosomal protein L5





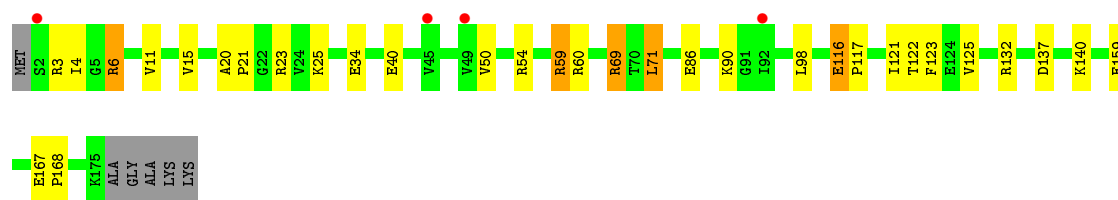
• Molecule 6: 50S ribosomal protein L5

Chain 2G: 34% 53% 41% 5%



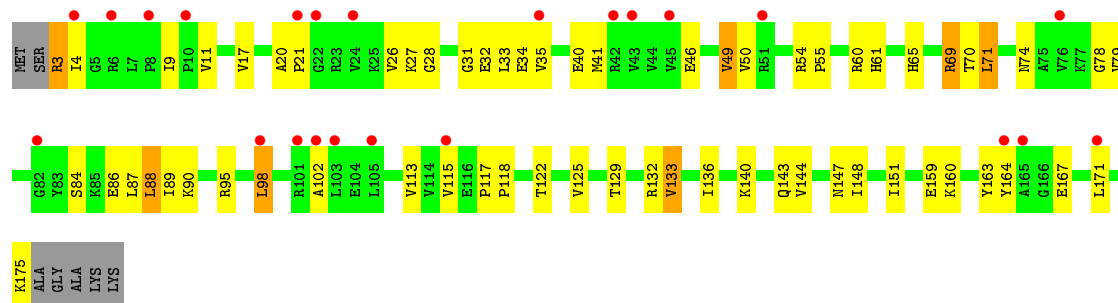
• Molecule 7: 50S ribosomal protein L6

Chain 1H: 2% 79% 15%



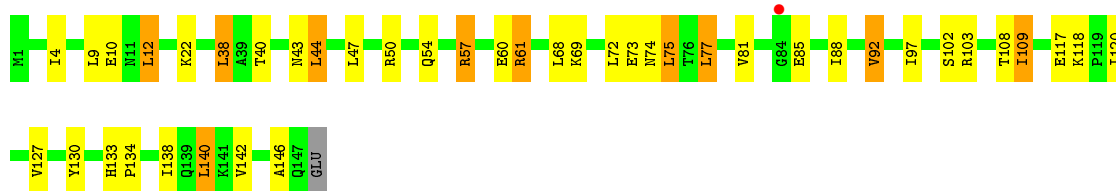
• Molecule 7: 50S ribosomal protein L6

Chain 2H: 13% 61% 31%

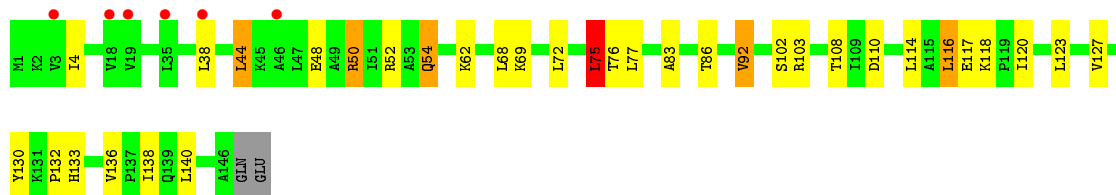
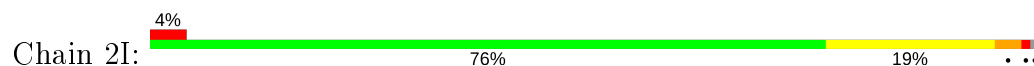


• Molecule 8: 50S ribosomal protein L9

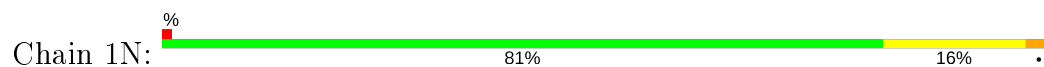
Chain 1I: % 71% 22% 7%



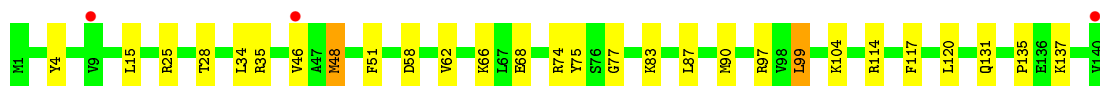
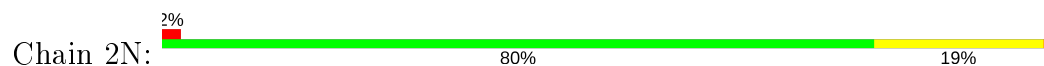
• Molecule 8: 50S ribosomal protein L9



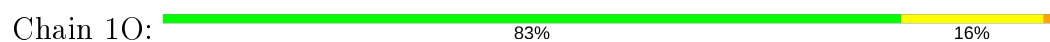
• Molecule 9: 50S ribosomal protein L13



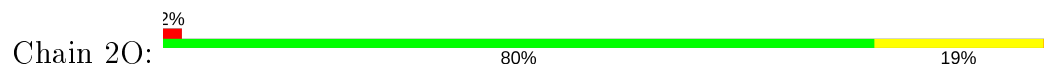
• Molecule 9: 50S ribosomal protein L13



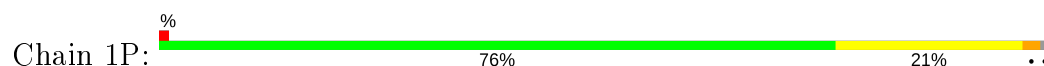
• Molecule 10: 50S ribosomal protein L14

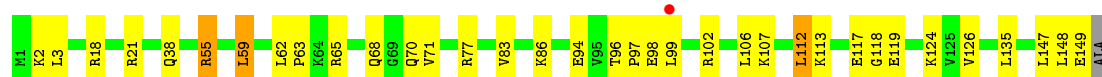


• Molecule 10: 50S ribosomal protein L14

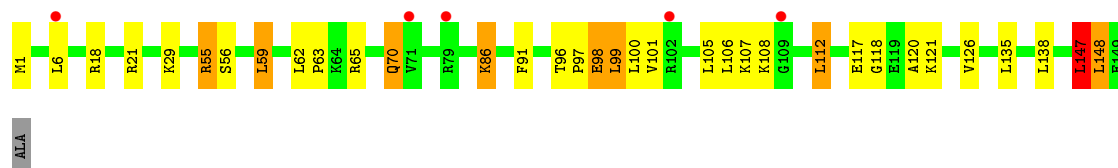
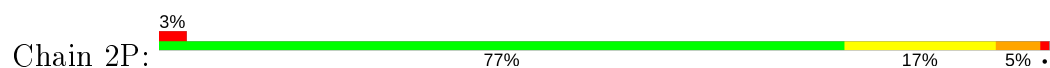


• Molecule 11: 50S ribosomal protein L15

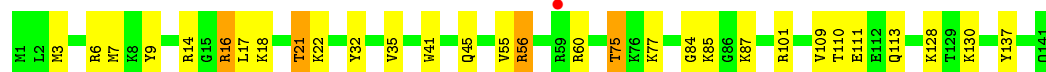
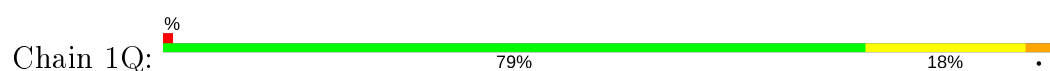




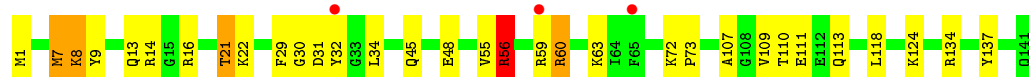
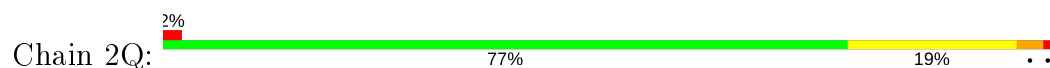
- Molecule 11: 50S ribosomal protein L15



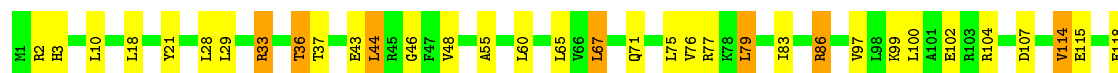
- Molecule 12: 50S ribosomal protein L16



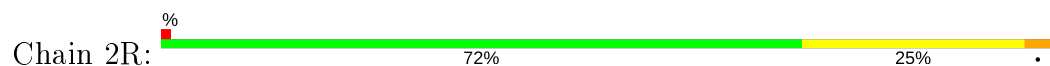
- Molecule 12: 50S ribosomal protein L16



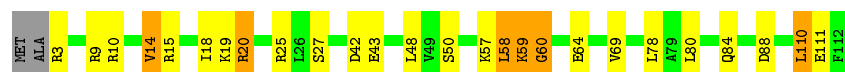
- Molecule 13: 50S ribosomal protein L17



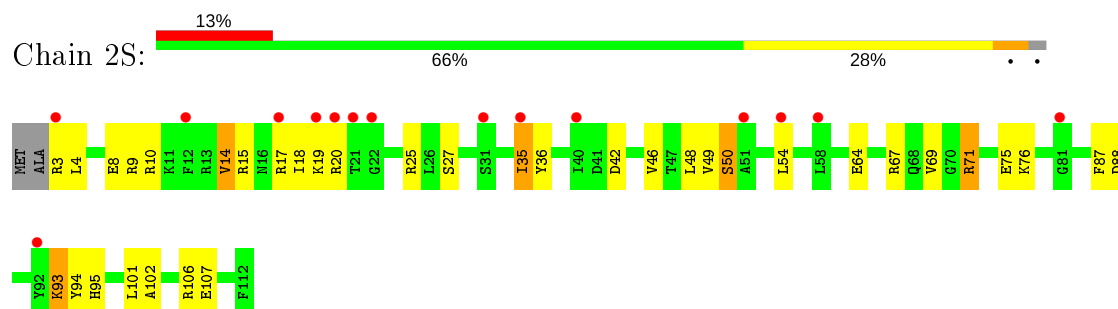
- Molecule 13: 50S ribosomal protein L17



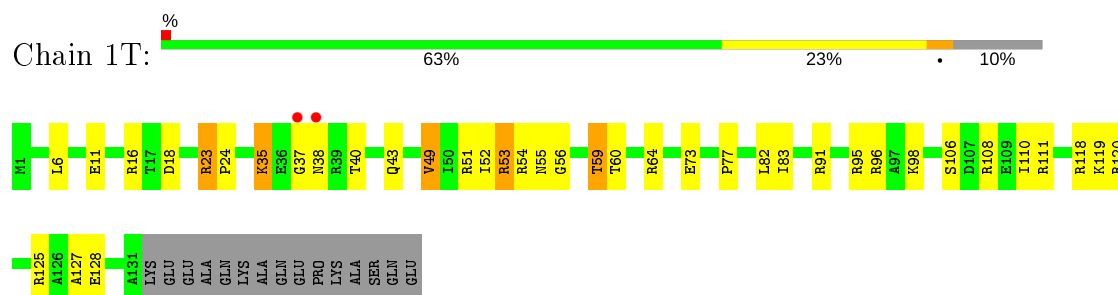
- Molecule 14: 50S ribosomal protein L18



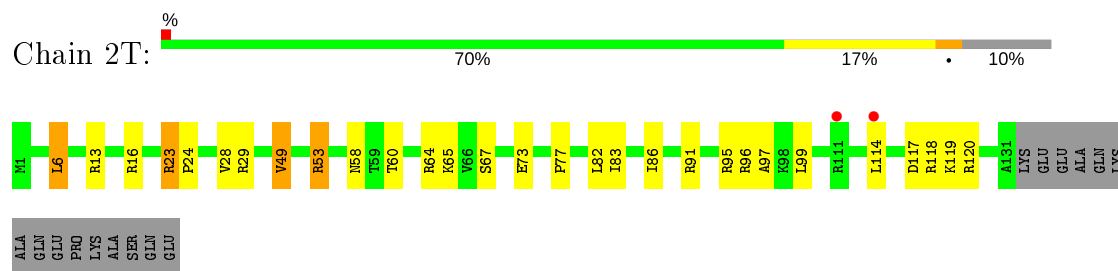
- Molecule 14: 50S ribosomal protein L18



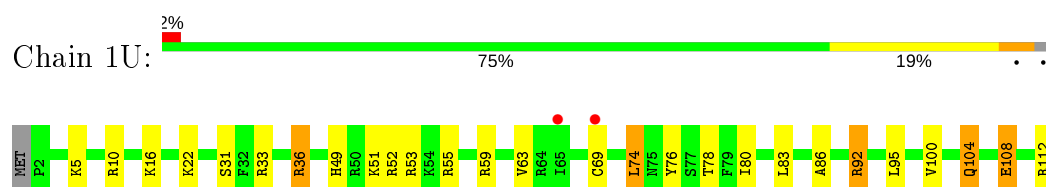
- Molecule 15: 50S ribosomal protein L19



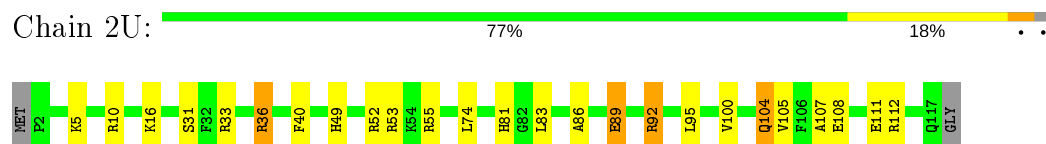
- Molecule 15: 50S ribosomal protein L19



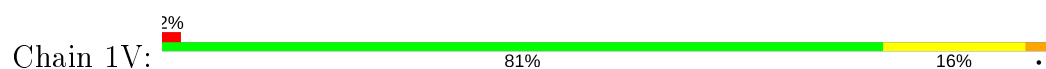
- Molecule 16: 50S ribosomal protein L20

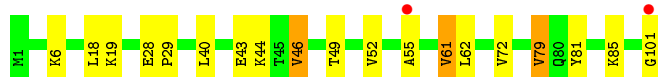


- Molecule 16: 50S ribosomal protein L20

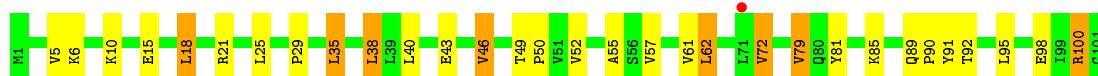


- Molecule 17: 50S ribosomal protein L21

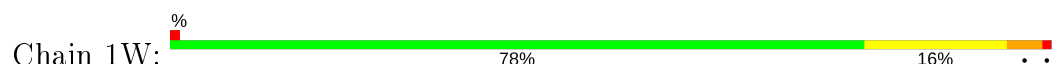




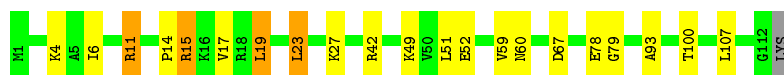
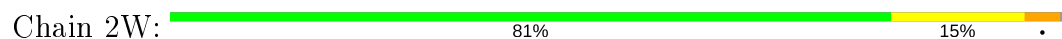
- Molecule 17: 50S ribosomal protein L21



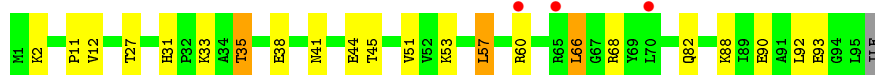
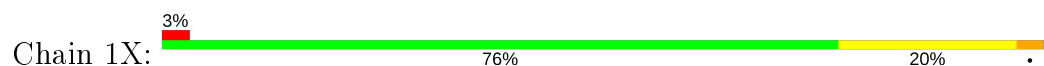
- Molecule 18: 50S ribosomal protein L22



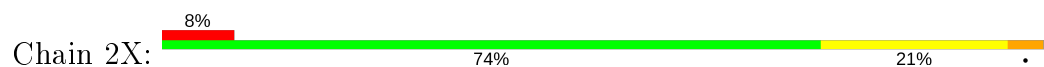
- Molecule 18: 50S ribosomal protein L22



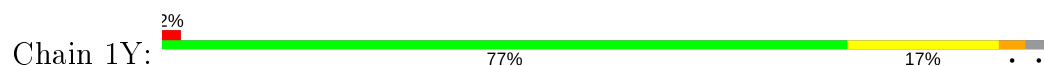
- Molecule 19: 50S ribosomal protein L23



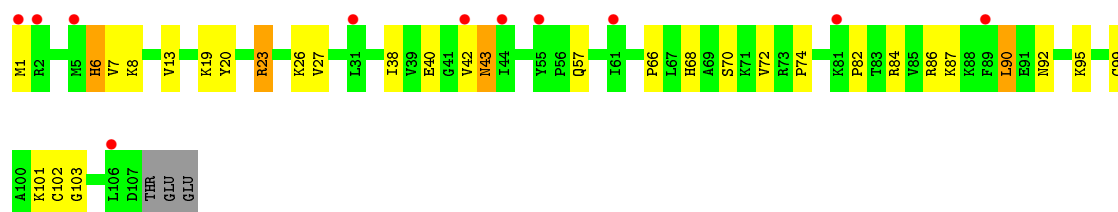
- Molecule 19: 50S ribosomal protein L23



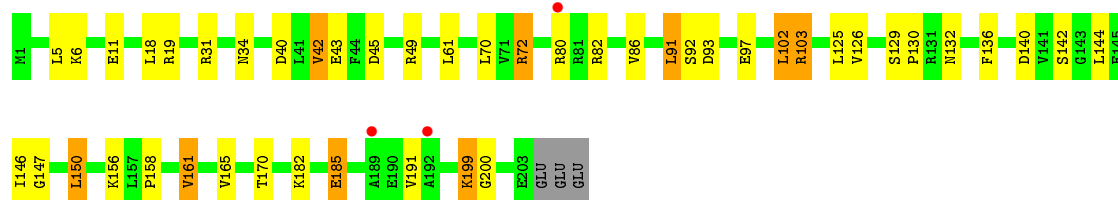
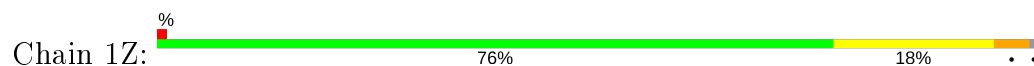
- Molecule 20: 50S ribosomal protein L24



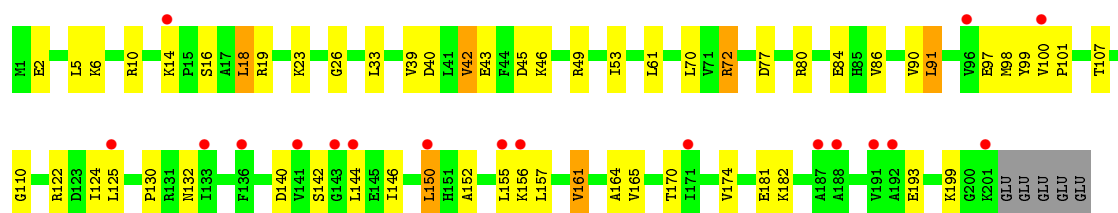
- Molecule 20: 50S ribosomal protein L24



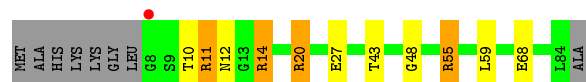
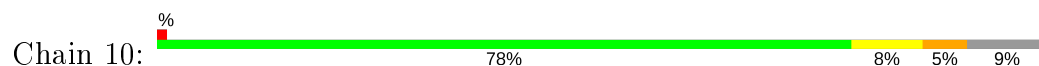
- Molecule 21: 50S ribosomal protein L25



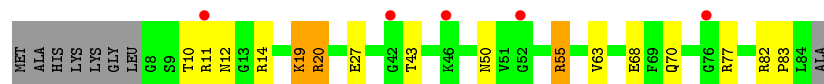
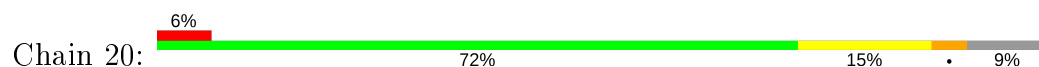
- Molecule 21: 50S ribosomal protein L25



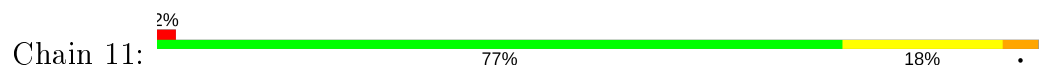
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28

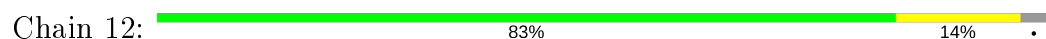




- Molecule 23: 50S ribosomal protein L28



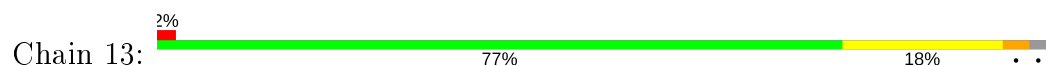
- Molecule 24: 50S ribosomal protein L29



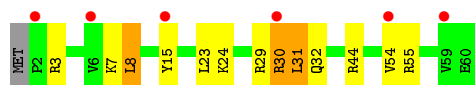
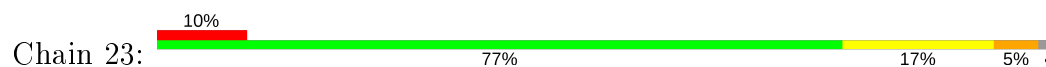
- Molecule 24: 50S ribosomal protein L29



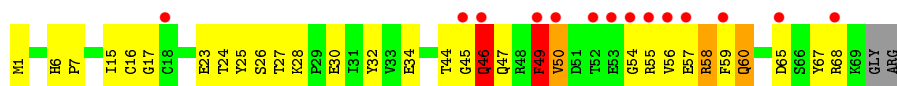
- Molecule 25: 50S ribosomal protein L30



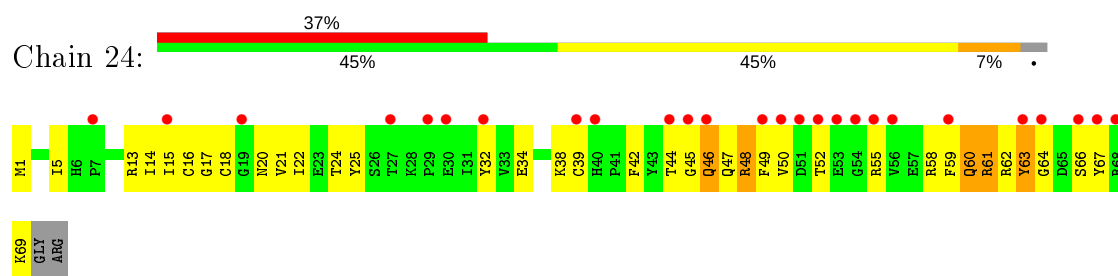
- Molecule 25: 50S ribosomal protein L30



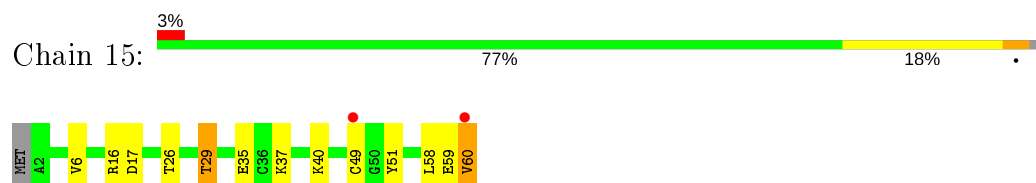
- Molecule 26: 50S ribosomal protein L31



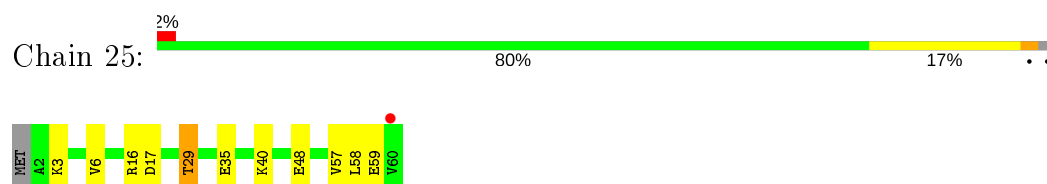
- Molecule 26: 50S ribosomal protein L31



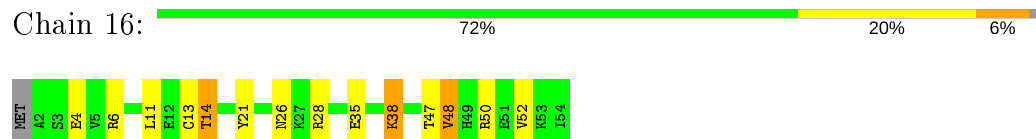
- Molecule 27: 50S ribosomal protein L32



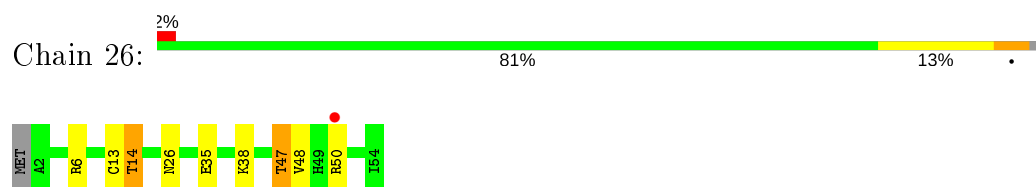
- Molecule 27: 50S ribosomal protein L32



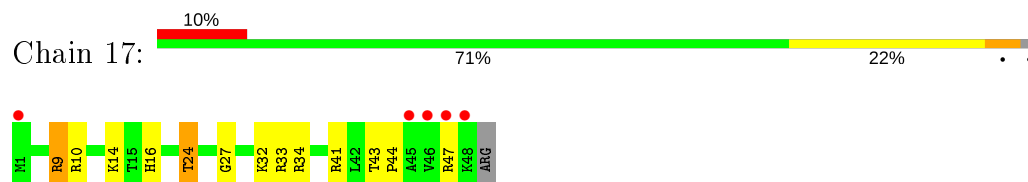
- Molecule 28: 50S ribosomal protein L33



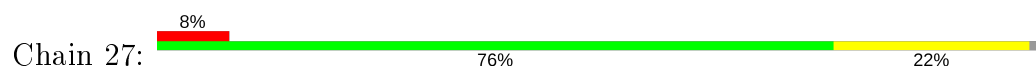
- Molecule 28: 50S ribosomal protein L33

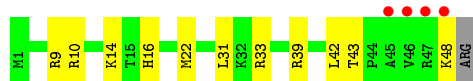


- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34





- Molecule 30: 50S ribosomal protein L35

Chain 18: 69% 28% ..



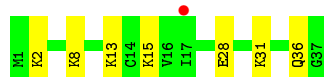
- Molecule 30: 50S ribosomal protein L35

Chain 28: 74% 25% .



- Molecule 31: 50S ribosomal protein L36

Chain 19: 3% 81% 19%



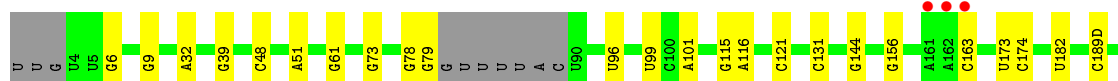
- Molecule 31: 50S ribosomal protein L36

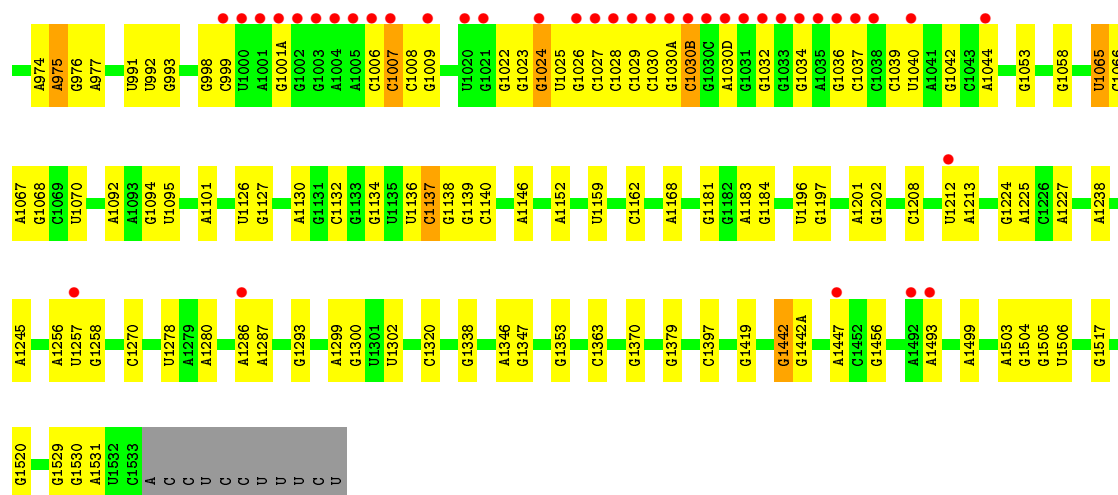
Chain 29: 5% 78% 22%



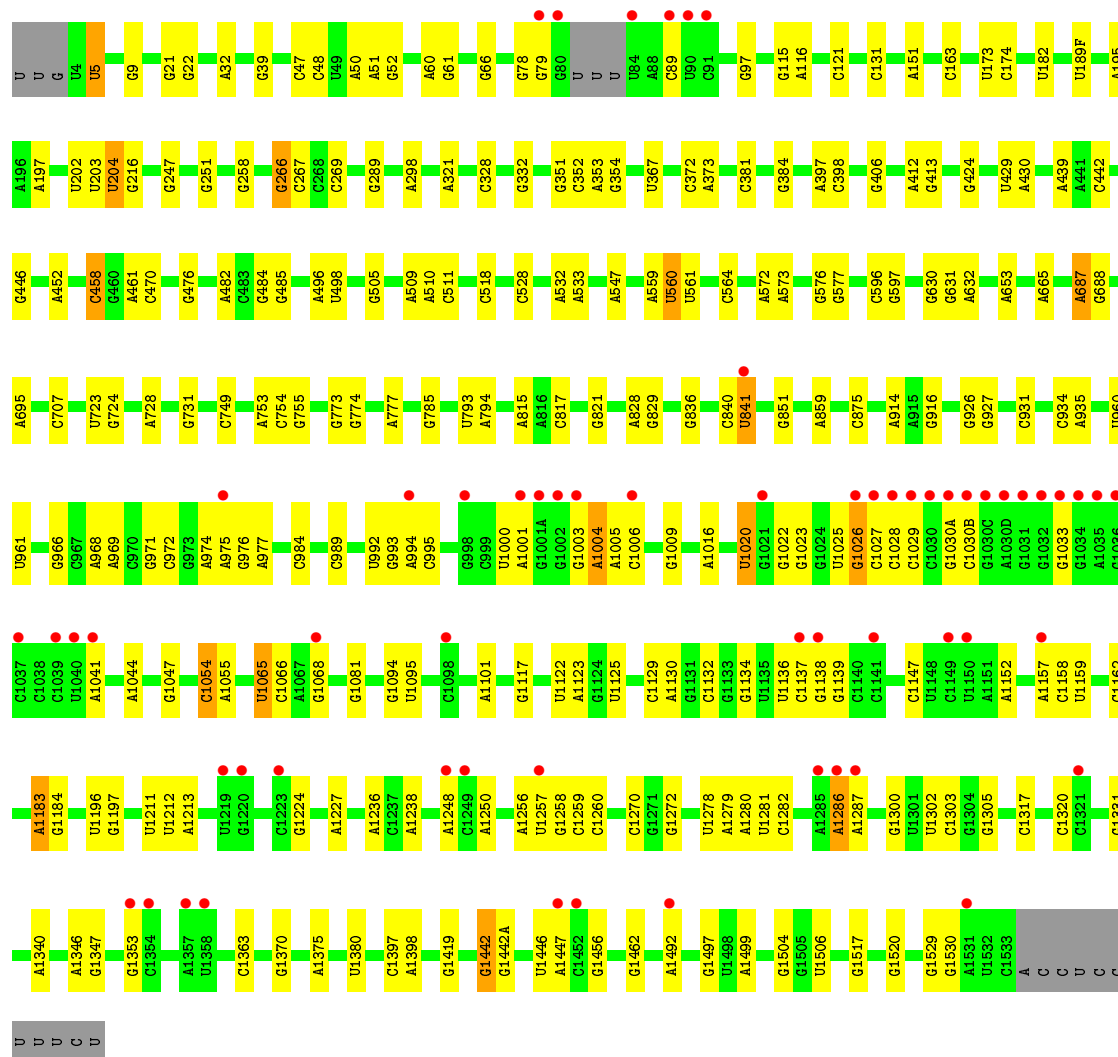
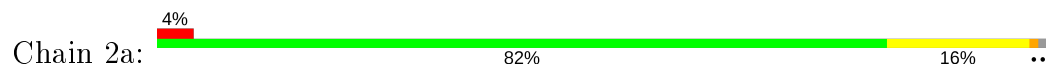
- Molecule 32: 16S Ribosomal RNA

Chain 1a: 3% 83% 15% ..

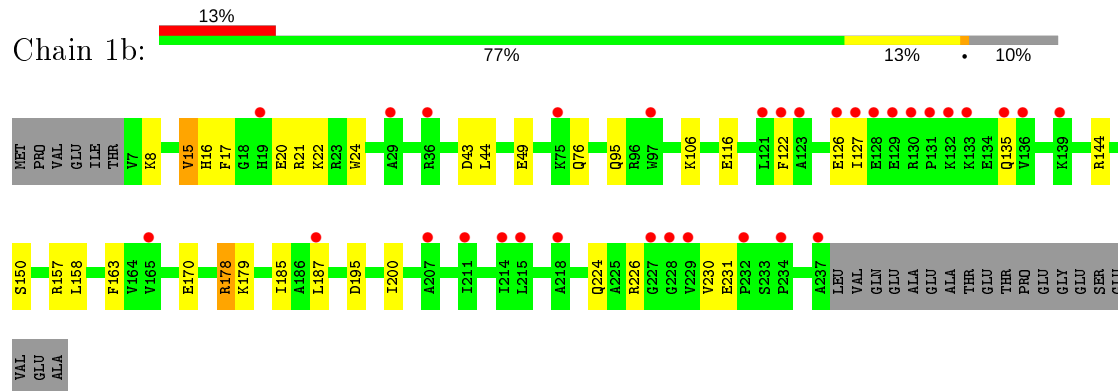




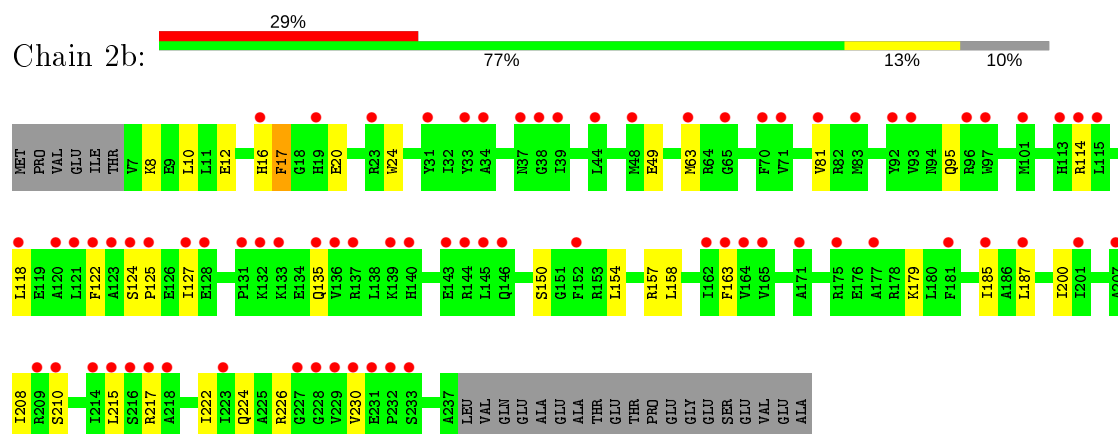
• Molecule 32: 16S Ribosomal RNA



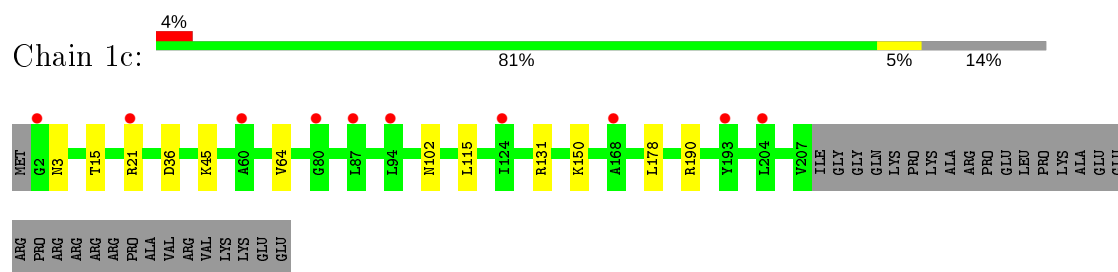
- Molecule 33: 30S ribosomal protein S2



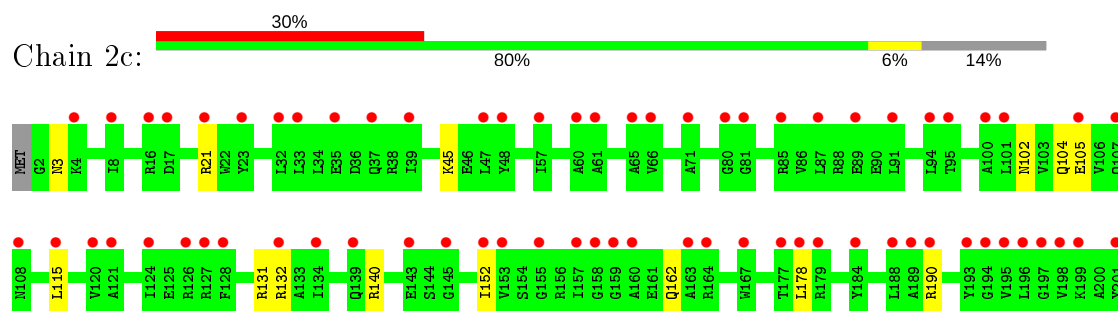
- Molecule 33: 30S ribosomal protein S2

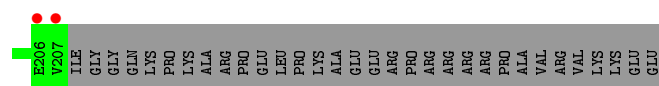


- Molecule 34: 30S ribosomal protein S3

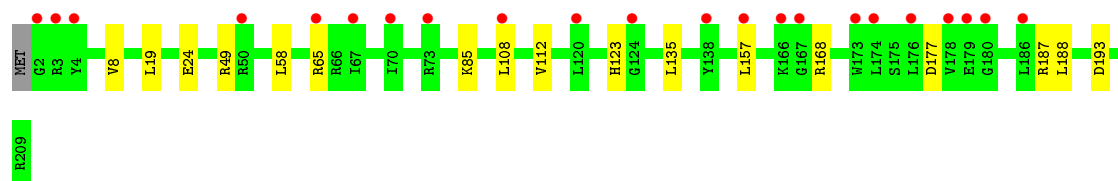
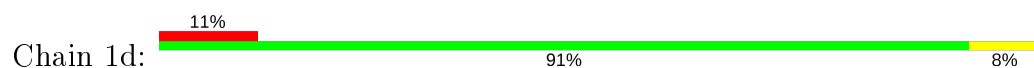


- Molecule 34: 30S ribosomal protein S3

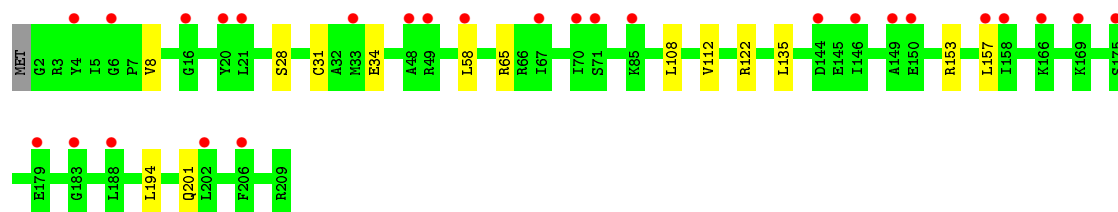




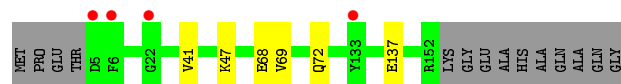
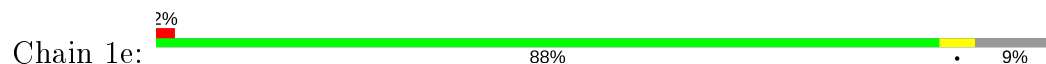
- Molecule 35: 30S ribosomal protein S4



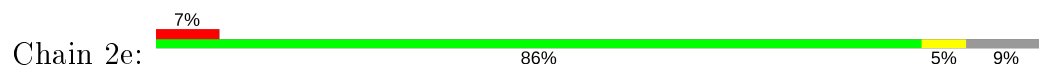
- Molecule 35: 30S ribosomal protein S4



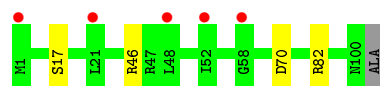
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5

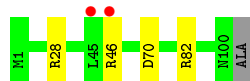


- Molecule 37: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S6

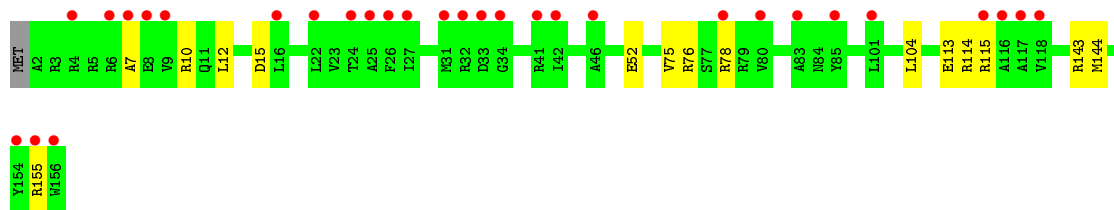
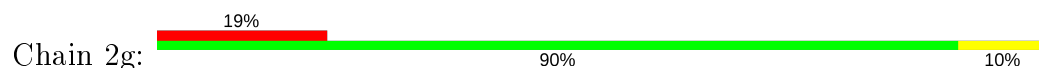




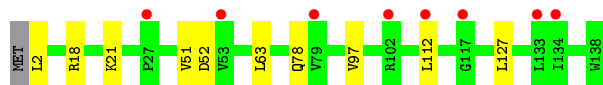
- Molecule 38: 30S ribosomal protein S7



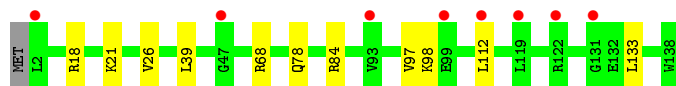
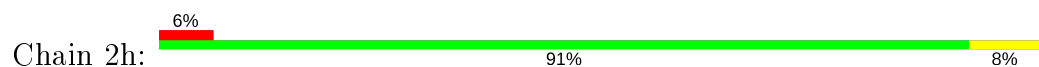
- Molecule 38: 30S ribosomal protein S7



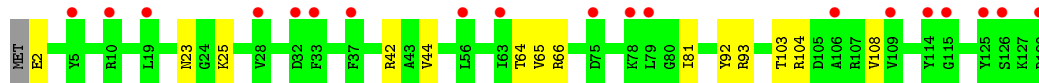
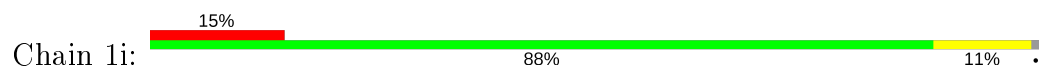
- Molecule 39: 30S ribosomal protein S8



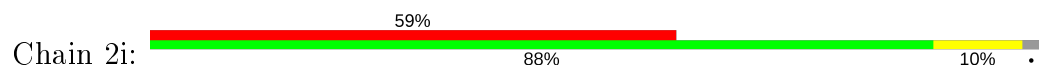
- Molecule 39: 30S ribosomal protein S8

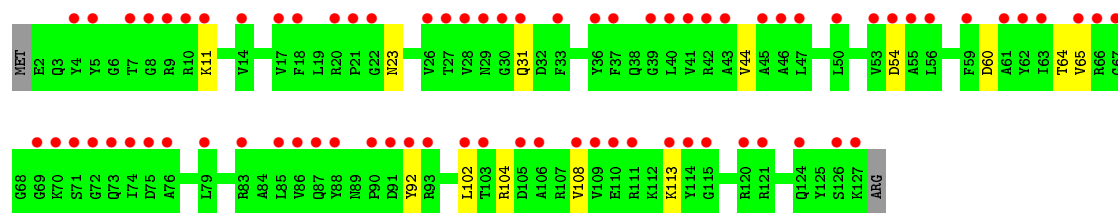


- Molecule 40: 30S ribosomal protein S9

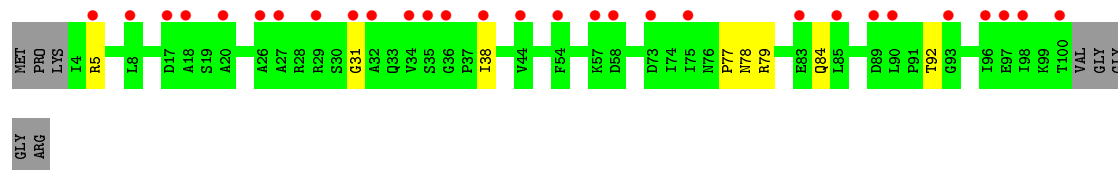
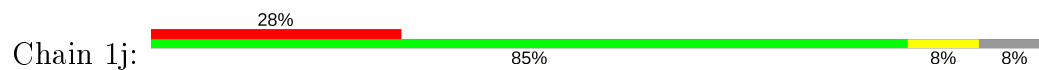


- Molecule 40: 30S ribosomal protein S9

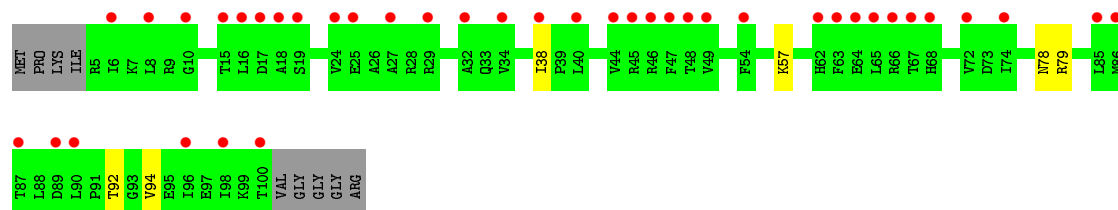
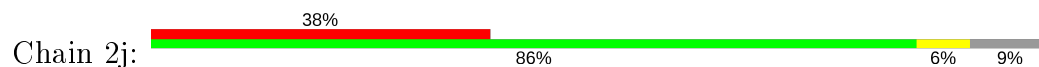




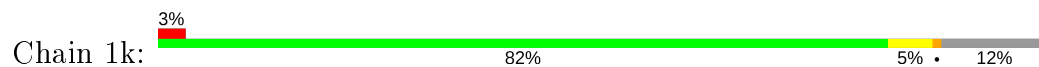
• Molecule 41: 30S ribosomal protein S10



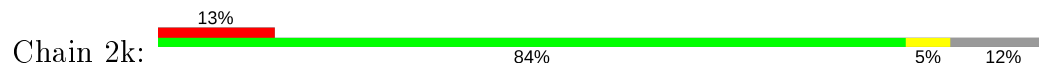
• Molecule 41: 30S ribosomal protein S10



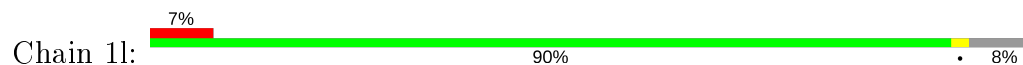
• Molecule 42: 30S ribosomal protein S11



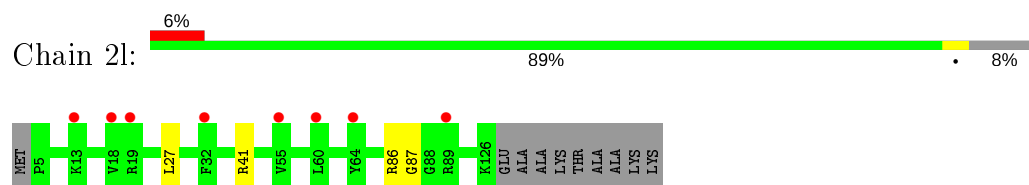
• Molecule 42: 30S ribosomal protein S11



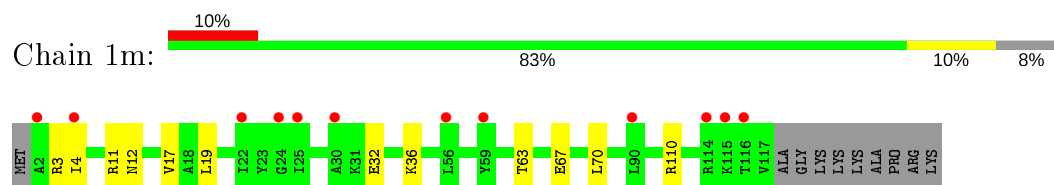
• Molecule 43: 30S ribosomal protein S12



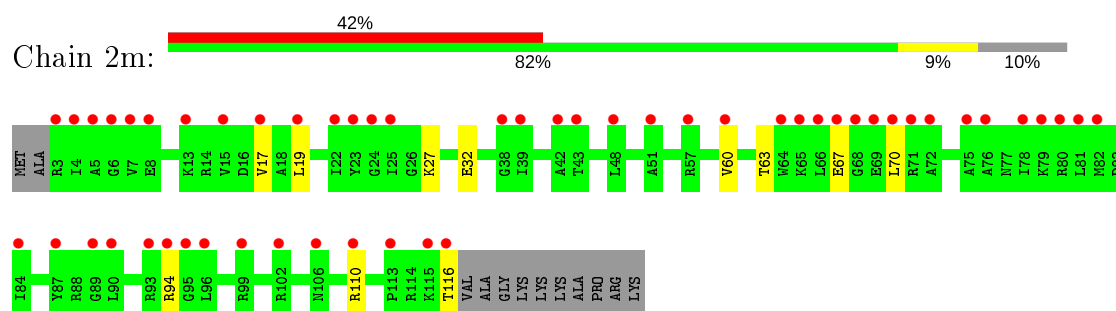
- Molecule 43: 30S ribosomal protein S12



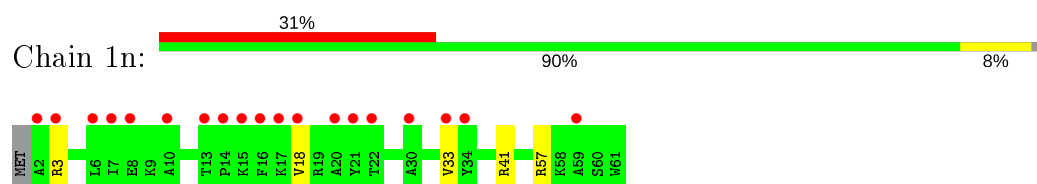
- Molecule 44: 30S ribosomal protein S13



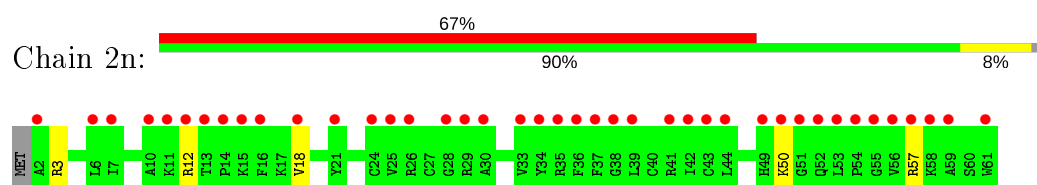
- Molecule 44: 30S ribosomal protein S13



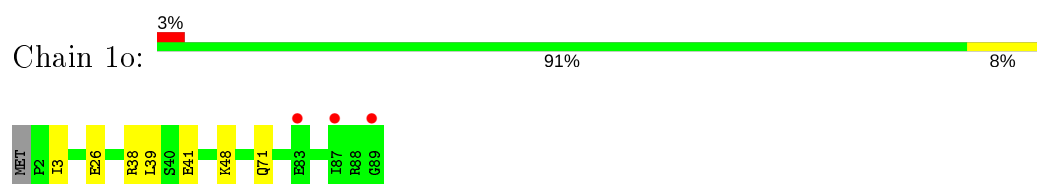
- Molecule 45: 30S ribosomal protein S14 type Z



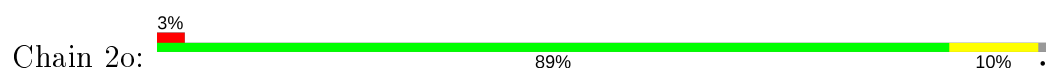
- Molecule 45: 30S ribosomal protein S14 type Z



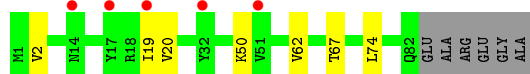
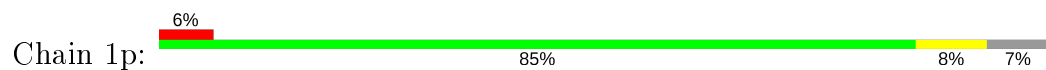
- Molecule 46: 30S ribosomal protein S15



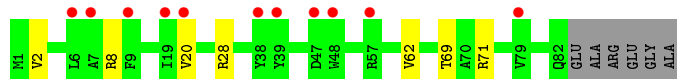
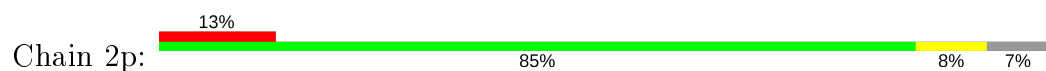
- Molecule 46: 30S ribosomal protein S15



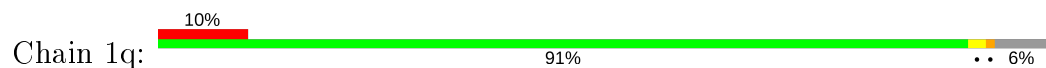
- Molecule 47: 30S ribosomal protein S16



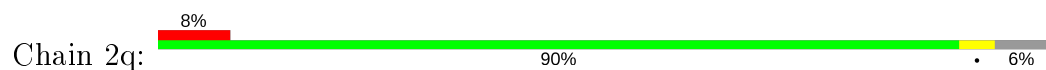
- Molecule 47: 30S ribosomal protein S16



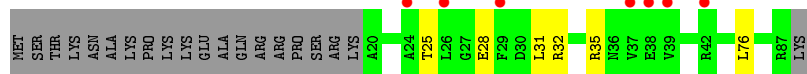
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



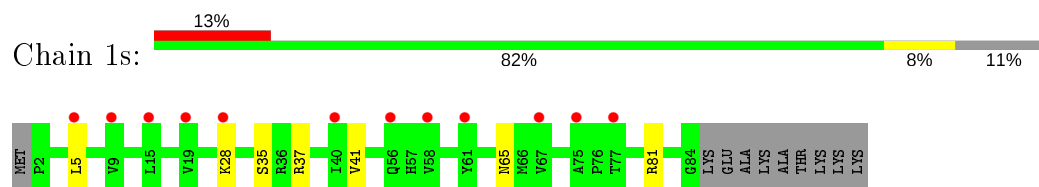
- Molecule 49: 30S ribosomal protein S18



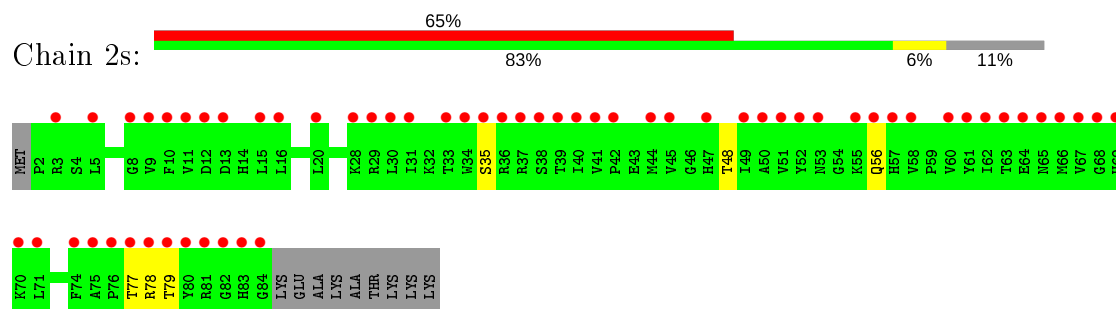
- Molecule 49: 30S ribosomal protein S18



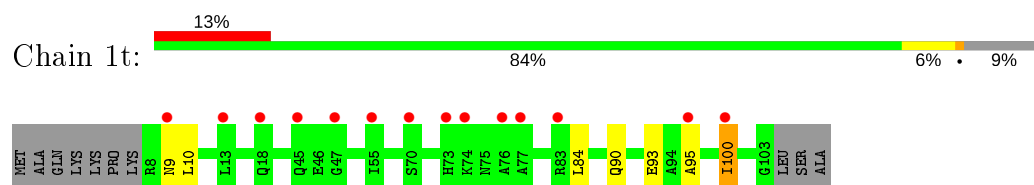
- Molecule 50: 30S ribosomal protein S19



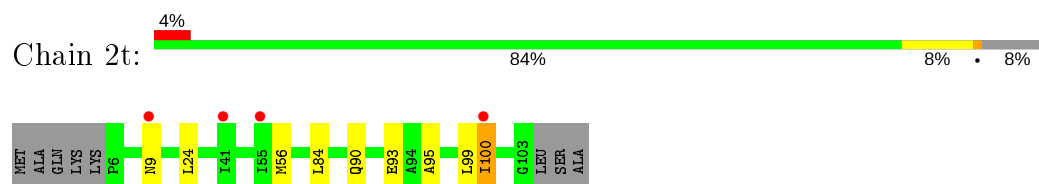
- Molecule 50: 30S ribosomal protein S19



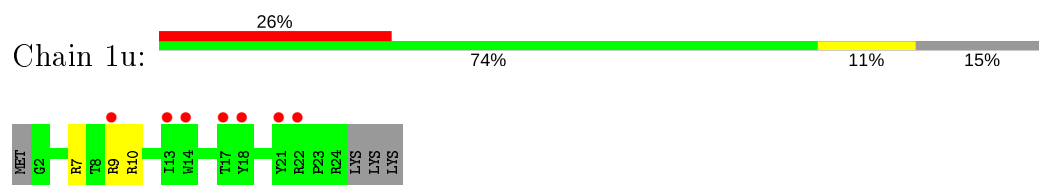
- Molecule 51: 30S ribosomal protein S20



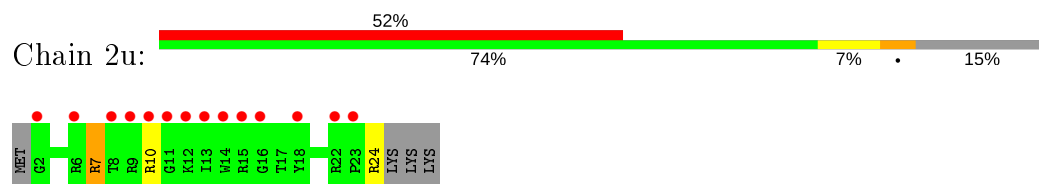
- Molecule 51: 30S ribosomal protein S20



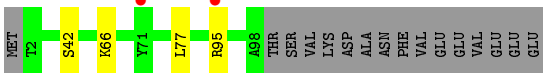
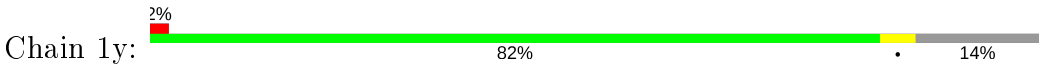
- Molecule 52: 30S ribosomal protein Thx



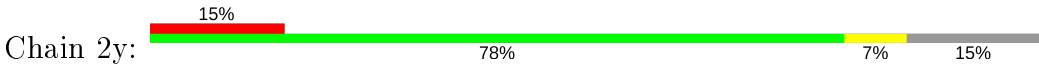
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



● Molecule 53: Ribosome-associated inhibitor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.16Å 448.37Å 618.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	173.22 – 2.30 309.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (173.22-2.30) 97.5 (309.06-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.207 , 0.247 0.207 , 0.247	Depositor DCC
R_{free} test set	123763 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	298502	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MPD, OMG, MA6, ZN, SF4, 0TD, MG, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, M2G, 7MG, 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	0.70	4/69029 (0.0%)	1.14	238/107746 (0.2%)
1	2A	0.58	5/68901 (0.0%)	1.09	188/107544 (0.2%)
2	1B	0.54	0/2876	0.98	2/4486 (0.0%)
2	2B	0.58	0/2878	0.99	2/4490 (0.0%)
3	1D	0.47	0/2181	0.69	1/2940 (0.0%)
3	2D	0.41	0/2186	0.64	0/2944
4	1E	0.48	0/1592	0.64	0/2149
4	2E	0.41	0/1592	0.67	1/2149 (0.0%)
5	1F	0.44	0/1619	0.67	2/2193 (0.1%)
5	2F	0.39	0/1615	0.61	0/2188
6	1G	0.33	0/1451	0.56	0/1961
6	2G	0.38	0/1449	0.54	0/1957
7	1H	0.38	0/1356	0.55	0/1834
7	2H	0.37	0/1350	0.57	1/1826 (0.1%)
8	1I	0.34	0/1109	0.58	0/1512
8	2I	0.32	0/1091	0.59	1/1490 (0.1%)
9	1N	0.44	0/1148	0.64	1/1547 (0.1%)
9	2N	0.33	0/1144	0.55	0/1543
10	1O	0.47	0/943	0.66	1/1269 (0.1%)
10	2O	0.38	0/943	0.61	1/1269 (0.1%)
11	1P	0.47	0/1152	0.70	0/1533
11	2P	0.37	0/1152	0.59	1/1533 (0.1%)
12	1Q	0.48	0/1143	0.63	0/1527
12	2Q	0.41	0/1143	0.59	1/1527 (0.1%)
13	1R	0.47	0/982	0.68	0/1312
13	2R	0.39	0/982	0.63	0/1312
14	1S	0.40	0/887	0.59	0/1180
14	2S	0.40	0/880	0.61	0/1172
15	1T	0.43	0/1105	0.65	0/1477
15	2T	0.39	0/1097	0.61	0/1468
16	1U	0.47	0/977	0.66	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.42	0/977	0.62	0/1301
17	1V	0.44	0/786	0.61	0/1053
17	2V	0.42	0/782	0.62	0/1049
18	1W	0.48	0/897	0.65	1/1205 (0.1%)
18	2W	0.45	0/897	0.59	0/1205
19	1X	0.49	0/764	0.65	1/1025 (0.1%)
19	2X	0.44	0/764	0.62	1/1025 (0.1%)
20	1Y	0.43	0/823	0.65	0/1099
20	2Y	0.38	0/823	0.59	0/1100
21	1Z	0.36	0/1620	0.54	0/2200
21	2Z	0.37	0/1590	0.56	0/2162
22	10	0.48	0/616	0.67	1/821 (0.1%)
22	20	0.35	0/616	0.54	0/821
23	11	0.41	0/761	0.60	0/1013
23	21	0.40	0/766	0.59	0/1018
24	12	0.38	0/590	0.54	0/781
24	22	0.40	0/594	0.50	0/785
25	13	0.45	0/474	0.62	0/635
25	23	0.36	0/469	0.61	0/630
26	14	0.40	0/559	0.71	0/754
26	24	0.44	0/549	0.67	0/741
27	15	0.46	0/473	0.67	0/639
27	25	0.38	0/469	0.57	0/635
28	16	0.43	0/460	0.55	0/613
28	26	0.40	0/456	0.53	0/608
29	17	0.49	0/426	0.76	1/561 (0.2%)
29	27	0.42	0/426	0.66	0/561
30	18	0.47	0/525	0.65	1/691 (0.1%)
30	28	0.42	0/525	0.65	0/691
31	19	0.44	0/310	0.58	0/407
31	29	0.37	0/310	0.54	0/407
32	1a	0.46	0/35795	0.95	28/55864 (0.1%)
32	2a	0.43	0/35890	0.92	43/56012 (0.1%)
33	1b	0.35	0/1876	0.61	1/2533 (0.0%)
33	2b	0.37	0/1860	0.59	0/2518
34	1c	0.33	0/1582	0.53	0/2137
34	2c	0.36	0/1566	0.54	0/2119
35	1d	0.35	0/1695	0.55	0/2274
35	2d	0.33	0/1698	0.52	0/2277
36	1e	0.34	0/1149	0.57	0/1548
36	2e	0.35	0/1149	0.55	0/1548
37	1f	0.37	0/827	0.57	0/1120
37	2f	0.35	0/829	0.55	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.31	0/1254	0.48	0/1683
38	2g	0.33	0/1248	0.51	0/1676
39	1h	0.31	0/1118	0.53	0/1506
39	2h	0.30	0/1108	0.54	0/1494
40	1i	0.32	0/1005	0.56	0/1351
40	2i	0.37	0/985	0.57	0/1329
41	1j	0.31	0/732	0.57	0/993
41	2j	0.33	0/723	0.55	0/984
42	1k	0.34	0/849	0.54	0/1150
42	2k	0.34	0/848	0.58	0/1149
43	1l	0.35	0/937	0.54	0/1260
43	2l	0.35	0/937	0.62	1/1260 (0.1%)
44	1m	0.33	0/924	0.57	0/1242
44	2m	0.31	0/905	0.57	0/1217
45	1n	0.36	0/501	0.48	0/664
45	2n	0.35	0/501	0.50	0/664
46	1o	0.33	0/739	0.55	0/985
46	2o	0.32	0/739	0.53	0/985
47	1p	0.32	0/697	0.59	0/939
47	2p	0.34	0/693	0.55	0/935
48	1q	0.34	0/836	0.54	0/1117
48	2q	0.35	0/836	0.54	0/1117
49	1r	0.33	0/560	0.59	0/746
49	2r	0.34	0/560	0.53	0/746
50	1s	0.30	0/663	0.57	0/895
50	2s	0.35	0/660	0.56	0/893
51	1t	0.34	0/734	0.56	0/969
51	2t	0.30	0/736	0.49	0/976
52	1u	0.30	0/203	0.47	0/266
52	2u	0.35	0/203	0.54	0/266
53	1y	0.35	0/776	0.53	0/1048
53	2y	0.31	0/761	0.48	0/1030
All	All	0.53	9/309937 (0.0%)	0.95	520/463223 (0.1%)

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
14	1S	0	1
19	1X	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	2X	0	1
33	1b	0	1
43	2l	0	1
All	All	0	5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	354	A	N9-C4	-7.97	1.33	1.37
1	2A	2104	G	N1-C2	-7.56	1.31	1.37
1	1A	2261	U	C4-O4	-6.50	1.18	1.23
1	2A	1086	A	N9-C4	6.07	1.41	1.37
1	2A	2104	G	C6-N1	-5.82	1.35	1.39

The worst 5 of 520 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2185	C	N1-C2-O2	19.49	130.60	118.90
1	2A	1079	C	N1-C2-O2	17.91	129.65	118.90
1	2A	2104	G	C5-C6-O6	17.73	139.24	128.60
1	2A	2104	G	N3-C2-N2	17.60	132.22	119.90
1	1A	991	G	O5'-P-OP1	-15.11	92.10	105.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	1S	58	LEU	Peptide
19	1X	93	GLU	Peptide
33	1b	231	GLU	Peptide
19	2X	93	GLU	Peptide
43	2l	86	ARG	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	31203	548	0
1	2A	61758	0	31151	788	0
2	1B	2572	0	1305	25	0
2	2B	2573	0	1306	36	0
3	1D	2131	0	2207	42	0
3	2D	2136	0	2218	50	0
4	1E	1559	0	1618	37	0
4	2E	1559	0	1618	42	0
5	1F	1584	0	1625	40	0
5	2F	1580	0	1619	38	0
6	1G	1426	0	1445	40	0
6	2G	1424	0	1441	58	0
7	1H	1330	0	1407	19	0
7	2H	1324	0	1402	38	0
8	1I	1094	0	1127	26	0
8	2I	1076	0	1094	21	0
9	1N	1121	0	1195	13	0
9	2N	1117	0	1184	17	0
10	1O	933	0	996	15	0
10	2O	933	0	996	15	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	30	0
12	1Q	1122	0	1179	22	0
12	2Q	1122	0	1179	22	0
13	1R	968	0	1033	21	0
13	2R	968	0	1033	20	0
14	1S	877	0	938	20	0
14	2S	870	0	923	29	0
15	1T	1091	0	1151	35	0
15	2T	1083	0	1136	23	0
16	1U	959	0	1019	22	0
16	2U	959	0	1019	21	0
17	1V	775	0	841	13	0
17	2V	771	0	830	23	0
18	1W	886	0	940	14	0
18	2W	886	0	940	15	0
19	1X	750	0	814	16	0
19	2X	750	0	814	16	0
20	1Y	810	0	892	18	0
20	2Y	810	0	887	23	0
21	1Z	1587	0	1598	22	0
21	2Z	1557	0	1564	32	0
22	10	608	0	622	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	608	0	622	11	0
23	11	754	0	823	13	0
23	21	759	0	837	22	0
24	12	588	0	643	4	0
24	22	592	0	654	12	0
25	13	469	0	518	7	0
25	23	464	0	514	6	0
26	14	546	0	522	19	0
26	24	536	0	514	30	0
27	15	459	0	476	7	0
27	25	455	0	465	6	0
28	16	453	0	473	8	0
28	26	449	0	469	4	0
29	17	418	0	467	14	0
29	27	418	0	467	9	0
30	18	517	0	582	21	0
30	28	517	0	582	19	0
31	19	307	0	335	5	0
31	29	307	0	335	5	0
32	1a	32246	0	16296	0	0
32	2a	32331	0	16339	0	0
33	1b	1842	0	1862	0	0
33	2b	1825	0	1828	0	0
34	1c	1558	0	1557	0	0
34	2c	1542	0	1517	0	0
35	1d	1665	0	1687	0	0
35	2d	1668	0	1703	0	0
36	1e	1133	0	1191	0	0
36	2e	1133	0	1191	0	0
37	1f	814	0	808	0	0
37	2f	816	0	808	0	0
38	1g	1235	0	1249	0	0
38	2g	1229	0	1238	0	0
39	1h	1098	0	1143	0	0
39	2h	1088	0	1126	0	0
40	1i	986	0	990	0	0
40	2i	966	0	953	0	0
41	1j	719	0	672	0	0
41	2j	710	0	661	0	0
42	1k	834	0	838	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	0	0
44	1m	914	0	954	0	0
44	2m	895	0	920	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	648	0	658	0	0
50	2s	645	0	635	0	0
51	1t	732	0	809	0	0
51	2t	733	0	795	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1y	764	0	786	0	0
53	2y	749	0	757	0	0
54	10	5	0	0	0	0
54	11	4	0	0	0	0
54	13	2	0	0	0	0
54	14	1	0	0	0	0
54	15	2	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	1075	0	0	0	0
54	1B	30	0	0	0	0
54	1D	14	0	0	0	0
54	1E	6	0	0	0	0
54	1F	10	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	3	0	0	0	0
54	1O	1	0	0	0	0
54	1P	2	0	0	0	0
54	1Q	4	0	0	0	0
54	1R	3	0	0	0	0
54	1T	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1U	2	0	0	0	0
54	1V	3	0	0	0	0
54	1W	2	0	0	0	0
54	1X	1	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	280	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	4	0	0	0	0
54	1f	1	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	2	0	0	0	0
54	1o	1	0	0	0	0
54	1q	2	0	0	0	0
54	1r	1	0	0	0	0
54	1t	1	0	0	0	0
54	1y	4	0	0	0	0
54	20	2	0	0	0	0
54	21	1	0	0	0	0
54	26	1	0	0	0	0
54	27	1	0	0	0	0
54	28	2	0	0	0	0
54	2A	761	0	0	0	0
54	2B	19	0	0	0	0
54	2D	9	0	0	0	0
54	2E	5	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	2	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	3	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	193	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2e	1	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2l	1	0	0	0	0
54	2r	1	0	0	0	0
54	2t	1	0	0	0	0
55	18	8	0	14	5	0
55	1A	8	0	14	1	0
55	1T	8	0	14	0	0
55	1a	8	0	14	0	0
55	2A	16	0	28	2	0
55	2B	8	0	14	0	0
56	1B	12	0	12	1	0
56	1F	12	0	12	3	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0
58	2d	8	0	0	0	0
59	10	25	0	0	0	0
59	11	25	0	0	0	0
59	12	15	0	0	0	0
59	13	25	0	0	0	0
59	14	4	0	0	0	0
59	15	25	0	0	0	0
59	16	22	0	0	0	0
59	17	19	0	0	2	0
59	18	31	0	0	2	0
59	19	9	0	0	1	0
59	1A	4154	0	0	66	0
59	1B	109	0	0	1	0
59	1D	119	0	0	2	0
59	1E	81	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1F	66	0	0	3	0
59	1G	20	0	0	2	0
59	1H	16	0	0	0	0
59	1I	9	0	0	0	0
59	1N	55	0	0	0	0
59	1O	29	0	0	1	0
59	1P	56	0	0	1	0
59	1Q	46	0	0	2	0
59	1R	37	0	0	2	0
59	1S	11	0	0	0	0
59	1T	39	0	0	3	0
59	1U	49	0	0	5	0
59	1V	34	0	0	3	0
59	1W	27	0	0	0	0
59	1X	27	0	0	0	0
59	1Y	20	0	0	2	0
59	1Z	13	0	0	1	0
59	1a	599	0	0	0	0
59	1b	1	0	0	0	0
59	1c	1	0	0	0	0
59	1d	8	0	0	0	0
59	1e	5	0	0	0	0
59	1f	3	0	0	0	0
59	1h	1	0	0	0	0
59	1i	1	0	0	0	0
59	1j	1	0	0	0	0
59	1k	1	0	0	0	0
59	1l	5	0	0	0	0
59	1m	2	0	0	0	0
59	1o	7	0	0	0	0
59	1p	3	0	0	0	0
59	1t	1	0	0	0	0
59	1y	7	0	0	0	0
59	20	13	0	0	0	0
59	21	22	0	0	1	0
59	22	4	0	0	1	0
59	23	3	0	0	0	0
59	24	2	0	0	2	0
59	25	10	0	0	0	0
59	26	5	0	0	0	0
59	27	9	0	0	1	0
59	28	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	29	3	0	0	0	0
59	2A	2665	0	0	78	0
59	2B	69	0	0	8	0
59	2D	59	0	0	0	0
59	2E	33	0	0	2	0
59	2F	26	0	0	0	0
59	2G	9	0	0	0	0
59	2H	4	0	0	0	0
59	2I	4	0	0	1	0
59	2N	6	0	0	0	0
59	2O	23	0	0	3	0
59	2P	30	0	0	1	0
59	2Q	28	0	0	1	0
59	2R	21	0	0	1	0
59	2S	7	0	0	1	0
59	2T	11	0	0	0	0
59	2U	20	0	0	1	0
59	2V	6	0	0	0	0
59	2W	20	0	0	1	0
59	2X	10	0	0	0	0
59	2Y	4	0	0	0	0
59	2Z	16	0	0	2	0
59	2a	459	0	0	0	0
59	2d	6	0	0	0	0
59	2e	2	0	0	0	0
59	2f	1	0	0	0	0
59	2j	2	0	0	0	0
59	2l	5	0	0	0	0
59	2m	2	0	0	0	0
59	2o	2	0	0	0	0
59	2p	3	0	0	0	0
59	2q	1	0	0	0	0
59	2r	5	0	0	0	0
59	2t	2	0	0	0	0
59	2y	5	0	0	0	0
All	All	298502	0	194517	2295	0

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

The worst 5 of 2295 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	1.32	1.27
1:2A:2128:C:N4	1:2A:2160:G:H1	1.46	1.11
1:2A:2602:A:H1'	1:2A:2603:G:H5''	1.36	1.08
1:1A:1128:U:O4	1:1A:1132:A:N1	1.98	0.96
26:24:59:PHE:HA	26:24:61:ARG:N	1.80	0.95

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	35
4	2E	202/206 (98%)	196 (97%)	6 (3%)	0	100	100
5	1F	201/210 (96%)	197 (98%)	4 (2%)	0	100	100
5	2F	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	15	17
6	1G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	25	31
6	2G	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	25	31
7	1H	172/180 (96%)	167 (97%)	5 (3%)	0	100	100
7	2H	171/180 (95%)	165 (96%)	6 (4%)	0	100	100
8	1I	145/148 (98%)	133 (92%)	11 (8%)	1 (1%)	22	26
8	2I	144/148 (97%)	135 (94%)	9 (6%)	0	100	100
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	2N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
11	2P	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	22	26
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	20
14	2S	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	1T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
15	2T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
17	2V	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
19	2X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
20	1Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	2Y	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
21	1Z	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
21	2Z	199/206 (97%)	194 (98%)	5 (2%)	0	100	100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	20	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	14	15
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	15
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	56 (84%)	5 (8%)	6 (9%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	4	2
33	2b	229/256 (90%)	205 (90%)	19 (8%)	5 (2%)	6	5
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	187 (92%)	17 (8%)	0	100	100
35	1d	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
35	2d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
36	1e	146/162 (90%)	144 (99%)	2 (1%)	0	100	100
36	2e	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
38	2g	153/156 (98%)	148 (97%)	4 (3%)	1 (1%)	22	26
39	1h	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	115 (92%)	9 (7%)	1 (1%)	19	23
40	2i	124/128 (97%)	113 (91%)	8 (6%)	3 (2%)	6	4
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	1
41	2j	94/105 (90%)	85 (90%)	7 (7%)	2 (2%)	7	5
42	1k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8	7
42	2k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
43	2l	119/132 (90%)	116 (98%)	3 (2%)	0	100	100
44	1m	114/126 (90%)	105 (92%)	7 (6%)	2 (2%)	8	7
44	2m	112/126 (89%)	105 (94%)	6 (5%)	1 (1%)	17	20
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	1p	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
47	2p	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
48	1q	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	15	17
48	2q	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
50	2s	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
51	1t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	5
51	2t	96/106 (91%)	88 (92%)	6 (6%)	2 (2%)	7	5
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	1
53	1y	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
53	2y	94/113 (83%)	89 (95%)	4 (4%)	1 (1%)	14	15
All	All	11629/12354 (94%)	11139 (96%)	435 (4%)	55 (0%)	29	35

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	14	49	PHE
33	1b	16	HIS
33	1b	17	PHE
33	1b	22	LYS
51	1t	95	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	199 (93%)	15 (7%)	15	19
3	2D	215/218 (99%)	201 (94%)	14 (6%)	17	23
4	1E	164/166 (99%)	148 (90%)	16 (10%)	8	9
4	2E	164/166 (99%)	146 (89%)	18 (11%)	6	7
5	1F	160/166 (96%)	142 (89%)	18 (11%)	6	6
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	10
6	1G	144/156 (92%)	128 (89%)	16 (11%)	6	7
6	2G	142/156 (91%)	122 (86%)	20 (14%)	3	3
7	1H	144/148 (97%)	136 (94%)	8 (6%)	21	29
7	2H	143/148 (97%)	129 (90%)	14 (10%)	8	9
8	1I	111/124 (90%)	92 (83%)	19 (17%)	2	2
8	2I	108/124 (87%)	95 (88%)	13 (12%)	5	5
9	1N	119/119 (100%)	107 (90%)	12 (10%)	7	9
9	2N	118/119 (99%)	107 (91%)	11 (9%)	9	10
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	57
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	57
11	1P	115/116 (99%)	105 (91%)	10 (9%)	10	12
11	2P	115/116 (99%)	106 (92%)	9 (8%)	12	16
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	8	9
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9	11
13	1R	101/101 (100%)	87 (86%)	14 (14%)	3	3
13	2R	101/101 (100%)	88 (87%)	13 (13%)	4	4
14	1S	87/88 (99%)	77 (88%)	10 (12%)	5	6
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	5
15	1T	115/127 (91%)	106 (92%)	9 (8%)	12	16
15	2T	113/127 (89%)	106 (94%)	7 (6%)	18	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	83 (89%)	10 (11%)	6	7
16	2U	93/94 (99%)	86 (92%)	7 (8%)	13	17
17	1V	81/82 (99%)	73 (90%)	8 (10%)	8	9
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	9
18	1W	90/92 (98%)	79 (88%)	11 (12%)	5	5
18	2W	90/92 (98%)	81 (90%)	9 (10%)	7	9
19	1X	77/78 (99%)	73 (95%)	4 (5%)	23	32
19	2X	77/78 (99%)	72 (94%)	5 (6%)	17	23
20	1Y	86/91 (94%)	82 (95%)	4 (5%)	26	37
20	2Y	86/91 (94%)	78 (91%)	8 (9%)	9	10
21	1Z	169/179 (94%)	148 (88%)	21 (12%)	4	5
21	2Z	165/179 (92%)	147 (89%)	18 (11%)	6	7
22	10	61/67 (91%)	57 (93%)	4 (7%)	16	22
22	20	61/67 (91%)	57 (93%)	4 (7%)	16	22
23	11	79/83 (95%)	70 (89%)	9 (11%)	5	6
23	21	81/83 (98%)	74 (91%)	7 (9%)	10	12
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	38
24	22	66/67 (98%)	61 (92%)	5 (8%)	13	16
25	13	51/52 (98%)	47 (92%)	4 (8%)	12	16
25	23	50/52 (96%)	42 (84%)	8 (16%)	2	2
26	14	58/63 (92%)	49 (84%)	9 (16%)	2	2
26	24	54/63 (86%)	43 (80%)	11 (20%)	1	1
27	15	51/52 (98%)	44 (86%)	7 (14%)	3	3
27	25	50/52 (96%)	43 (86%)	7 (14%)	3	3
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	5
28	26	50/52 (96%)	47 (94%)	3 (6%)	19	26
29	17	41/42 (98%)	39 (95%)	2 (5%)	25	35
29	27	41/42 (98%)	40 (98%)	1 (2%)	49	66
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	29
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	17
31	19	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	191/220 (87%)	163 (85%)	28 (15%)	3	3
33	2b	187/220 (85%)	156 (83%)	31 (17%)	2	2
34	1c	144/188 (77%)	132 (92%)	12 (8%)	11	14
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7	9
35	1d	171/181 (94%)	154 (90%)	17 (10%)	8	9
35	2d	172/181 (95%)	158 (92%)	14 (8%)	11	15
36	1e	114/123 (93%)	108 (95%)	6 (5%)	22	31
36	2e	114/123 (93%)	106 (93%)	8 (7%)	15	19
37	1f	85/90 (94%)	81 (95%)	4 (5%)	26	37
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	37
38	1g	120/127 (94%)	112 (93%)	8 (7%)	16	21
38	2g	119/127 (94%)	105 (88%)	14 (12%)	5	5
39	1h	116/119 (98%)	106 (91%)	10 (9%)	10	12
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	10
40	1i	91/99 (92%)	78 (86%)	13 (14%)	3	3
40	2i	88/99 (89%)	78 (89%)	10 (11%)	5	6
41	1j	68/92 (74%)	64 (94%)	4 (6%)	19	27
41	2j	68/92 (74%)	64 (94%)	4 (6%)	19	27
42	1k	83/99 (84%)	76 (92%)	7 (8%)	11	13
42	2k	83/99 (84%)	78 (94%)	5 (6%)	19	26
43	1l	96/108 (89%)	93 (97%)	3 (3%)	40	55
43	2l	96/108 (89%)	94 (98%)	2 (2%)	53	70
44	1m	90/101 (89%)	80 (89%)	10 (11%)	6	7
44	2m	87/101 (86%)	77 (88%)	10 (12%)	5	6
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	8
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	8
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9	11
46	2o	78/80 (98%)	69 (88%)	9 (12%)	5	6
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	9
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	91 (97%)	3 (3%)	39	54
48	2q	94/97 (97%)	90 (96%)	4 (4%)	29	40
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	8
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	8
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7	8
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	11
51	1t	71/82 (87%)	65 (92%)	6 (8%)	10	13
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5	6
52	1u	18/22 (82%)	15 (83%)	3 (17%)	2	2
52	2u	18/22 (82%)	15 (83%)	3 (17%)	2	2
53	1y	82/98 (84%)	78 (95%)	4 (5%)	25	35
53	2y	79/98 (81%)	72 (91%)	7 (9%)	9	11
All	All	9524/10260 (93%)	8644 (91%)	880 (9%)	9	11

5 of 880 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	1o	48	LYS
6	2G	60	LEU
43	2l	27	LEU
48	1q	85	VAL
3	2D	229	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
3	2D	87	ASN
13	2R	91	GLN
48	2q	16	GLN
3	2D	164	GLN
6	2G	26	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	403 (14%)	41 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2A	2855/2915 (97%)	483 (16%)	41 (1%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	119/121 (98%)	14 (11%)	0
32	1a	1494/1521 (98%)	229 (15%)	0
32	2a	1498/1521 (98%)	251 (16%)	0
All	All	8947/9114 (98%)	1390 (15%)	82 (0%)

5 of 1390 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	70	A

5 of 82 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2614	A
1	2A	277	C
1	2A	2406	U
1	1A	2623	U
1	2A	9	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	2a	1519	32	19,26,27	1.07	1 (5%)	18,38,41	1.81	4 (22%)
1	5MC	2A	1962	1,54	15,22,23	1.26	1 (6%)	19,32,35	1.44	3 (15%)
32	M2G	1a	966	32	20,27,28	1.41	3 (15%)	22,40,43	2.18	7 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	2a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.64	6 (33%)
32	5MC	2a	1404	32	15,22,23	1.46	1 (6%)	19,32,35	1.37	4 (21%)
32	7MG	1a	527	32,54	22,26,27	1.70	4 (18%)	28,39,42	2.63	9 (32%)
32	5MC	1a	1407	32	15,22,23	1.48	1 (6%)	19,32,35	1.33	2 (10%)
1	PSU	2A	2605	1	17,21,22	1.53	4 (23%)	20,30,33	3.17	6 (30%)
1	PSU	2A	1911	1	17,21,22	1.59	3 (17%)	20,30,33	3.16	6 (30%)
32	MA6	1a	1518	32	19,26,27	0.96	1 (5%)	18,38,41	1.65	4 (22%)
1	PSU	1A	2617	1	17,21,22	1.69	3 (17%)	20,30,33	3.15	6 (30%)
32	2MG	1a	1207	32,54	19,26,27	1.29	2 (10%)	21,38,41	2.71	11 (52%)
1	2MU	2A	2552	1,54	14,22,24	0.80	0	14,31,36	0.77	0
32	5MC	2a	1407	32	15,22,23	1.32	1 (6%)	19,32,35	1.31	3 (15%)
1	PSU	1A	1939	1	17,21,22	1.52	4 (23%)	20,30,33	3.21	6 (30%)
32	UR3	1a	1498	32	14,22,23	0.76	0	15,32,35	0.69	0
1	5MC	1A	1984	1,54	15,22,23	1.33	1 (6%)	19,32,35	1.32	3 (15%)
1	5MC	2A	1942	1	15,22,23	1.40	1 (6%)	19,32,35	1.40	3 (15%)
43	0TD	1l	92	43	4,9,10	4.44	3 (75%)	3,11,13	5.66	2 (66%)
1	2MA	2A	2503	1,54	17,25,26	1.19	2 (11%)	19,37,40	1.87	3 (15%)
1	PSU	1A	1933	1	17,21,22	1.49	3 (17%)	20,30,33	3.17	7 (35%)
1	2MA	1A	2515	1,54	17,25,26	0.98	1 (5%)	19,37,40	2.00	3 (15%)
43	0TD	2l	92	43	4,9,10	3.21	1 (25%)	3,11,13	2.56	1 (33%)
1	OMG	2A	2251	1,54	18,26,27	1.19	2 (11%)	20,38,41	2.34	7 (35%)
32	5MC	2a	1400	32	15,22,23	1.40	1 (6%)	19,32,35	1.26	3 (15%)
1	4OC	2A	1920	1	15,22,24	0.67	0	17,31,35	1.31	1 (5%)
32	MA6	1a	1519	32	19,26,27	0.99	1 (5%)	18,38,41	1.59	4 (22%)
32	5MC	2a	967	32	15,22,23	1.45	1 (6%)	19,32,35	1.20	2 (10%)
1	5MC	1A	1964	1,54	15,22,23	1.23	1 (6%)	19,32,35	1.38	3 (15%)
32	4OC	1a	1402	32	16,23,24	0.62	0	17,32,35	1.02	1 (5%)
1	4OC	1A	1942	1,54	15,22,24	0.76	0	17,31,35	1.33	2 (11%)
32	UR3	2a	1498	32,54	14,22,23	0.77	0	15,32,35	0.75	1 (6%)
32	7MG	2a	527	32	22,26,27	1.75	4 (18%)	28,39,42	2.69	8 (28%)
1	5MU	1A	1961	1	15,22,23	1.12	1 (6%)	16,32,35	1.66	2 (12%)
1	PSU	2A	1917	1	17,21,22	1.67	2 (11%)	20,30,33	3.14	6 (30%)
32	2MG	2a	1207	32	19,26,27	1.25	2 (10%)	21,38,41	2.32	8 (38%)
32	PSU	2a	516	32,54	17,21,22	1.72	3 (17%)	20,30,33	3.10	7 (35%)
1	OMG	1A	2263	1,54	18,26,27	1.27	2 (11%)	20,38,41	2.28	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	1A	1937	1,54	15,22,23	1.02	1 (6%)	16,32,35	1.98	1 (6%)
1	5MU	2A	1915	1	15,22,23	1.08	1 (6%)	16,32,35	1.98	1 (6%)
1	5MU	2A	1939	1,54	15,22,23	1.07	1 (6%)	16,32,35	1.53	2 (12%)
32	5MC	1a	967	32	15,22,23	1.33	1 (6%)	19,32,35	1.35	3 (15%)
32	PSU	1a	516	32,54	17,21,22	1.41	4 (23%)	20,30,33	3.13	6 (30%)
32	5MC	1a	1404	32	15,22,23	1.34	1 (6%)	19,32,35	1.27	2 (10%)
32	M2G	2a	966	32,54	20,27,28	1.41	3 (15%)	22,40,43	2.39	7 (31%)
32	5MC	1a	1400	32	15,22,23	1.41	1 (6%)	19,32,35	1.57	4 (21%)
1	2MU	1A	2564	1,54	14,22,24	0.82	1 (7%)	14,31,36	0.73	1 (7%)
32	4OC	2a	1402	32	16,23,24	0.66	0	17,32,35	1.26	2 (11%)

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	MA6	2a	1519	32	-	5/7/29/30	0/3/3/3
1	5MC	2A	1962	1,54	-	2/5/25/26	0/2/2/2
32	M2G	1a	966	32	-	1/7/29/30	0/3/3/3
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32,54	-	2/7/37/38	0/3/3/3
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32,54	-	0/5/27/28	0/3/3/3
1	2MU	2A	2552	1,54	-	0/7/27/28	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
1	5MC	1A	1984	1,54	-	2/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
1	2MA	2A	2503	1,54	-	1/3/25/26	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	1,54	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	0TD	2l	92	43	-	3/3/12/14	-
1	OMG	2A	2251	1,54	-	1/5/27/28	0/3/3/3
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
1	5MC	1A	1964	1,54	-	0/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	4OC	1A	1942	1,54	-	1/7/27/30	0/2/2/2
32	UR3	2a	1498	32,54	-	0/5/25/26	0/2/2/2
32	7MG	2a	527	32	-	0/7/37/38	0/3/3/3
1	5MU	1A	1961	1	-	0/5/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	1,54	-	1/5/27/28	0/3/3/3
1	5MU	1A	1937	1,54	-	0/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
1	5MU	2A	1939	1,54	-	0/5/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/5/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	M2G	2a	966	32,54	-	0/7/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/5/25/26	0/2/2/2
1	2MU	1A	2564	1,54	-	0/7/27/28	0/2/2/2
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-7.89	1.65	1.84
43	2l	92	0TD	CB-SB	-6.07	1.69	1.84
32	2a	967	5MC	C5-C4	5.26	1.49	1.41
1	1A	2617	PSU	C5-C1'	-5.20	1.47	1.52
32	2a	1404	5MC	C5-C4	5.16	1.49	1.41

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	PSU	N1-C2-N3	-9.24	121.08	128.43
1	2A	2605	PSU	N1-C2-N3	-9.14	121.17	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	516	PSU	N1-C2-N3	-9.12	121.18	128.43
1	1A	1933	PSU	N1-C2-N3	-8.95	121.31	128.43
32	2a	527	7MG	N3-C4-N9	8.77	138.17	126.91

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	C5-C6-N6-C9
32	2a	1519	MA6	C5-C6-N6-C10
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
1	1A	1942	4OC	C2'-C1'-N1-C6

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	2552	2MU	1	0
1	2A	2503	2MA	1	0
1	2A	2251	OMG	1	0
1	1A	1961	5MU	1	0
1	2A	1915	5MU	1	0
1	2A	1939	5MU	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2540 ligands modelled in this entry, 2529 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	MPD	2A	3747	-	7,7,7	0.38	0	9,10,10	0.48	0
55	MPD	1A	4028	-	7,7,7	0.28	0	9,10,10	0.19	0
55	MPD	1T	8004	-	7,7,7	0.30	0	9,10,10	0.35	0
55	MPD	18	102	-	7,7,7	0.24	0	9,10,10	0.57	0
55	MPD	2A	3748	-	7,7,7	0.31	0	9,10,10	0.26	0
55	MPD	1a	1880	-	7,7,7	0.59	0	9,10,10	0.65	0
58	SF4	1d	501	35	0,12,12	0.00	-	-		
58	SF4	2d	501	35	0,12,12	0.00	-	-		
55	MPD	2B	3020	-	7,7,7	0.32	0	9,10,10	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	MPD	2A	3747	-	-	0/5/5/5	-
55	MPD	1A	4028	-	-	0/5/5/5	-
55	MPD	1T	8004	-	-	2/5/5/5	-
55	MPD	18	102	-	-	1/5/5/5	-
55	MPD	2A	3748	-	-	5/5/5/5	-
55	MPD	1a	1880	-	-	1/5/5/5	-
58	SF4	1d	501	35	-	-	0/6/5/5
58	SF4	2d	501	35	-	-	0/6/5/5
55	MPD	2B	3020	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	2A	3748	MPD	O2-C2-C3-C4
55	2A	3748	MPD	C2-C3-C4-O4
55	1a	1880	MPD	C2-C3-C4-C5
55	2A	3748	MPD	C2-C3-C4-C5
55	18	102	MPD	C2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2A	3747	MPD	2	0
55	1A	4028	MPD	1	0
55	18	102	MPD	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2861/2915 (98%)	0.88	90 (3%) 49 56	23, 40, 90, 101	0
1	2A	2856/2915 (97%)	0.35	130 (4%) 32 39	26, 44, 91, 104	0
2	1B	120/121 (99%)	0.57	0 100 100	34, 56, 71, 86	0
2	2B	120/121 (99%)	0.02	1 (0%) 86 89	41, 61, 74, 87	0
3	1D	275/276 (99%)	0.71	5 (1%) 68 74	23, 37, 53, 78	0
3	2D	275/276 (99%)	0.37	4 (1%) 73 79	25, 41, 55, 77	0
4	1E	204/206 (99%)	0.78	1 (0%) 91 94	22, 43, 63, 72	0
4	2E	204/206 (99%)	0.33	3 (1%) 73 79	26, 47, 65, 74	0
5	1F	203/210 (96%)	0.75	2 (0%) 82 86	20, 46, 72, 84	0
5	2F	203/210 (96%)	0.13	0 100 100	25, 52, 73, 85	0
6	1G	181/182 (99%)	0.44	6 (3%) 46 53	54, 70, 81, 90	0
6	2G	181/182 (99%)	1.65	62 (34%) 0 0	58, 73, 83, 91	0
7	1H	174/180 (96%)	0.75	4 (2%) 60 67	45, 62, 73, 78	0
7	2H	173/180 (96%)	0.82	23 (13%) 3 4	54, 67, 76, 80	0
8	1I	147/148 (99%)	0.26	1 (0%) 87 91	43, 71, 80, 84	0
8	2I	146/148 (98%)	0.37	6 (4%) 37 44	47, 71, 81, 84	0
9	1N	140/140 (100%)	0.57	1 (0%) 87 91	25, 36, 60, 81	0
9	2N	140/140 (100%)	0.49	3 (2%) 63 70	39, 58, 74, 81	0
10	1O	122/122 (100%)	0.52	0 100 100	25, 37, 57, 64	0
10	2O	122/122 (100%)	0.42	2 (1%) 72 77	38, 52, 66, 74	0
11	1P	149/150 (99%)	0.48	1 (0%) 87 91	19, 43, 67, 78	0
11	2P	149/150 (99%)	0.40	5 (3%) 45 52	32, 62, 79, 85	0
12	1Q	141/141 (100%)	0.75	1 (0%) 87 91	28, 44, 58, 72	0
12	2Q	141/141 (100%)	0.25	3 (2%) 63 70	33, 49, 61, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.72	0 100 100	27, 38, 54, 63	0
13	2R	118/118 (100%)	0.36	1 (0%) 86 89	32, 42, 56, 64	0
14	1S	110/112 (98%)	0.58	0 100 100	42, 56, 67, 71	0
14	2S	110/112 (98%)	0.63	15 (13%) 3 4	48, 60, 70, 74	0
15	1T	131/146 (89%)	0.62	2 (1%) 73 79	34, 47, 72, 82	0
15	2T	131/146 (89%)	0.32	2 (1%) 73 79	39, 49, 74, 83	0
16	1U	116/118 (98%)	0.93	2 (1%) 70 76	25, 36, 53, 68	0
16	2U	116/118 (98%)	0.29	0 100 100	30, 43, 57, 70	0
17	1V	101/101 (100%)	0.82	2 (1%) 65 71	26, 48, 63, 73	0
17	2V	101/101 (100%)	0.16	1 (0%) 82 86	30, 54, 67, 74	0
18	1W	112/113 (99%)	0.74	1 (0%) 84 88	28, 34, 55, 87	0
18	2W	112/113 (99%)	0.29	0 100 100	32, 38, 58, 87	0
19	1X	95/96 (98%)	0.80	3 (3%) 47 54	32, 42, 63, 74	0
19	2X	95/96 (98%)	0.68	8 (8%) 11 15	37, 47, 67, 76	0
20	1Y	107/110 (97%)	0.72	2 (1%) 66 73	39, 54, 69, 78	0
20	2Y	107/110 (97%)	0.86	11 (10%) 6 9	43, 58, 72, 80	0
21	1Z	203/206 (98%)	0.59	3 (1%) 73 79	45, 63, 78, 83	0
21	2Z	201/206 (97%)	0.60	18 (8%) 9 12	50, 66, 78, 82	0
22	10	77/85 (90%)	0.46	1 (1%) 77 81	26, 35, 52, 63	0
22	20	77/85 (90%)	0.85	5 (6%) 18 24	41, 57, 68, 81	0
23	11	97/98 (98%)	0.56	2 (2%) 63 70	26, 41, 68, 76	0
23	21	97/98 (98%)	0.52	1 (1%) 82 86	35, 51, 72, 75	0
24	12	70/72 (97%)	0.64	0 100 100	40, 53, 65, 82	0
24	22	70/72 (97%)	0.42	1 (1%) 75 80	45, 59, 68, 81	0
25	13	59/60 (98%)	0.75	1 (1%) 70 76	28, 40, 67, 80	0
25	23	59/60 (98%)	0.88	6 (10%) 6 9	34, 45, 70, 80	0
26	14	69/71 (97%)	1.04	14 (20%) 1 1	67, 81, 90, 94	0
26	24	69/71 (97%)	2.18	26 (37%) 0 0	70, 82, 90, 94	0
27	15	59/60 (98%)	0.77	2 (3%) 45 52	22, 37, 59, 69	0
27	25	59/60 (98%)	0.14	1 (1%) 70 76	25, 40, 61, 70	0
28	16	53/54 (98%)	0.64	0 100 100	34, 45, 61, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.23	1 (1%) 66 73	39, 49, 61, 66	0
29	17	48/49 (97%)	1.02	5 (10%) 6 9	22, 30, 58, 68	0
29	27	48/49 (97%)	0.84	4 (8%) 11 15	26, 33, 60, 68	0
30	18	64/65 (98%)	0.70	0 100 100	30, 38, 45, 61	0
30	28	64/65 (98%)	0.37	0 100 100	33, 42, 49, 64	0
31	19	37/37 (100%)	0.47	1 (2%) 54 62	29, 39, 55, 56	0
31	29	37/37 (100%)	0.86	2 (5%) 25 32	45, 60, 72, 75	0
32	1a	1488/1521 (97%)	0.33	45 (3%) 50 57	34, 63, 89, 102	0
32	2a	1492/1521 (98%)	0.38	61 (4%) 37 44	44, 73, 92, 103	0
33	1b	231/256 (90%)	0.75	32 (13%) 2 4	65, 78, 86, 91	0
33	2b	231/256 (90%)	1.62	74 (32%) 0 0	67, 79, 87, 93	0
34	1c	206/239 (86%)	0.57	10 (4%) 29 36	63, 74, 83, 89	0
34	2c	206/239 (86%)	1.65	71 (34%) 0 0	65, 76, 84, 90	0
35	1d	208/209 (99%)	0.82	22 (10%) 6 8	55, 69, 79, 84	0
35	2d	208/209 (99%)	1.03	27 (12%) 3 4	57, 69, 78, 84	0
36	1e	148/162 (91%)	0.44	4 (2%) 54 62	46, 61, 72, 87	0
36	2e	148/162 (91%)	0.71	12 (8%) 12 16	56, 70, 79, 87	0
37	1f	100/101 (99%)	0.55	5 (5%) 28 35	53, 64, 74, 79	0
37	2f	100/101 (99%)	0.24	2 (2%) 65 71	53, 64, 74, 79	0
38	1g	155/156 (99%)	0.48	6 (3%) 39 46	62, 72, 81, 84	0
38	2g	155/156 (99%)	1.08	30 (19%) 1 1	66, 74, 81, 84	0
39	1h	137/138 (99%)	0.73	8 (5%) 23 29	54, 67, 74, 77	0
39	2h	137/138 (99%)	0.61	8 (5%) 23 29	56, 68, 75, 78	0
40	1i	127/128 (99%)	1.07	19 (14%) 2 3	60, 78, 85, 88	0
40	2i	126/128 (98%)	2.58	76 (60%) 0 0	64, 79, 86, 89	0
41	1j	97/105 (92%)	1.42	29 (29%) 0 0	59, 79, 88, 91	0
41	2j	96/105 (91%)	1.93	40 (41%) 0 0	65, 80, 88, 91	0
42	1k	114/129 (88%)	0.57	4 (3%) 44 51	46, 63, 77, 79	0
42	2k	114/129 (88%)	1.02	17 (14%) 2 3	48, 65, 77, 80	0
43	1l	121/132 (91%)	0.66	9 (7%) 14 19	48, 58, 70, 75	0
43	2l	121/132 (91%)	0.64	8 (6%) 18 23	51, 60, 70, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.78	12 (10%) 6 9	54, 71, 79, 84	0
44	2m	114/126 (90%)	2.05	53 (46%) 0 0	73, 82, 87, 91	0
45	1n	60/61 (98%)	1.70	19 (31%) 0 0	64, 71, 78, 79	0
45	2n	60/61 (98%)	2.90	41 (68%) 0 0	67, 74, 80, 87	0
46	1o	88/89 (98%)	0.48	3 (3%) 45 52	46, 64, 77, 79	0
46	2o	88/89 (98%)	0.37	3 (3%) 45 52	50, 65, 78, 80	0
47	1p	82/88 (93%)	0.69	5 (6%) 21 27	58, 68, 78, 81	0
47	2p	82/88 (93%)	0.98	11 (13%) 3 4	59, 68, 77, 83	0
48	1q	99/105 (94%)	0.82	11 (11%) 5 7	53, 66, 75, 79	0
48	2q	99/105 (94%)	0.86	8 (8%) 12 16	53, 66, 76, 80	0
49	1r	68/88 (77%)	0.66	7 (10%) 6 9	55, 65, 77, 79	0
49	2r	68/88 (77%)	0.48	2 (2%) 51 58	55, 66, 77, 79	0
50	1s	83/93 (89%)	1.04	12 (14%) 2 3	67, 77, 83, 85	0
50	2s	83/93 (89%)	3.24	60 (72%) 0 0	70, 79, 84, 86	0
51	1t	96/106 (90%)	1.04	14 (14%) 2 3	57, 68, 79, 83	0
51	2t	98/106 (92%)	0.63	4 (4%) 37 44	57, 69, 81, 83	0
52	1u	23/27 (85%)	1.44	7 (30%) 0 0	69, 72, 76, 78	0
52	2u	23/27 (85%)	2.48	14 (60%) 0 0	71, 74, 77, 80	0
53	1y	97/113 (85%)	0.45	2 (2%) 63 70	44, 56, 70, 74	0
53	2y	96/113 (84%)	1.06	17 (17%) 1 1	57, 71, 79, 83	0
All	All	20766/21468 (96%)	0.67	1422 (6%) 17 22	19, 58, 85, 104	0

The worst 5 of 1422 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	24	50	VAL	10.3
1	2A	2142	C	10.0
1	1A	1122	C	10.0
33	2b	127	ILE	9.8
1	2A	2147	G	9.5

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	2MG	2a	1207	24/25	0.90	0.19	75,83,90,94	0
1	5MU	1A	1937	21/22	0.90	0.17	65,79,86,95	0
1	5MU	2A	1915	21/22	0.90	0.13	70,82,87,103	0
32	M2G	2a	966	25/26	0.91	0.14	52,68,81,90	0
1	PSU	1A	1939	20/21	0.92	0.17	63,73,82,86	0
1	PSU	2A	1917	20/21	0.92	0.16	62,74,84,89	0
1	PSU	2A	1911	20/21	0.92	0.12	62,68,73,82	0
43	0TD	2l	92	10/11	0.93	0.11	57,63,66,74	0
32	5MC	2a	1404	21/22	0.94	0.17	54,61,64,67	0
43	0TD	1l	92	10/11	0.94	0.18	54,59,68,68	0
32	PSU	2a	516	20/21	0.94	0.12	69,76,81,82	0
1	PSU	1A	1933	20/21	0.95	0.14	59,66,68,81	0
32	7MG	2a	527	24/25	0.95	0.14	57,66,70,73	0
32	2MG	1a	1207	24/25	0.95	0.14	60,68,71,74	0
32	5MC	1a	967	21/22	0.95	0.16	51,61,73,83	0
32	5MC	2a	967	21/22	0.95	0.13	61,68,77,86	0
32	4OC	2a	1402	22/23	0.95	0.15	53,64,74,82	0
32	MA6	2a	1518	24/25	0.96	0.16	47,58,65,68	0
32	5MC	2a	1407	21/22	0.96	0.12	46,62,69,70	0
32	UR3	2a	1498	21/22	0.96	0.15	53,60,65,73	0
32	UR3	1a	1498	21/22	0.96	0.16	35,46,53,56	0
32	5MC	2a	1400	21/22	0.96	0.20	62,68,74,77	0
1	4OC	2A	1920	21/23	0.96	0.13	57,62,67,67	0
32	MA6	1a	1518	24/25	0.97	0.18	37,44,51,56	0
32	M2G	1a	966	25/26	0.97	0.15	48,53,59,65	0
32	MA6	2a	1519	24/25	0.97	0.19	51,61,64,69	0
1	4OC	1A	1942	21/23	0.97	0.16	52,60,63,65	0
32	PSU	1a	516	20/21	0.97	0.14	49,58,65,67	0
32	5MC	1a	1404	21/22	0.97	0.15	33,43,49,51	0
1	5MC	2A	1942	21/22	0.97	0.15	36,45,52,53	0
32	5MC	1a	1400	21/22	0.97	0.15	37,50,57,58	0
32	MA6	1a	1519	24/25	0.97	0.18	40,45,52,52	0
1	5MU	2A	1939	21/22	0.98	0.15	28,33,37,42	0
32	7MG	1a	527	24/25	0.98	0.16	40,48,55,55	0
32	5MC	1a	1407	21/22	0.98	0.16	41,48,54,56	0
1	PSU	2A	2605	20/21	0.98	0.17	27,31,39,41	0
1	2MA	2A	2503	23/24	0.98	0.17	21,28,32,37	0
1	OMG	2A	2251	24/25	0.98	0.15	27,31,35,37	0
1	5MC	1A	1964	21/22	0.98	0.17	34,41,47,52	0
32	4OC	1a	1402	22/23	0.98	0.16	41,47,51,56	0
1	2MU	2A	2552	21/23	0.98	0.17	27,33,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	2MA	1A	2515	23/24	0.98	0.21	17,23,28,31	0
1	5MC	2A	1962	21/22	0.98	0.15	32,38,44,54	0
1	5MU	1A	1961	21/22	0.98	0.19	24,30,34,37	0
1	PSU	1A	2617	20/21	0.99	0.18	23,29,35,38	0
1	5MC	1A	1984	21/22	0.99	0.17	29,36,41,47	0
1	2MU	1A	2564	21/23	0.99	0.19	24,29,33,36	0
1	OMG	1A	2263	24/25	0.99	0.21	22,28,29,33	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3598	1/1	0.21	0.21	72,72,72,72	0
54	MG	2A	3659	1/1	0.22	0.12	76,76,76,76	0
54	MG	10	104	1/1	0.29	0.13	64,64,64,64	0
54	MG	2A	3509	1/1	0.32	0.28	75,75,75,75	0
54	MG	1A	3950	1/1	0.37	0.20	77,77,77,77	0
54	MG	1a	1817	1/1	0.38	0.07	98,98,98,98	0
54	MG	1A	3708	1/1	0.38	0.17	64,64,64,64	0
54	MG	2A	3697	1/1	0.39	0.08	67,67,67,67	0
54	MG	1a	1773	1/1	0.40	0.09	85,85,85,85	0
54	MG	2A	3626	1/1	0.41	0.22	47,47,47,47	0
54	MG	1A	3836	1/1	0.41	0.12	57,57,57,57	0
54	MG	2A	3663	1/1	0.43	0.16	74,74,74,74	0
54	MG	2B	3007	1/1	0.43	0.22	76,76,76,76	0
54	MG	1A	3889	1/1	0.44	0.23	47,47,47,47	0
54	MG	1B	221	1/1	0.45	0.13	48,48,48,48	0
54	MG	2A	3638	1/1	0.45	0.13	55,55,55,55	0
54	MG	1A	3990	1/1	0.45	0.13	83,83,83,83	0
54	MG	2Q	3002	1/1	0.46	0.11	63,63,63,63	0
54	MG	2A	3488	1/1	0.48	0.09	58,58,58,58	0
54	MG	2A	3640	1/1	0.48	0.05	63,63,63,63	0
54	MG	2A	3375	1/1	0.49	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3496	1/1	0.49	0.10	56,56,56,56	0
54	MG	2a	1750	1/1	0.49	0.10	79,79,79,79	0
54	MG	1a	1744	1/1	0.50	0.71	88,88,88,88	0
54	MG	1A	3409	1/1	0.51	0.22	58,58,58,58	0
54	MG	1a	1870	1/1	0.52	0.13	93,93,93,93	0
54	MG	1A	3377	1/1	0.52	0.15	67,67,67,67	0
54	MG	2A	3569	1/1	0.52	0.17	55,55,55,55	0
54	MG	2A	3681	1/1	0.53	0.08	70,70,70,70	0
54	MG	2a	1747	1/1	0.53	0.14	78,78,78,78	0
54	MG	2A	3586	1/1	0.54	0.07	62,62,62,62	0
54	MG	2B	3012	1/1	0.55	0.13	77,77,77,77	0
54	MG	2a	1749	1/1	0.55	0.10	85,85,85,85	0
54	MG	2A	3593	1/1	0.55	0.14	48,48,48,48	0
54	MG	2A	3588	1/1	0.56	0.14	88,88,88,88	0
54	MG	2A	3584	1/1	0.56	0.21	49,49,49,49	0
54	MG	2a	1789	1/1	0.56	0.19	80,80,80,80	0
54	MG	1a	1676	1/1	0.56	0.26	75,75,75,75	0
54	MG	1A	3513	1/1	0.57	0.19	58,58,58,58	0
54	MG	2A	3464	1/1	0.57	0.15	63,63,63,63	0
54	MG	2A	3727	1/1	0.57	0.09	70,70,70,70	0
54	MG	2A	3495	1/1	0.57	0.10	54,54,54,54	0
54	MG	10	101	1/1	0.58	0.07	52,52,52,52	0
54	MG	1A	3499	1/1	0.58	0.11	55,55,55,55	0
54	MG	2A	3642	1/1	0.59	0.23	77,77,77,77	0
54	MG	1a	1673	1/1	0.59	0.14	71,71,71,71	0
54	MG	2A	3729	1/1	0.60	0.11	59,59,59,59	0
54	MG	2A	3478	1/1	0.60	0.45	64,64,64,64	0
54	MG	1A	3171	1/1	0.61	0.17	56,56,56,56	0
54	MG	1B	202	1/1	0.61	0.20	63,63,63,63	0
54	MG	1A	3612	1/1	0.62	0.70	66,66,66,66	0
54	MG	1a	1875	1/1	0.62	0.10	77,77,77,77	0
54	MG	1a	1783	1/1	0.62	0.23	87,87,87,87	0
54	MG	1A	3799	1/1	0.62	0.10	51,51,51,51	0
54	MG	1A	3616	1/1	0.62	0.14	55,55,55,55	0
57	ZN	2Y	501	1/1	0.63	0.24	169,169,169,169	0
54	MG	2a	1755	1/1	0.63	0.23	82,82,82,82	0
54	MG	2a	1649	1/1	0.64	0.10	75,75,75,75	0
54	MG	1A	3924	1/1	0.64	0.11	61,61,61,61	0
54	MG	2A	3481	1/1	0.64	0.16	69,69,69,69	0
54	MG	1A	3450	1/1	0.64	0.15	57,57,57,57	0
54	MG	2a	1729	1/1	0.64	0.10	71,71,71,71	0
54	MG	2A	3597	1/1	0.64	0.05	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3374	1/1	0.64	0.10	57,57,57,57	0
54	MG	2B	3015	1/1	0.64	0.23	87,87,87,87	0
54	MG	1A	3985	1/1	0.64	0.11	75,75,75,75	0
54	MG	1A	3580	1/1	0.64	0.07	59,59,59,59	0
54	MG	2A	3684	1/1	0.65	0.12	62,62,62,62	0
54	MG	2A	3431	1/1	0.65	0.44	57,57,57,57	0
54	MG	2A	3709	1/1	0.65	0.07	50,50,50,50	0
54	MG	1A	3431	1/1	0.65	0.12	61,61,61,61	0
54	MG	2A	3312	1/1	0.66	0.10	65,65,65,65	0
54	MG	2A	3484	1/1	0.66	0.18	66,66,66,66	0
54	MG	2a	1788	1/1	0.66	0.10	102,102,102,102	0
54	MG	2A	3171	1/1	0.66	0.18	56,56,56,56	0
54	MG	1A	3936	1/1	0.66	0.17	55,55,55,55	0
54	MG	2A	3633	1/1	0.67	0.74	68,68,68,68	0
54	MG	1A	3615	1/1	0.67	0.10	60,60,60,60	0
54	MG	2A	3465	1/1	0.67	0.15	67,67,67,67	0
54	MG	2A	3288	1/1	0.67	0.14	51,51,51,51	0
54	MG	2A	3468	1/1	0.67	0.27	72,72,72,72	0
54	MG	1A	3745	1/1	0.67	0.09	71,71,71,71	0
54	MG	2A	3325	1/1	0.67	0.14	50,50,50,50	0
54	MG	2A	3665	1/1	0.67	0.10	53,53,53,53	0
54	MG	1A	3593	1/1	0.67	0.14	62,62,62,62	0
54	MG	1a	1872	1/1	0.67	0.21	83,83,83,83	0
54	MG	1B	217	1/1	0.67	0.35	70,70,70,70	0
54	MG	1A	3772	1/1	0.67	0.10	50,50,50,50	0
54	MG	1A	3295	1/1	0.68	0.13	84,84,84,84	0
54	MG	2A	3680	1/1	0.68	0.24	53,53,53,53	0
54	MG	2D	306	1/1	0.68	0.18	60,60,60,60	0
54	MG	1A	3786	1/1	0.68	0.12	64,64,64,64	0
54	MG	1A	3833	1/1	0.68	0.13	60,60,60,60	0
54	MG	1A	3621	1/1	0.68	0.18	65,65,65,65	0
54	MG	2A	3685	1/1	0.68	0.08	60,60,60,60	0
54	MG	2A	3603	1/1	0.68	0.30	78,78,78,78	0
54	MG	1F	309	1/1	0.69	0.08	69,69,69,69	0
54	MG	2A	3609	1/1	0.69	0.12	58,58,58,58	0
54	MG	1a	1791	1/1	0.69	0.15	72,72,72,72	0
54	MG	2A	3622	1/1	0.69	0.08	69,69,69,69	0
54	MG	1A	3805	1/1	0.69	0.09	63,63,63,63	0
54	MG	2A	3513	1/1	0.69	0.19	58,58,58,58	0
54	MG	1A	3788	1/1	0.69	0.25	66,66,66,66	0
54	MG	1A	3485	1/1	0.69	0.09	72,72,72,72	0
54	MG	1A	4019	1/1	0.69	0.26	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1751	1/1	0.70	0.08	67,67,67,67	0
54	MG	2A	3384	1/1	0.70	0.09	46,46,46,46	0
54	MG	1a	1868	1/1	0.70	0.07	71,71,71,71	0
54	MG	1A	3511	1/1	0.70	0.27	64,64,64,64	0
54	MG	1A	3956	1/1	0.70	0.20	60,60,60,60	0
54	MG	1A	3530	1/1	0.70	0.30	69,69,69,69	0
54	MG	1A	3528	1/1	0.70	0.25	61,61,61,61	0
57	ZN	24	501	1/1	0.70	0.09	257,257,257,257	0
54	MG	2a	1681	1/1	0.70	0.08	74,74,74,74	0
54	MG	2A	3081	1/1	0.70	0.46	55,55,55,55	0
54	MG	1A	3553	1/1	0.70	0.15	68,68,68,68	0
54	MG	1d	506	1/1	0.70	0.19	93,93,93,93	0
54	MG	2a	1629	1/1	0.70	0.11	61,61,61,61	0
54	MG	2A	3505	1/1	0.70	0.09	73,73,73,73	0
54	MG	1A	3991	1/1	0.70	0.06	50,50,50,50	0
54	MG	2A	3223	1/1	0.70	0.22	58,58,58,58	0
54	MG	2a	1778	1/1	0.70	0.24	79,79,79,79	0
54	MG	1A	3579	1/1	0.71	0.25	74,74,74,74	0
54	MG	2A	3737	1/1	0.71	0.20	37,37,37,37	0
54	MG	1A	3719	1/1	0.71	0.15	47,47,47,47	0
54	MG	1E	304	1/1	0.71	0.18	59,59,59,59	0
54	MG	1A	3639	1/1	0.71	0.09	65,65,65,65	0
54	MG	1A	3858	1/1	0.71	0.17	68,68,68,68	0
54	MG	2A	3388	1/1	0.71	0.16	55,55,55,55	0
54	MG	2A	3367	1/1	0.71	0.12	66,66,66,66	0
54	MG	1R	203	1/1	0.71	0.23	48,48,48,48	0
54	MG	2A	3627	1/1	0.71	0.16	60,60,60,60	0
54	MG	2a	1707	1/1	0.71	0.11	65,65,65,65	0
54	MG	1a	1694	1/1	0.71	0.13	67,67,67,67	0
54	MG	2A	3658	1/1	0.71	0.09	52,52,52,52	0
54	MG	2A	3561	1/1	0.71	0.14	50,50,50,50	0
54	MG	1A	3759	1/1	0.72	0.20	45,45,45,45	0
54	MG	2A	3625	1/1	0.72	0.20	43,43,43,43	0
54	MG	2A	3349	1/1	0.72	0.17	46,46,46,46	0
54	MG	1a	1793	1/1	0.72	0.13	67,67,67,67	0
54	MG	20	101	1/1	0.72	0.14	64,64,64,64	0
54	MG	1A	3011	1/1	0.72	0.14	62,62,62,62	0
54	MG	1A	3763	1/1	0.72	0.19	53,53,53,53	0
54	MG	1A	4017	1/1	0.72	0.11	62,62,62,62	0
54	MG	1A	3294	1/1	0.72	0.09	74,74,74,74	0
54	MG	2a	1771	1/1	0.72	0.33	86,86,86,86	0
54	MG	2D	301	1/1	0.72	0.30	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3616	1/1	0.72	0.19	47,47,47,47	0
54	MG	1G	3002	1/1	0.72	0.12	62,62,62,62	0
54	MG	1A	3706	1/1	0.72	0.17	64,64,64,64	0
54	MG	1A	3888	1/1	0.73	0.10	58,58,58,58	0
54	MG	2a	1786	1/1	0.73	0.15	67,67,67,67	0
54	MG	2A	3578	1/1	0.73	0.20	71,71,71,71	0
54	MG	2A	3679	1/1	0.73	0.10	56,56,56,56	0
54	MG	2a	1752	1/1	0.73	0.19	67,67,67,67	0
54	MG	1A	3927	1/1	0.73	0.09	63,63,63,63	0
54	MG	1A	4006	1/1	0.73	0.17	55,55,55,55	0
54	MG	1A	3568	1/1	0.73	0.18	55,55,55,55	0
54	MG	1a	1841	1/1	0.73	0.20	61,61,61,61	0
54	MG	1a	1767	1/1	0.73	0.16	79,79,79,79	0
54	MG	1A	3825	1/1	0.73	0.10	70,70,70,70	0
54	MG	1b	3001	1/1	0.73	0.10	87,87,87,87	0
54	MG	2A	3187	1/1	0.73	0.69	61,61,61,61	0
54	MG	1a	1836	1/1	0.73	0.15	83,83,83,83	0
54	MG	14	502	1/1	0.74	0.12	83,83,83,83	0
54	MG	2A	3545	1/1	0.74	0.10	75,75,75,75	0
54	MG	1A	3367	1/1	0.74	0.12	54,54,54,54	0
54	MG	2a	1645	1/1	0.74	0.17	67,67,67,67	0
54	MG	2A	3629	1/1	0.74	0.15	62,62,62,62	0
54	MG	1A	3455	1/1	0.74	0.14	50,50,50,50	0
54	MG	1A	3634	1/1	0.74	0.37	43,43,43,43	0
54	MG	2a	1667	1/1	0.74	0.15	83,83,83,83	0
54	MG	2A	3360	1/1	0.74	0.11	72,72,72,72	0
54	MG	2a	1610	1/1	0.74	0.16	61,61,61,61	0
54	MG	1A	3576	1/1	0.74	0.23	57,57,57,57	0
54	MG	1a	1664	1/1	0.74	0.12	58,58,58,58	0
54	MG	1A	3196	1/1	0.74	0.19	72,72,72,72	0
54	MG	1A	3830	1/1	0.74	0.14	65,65,65,65	0
54	MG	1a	1788	1/1	0.74	0.11	85,85,85,85	0
54	MG	2A	3174	1/1	0.74	0.62	61,61,61,61	0
54	MG	2A	3720	1/1	0.74	0.24	55,55,55,55	0
54	MG	1A	3597	1/1	0.74	0.09	62,62,62,62	0
54	MG	2a	1605	1/1	0.74	0.16	63,63,63,63	0
54	MG	2a	1656	1/1	0.74	0.13	69,69,69,69	0
54	MG	2A	3563	1/1	0.74	0.07	50,50,50,50	0
54	MG	1A	3084	1/1	0.74	0.15	58,58,58,58	0
54	MG	2A	3556	1/1	0.74	0.09	62,62,62,62	0
54	MG	2A	3455	1/1	0.74	0.14	62,62,62,62	0
54	MG	1A	3902	1/1	0.75	0.06	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3418	1/1	0.75	0.10	71,71,71,71	0
54	MG	1A	3625	1/1	0.75	0.20	63,63,63,63	0
54	MG	2a	1754	1/1	0.75	0.33	84,84,84,84	0
54	MG	2A	3426	1/1	0.75	0.12	58,58,58,58	0
54	MG	2A	3502	1/1	0.75	0.18	61,61,61,61	0
54	MG	2A	3512	1/1	0.75	0.09	54,54,54,54	0
54	MG	1A	4025	1/1	0.75	0.12	70,70,70,70	0
54	MG	2a	1635	1/1	0.75	0.14	67,67,67,67	0
54	MG	1a	1869	1/1	0.76	0.11	74,74,74,74	0
54	MG	2A	3576	1/1	0.76	0.10	49,49,49,49	0
54	MG	1A	3655	1/1	0.76	0.11	40,40,40,40	0
55	MPD	1a	1880	8/8	0.76	0.20	48,59,72,72	0
54	MG	1A	3558	1/1	0.76	0.11	62,62,62,62	0
54	MG	1A	3866	1/1	0.76	0.11	64,64,64,64	0
54	MG	2A	3383	1/1	0.76	0.17	52,52,52,52	0
54	MG	2A	3190	1/1	0.76	0.14	61,61,61,61	0
54	MG	1A	3312	1/1	0.76	0.15	72,72,72,72	0
54	MG	1A	3766	1/1	0.76	0.20	56,56,56,56	0
54	MG	2a	1692	1/1	0.76	0.10	77,77,77,77	0
54	MG	2A	3551	1/1	0.76	0.12	61,61,61,61	0
54	MG	1a	1801	1/1	0.76	0.25	80,80,80,80	0
54	MG	2A	3162	1/1	0.76	0.28	57,57,57,57	0
54	MG	1a	1865	1/1	0.76	0.17	46,46,46,46	0
54	MG	2a	1792	1/1	0.76	0.14	67,67,67,67	0
54	MG	1A	3464	1/1	0.76	0.18	47,47,47,47	0
54	MG	2B	3001	1/1	0.76	0.11	68,68,68,68	0
54	MG	2A	3244	1/1	0.76	0.20	56,56,56,56	0
54	MG	2a	1664	1/1	0.76	0.16	79,79,79,79	0
54	MG	1A	4003	1/1	0.76	0.44	66,66,66,66	0
54	MG	2a	1601	1/1	0.76	0.25	69,69,69,69	0
54	MG	1A	3861	1/1	0.77	0.18	54,54,54,54	0
54	MG	2A	3688	1/1	0.77	0.11	67,67,67,67	0
54	MG	1A	3566	1/1	0.77	0.14	60,60,60,60	0
54	MG	1A	3443	1/1	0.77	0.07	48,48,48,48	0
54	MG	2A	3575	1/1	0.77	0.09	43,43,43,43	0
54	MG	1A	3152	1/1	0.77	0.19	66,66,66,66	0
54	MG	1A	3600	1/1	0.77	0.10	57,57,57,57	0
54	MG	2A	3251	1/1	0.77	0.16	53,53,53,53	0
54	MG	1a	1718	1/1	0.77	0.17	58,58,58,58	0
54	MG	1A	3497	1/1	0.77	0.16	45,45,45,45	0
54	MG	2B	3018	1/1	0.77	0.11	76,76,76,76	0
54	MG	2A	3645	1/1	0.77	0.04	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3438	1/1	0.77	0.20	56,56,56,56	0
54	MG	2A	3206	1/1	0.77	0.18	56,56,56,56	0
54	MG	1a	1614	1/1	0.77	0.19	74,74,74,74	0
54	MG	1A	3758	1/1	0.77	0.10	66,66,66,66	0
54	MG	2A	3234	1/1	0.77	0.41	65,65,65,65	0
54	MG	1A	3692	1/1	0.77	0.10	55,55,55,55	0
54	MG	2a	1604	1/1	0.77	0.17	66,66,66,66	0
54	MG	2A	3668	1/1	0.77	0.27	73,73,73,73	0
54	MG	2A	3129	1/1	0.77	0.11	63,63,63,63	0
54	MG	2a	1614	1/1	0.77	0.13	55,55,55,55	0
54	MG	1A	3988	1/1	0.77	0.10	81,81,81,81	0
54	MG	2a	1744	1/1	0.77	0.11	75,75,75,75	0
54	MG	2A	3023	1/1	0.77	0.14	54,54,54,54	0
54	MG	1A	3959	1/1	0.77	0.07	70,70,70,70	0
54	MG	2A	3526	1/1	0.78	0.13	66,66,66,66	0
54	MG	2A	3530	1/1	0.78	0.10	50,50,50,50	0
54	MG	1A	3685	1/1	0.78	0.08	70,70,70,70	0
54	MG	1a	1746	1/1	0.78	0.09	56,56,56,56	0
54	MG	2A	3635	1/1	0.78	0.16	65,65,65,65	0
54	MG	2a	1721	1/1	0.78	0.11	71,71,71,71	0
54	MG	1F	307	1/1	0.78	0.21	49,49,49,49	0
54	MG	1A	3592	1/1	0.78	0.08	54,54,54,54	0
54	MG	1A	3962	1/1	0.78	0.18	59,59,59,59	0
54	MG	1A	3375	1/1	0.78	0.14	49,49,49,49	0
54	MG	2A	3553	1/1	0.78	0.26	76,76,76,76	0
54	MG	2A	3535	1/1	0.78	0.42	71,71,71,71	0
54	MG	2A	3237	1/1	0.78	0.12	65,65,65,65	0
54	MG	2A	3231	1/1	0.78	0.13	61,61,61,61	0
54	MG	1A	3571	1/1	0.78	0.09	65,65,65,65	0
54	MG	2A	3082	1/1	0.78	0.39	59,59,59,59	0
54	MG	1a	1631	1/1	0.78	0.25	70,70,70,70	0
54	MG	2A	3671	1/1	0.78	0.14	36,36,36,36	0
54	MG	2a	1686	1/1	0.78	0.35	66,66,66,66	0
54	MG	2a	1626	1/1	0.78	0.20	70,70,70,70	0
54	MG	1A	3775	1/1	0.79	0.18	36,36,36,36	0
54	MG	2a	1715	1/1	0.79	0.09	71,71,71,71	0
54	MG	2A	3544	1/1	0.79	0.07	55,55,55,55	0
54	MG	1A	3747	1/1	0.79	0.10	62,62,62,62	0
54	MG	1A	3534	1/1	0.79	0.18	67,67,67,67	0
54	MG	2A	3473	1/1	0.79	0.06	51,51,51,51	0
54	MG	1A	3066	1/1	0.79	0.10	64,64,64,64	0
54	MG	1a	1787	1/1	0.79	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3641	1/1	0.79	0.14	62,62,62,62	0
54	MG	1A	3810	1/1	0.79	0.12	80,80,80,80	0
54	MG	1A	3525	1/1	0.79	0.15	57,57,57,57	0
54	MG	1A	3862	1/1	0.79	0.07	54,54,54,54	0
54	MG	1A	3770	1/1	0.79	0.22	34,34,34,34	0
54	MG	2A	3408	1/1	0.79	0.60	74,74,74,74	0
54	MG	1A	3975	1/1	0.79	0.17	52,52,52,52	0
54	MG	1a	1859	1/1	0.79	0.13	72,72,72,72	0
54	MG	2a	1774	1/1	0.79	0.12	66,66,66,66	0
54	MG	1a	1670	1/1	0.79	0.25	68,68,68,68	0
54	MG	2a	1646	1/1	0.79	0.09	77,77,77,77	0
54	MG	1a	1749	1/1	0.79	0.15	70,70,70,70	0
54	MG	1A	3794	1/1	0.79	0.14	65,65,65,65	0
54	MG	1B	208	1/1	0.79	0.33	72,72,72,72	0
54	MG	1A	3590	1/1	0.79	0.19	72,72,72,72	0
54	MG	2a	1737	1/1	0.79	0.08	67,67,67,67	0
54	MG	2a	1689	1/1	0.79	0.12	70,70,70,70	0
54	MG	1a	1700	1/1	0.79	0.10	66,66,66,66	0
54	MG	2A	3387	1/1	0.79	0.23	55,55,55,55	0
54	MG	1A	3620	1/1	0.79	0.24	40,40,40,40	0
54	MG	1A	3964	1/1	0.79	0.10	68,68,68,68	0
54	MG	1A	3680	1/1	0.79	0.15	66,66,66,66	0
57	ZN	14	501	1/1	0.79	0.25	225,225,225,225	0
54	MG	1A	3507	1/1	0.79	0.21	32,32,32,32	0
54	MG	1A	3649	1/1	0.79	0.12	59,59,59,59	0
54	MG	1a	1818	1/1	0.79	0.04	69,69,69,69	0
54	MG	2B	3004	1/1	0.79	0.15	77,77,77,77	0
54	MG	2A	3570	1/1	0.79	0.10	57,57,57,57	0
54	MG	1a	1843	1/1	0.79	0.10	67,67,67,67	0
54	MG	2A	3323	1/1	0.79	0.16	59,59,59,59	0
54	MG	1A	3967	1/1	0.79	0.33	81,81,81,81	0
54	MG	1A	3882	1/1	0.80	0.23	74,74,74,74	0
54	MG	1A	3360	1/1	0.80	0.14	55,55,55,55	0
54	MG	1A	3583	1/1	0.80	0.19	43,43,43,43	0
54	MG	1A	3573	1/1	0.80	0.22	59,59,59,59	0
54	MG	1A	3855	1/1	0.80	0.12	62,62,62,62	0
54	MG	1A	3529	1/1	0.80	0.13	55,55,55,55	0
54	MG	1A	3595	1/1	0.80	0.18	48,48,48,48	0
54	MG	2A	3712	1/1	0.80	0.18	67,67,67,67	0
54	MG	2A	3692	1/1	0.80	0.10	52,52,52,52	0
54	MG	1A	3344	1/1	0.80	0.18	59,59,59,59	0
54	MG	1A	3957	1/1	0.80	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3001	1/1	0.80	0.11	57,57,57,57	0
54	MG	2A	3463	1/1	0.80	0.15	55,55,55,55	0
54	MG	1A	3577	1/1	0.80	0.31	41,41,41,41	0
54	MG	1A	3643	1/1	0.80	0.26	72,72,72,72	0
54	MG	1A	3203	1/1	0.80	0.11	61,61,61,61	0
54	MG	1a	1785	1/1	0.80	0.15	76,76,76,76	0
54	MG	1A	3891	1/1	0.80	0.17	73,73,73,73	0
54	MG	1A	3027	1/1	0.80	0.15	60,60,60,60	0
54	MG	2A	3068	1/1	0.80	0.10	61,61,61,61	0
54	MG	1A	3589	1/1	0.80	0.14	57,57,57,57	0
54	MG	1A	3519	1/1	0.80	0.08	59,59,59,59	0
54	MG	1a	1659	1/1	0.80	0.11	76,76,76,76	0
54	MG	1a	1764	1/1	0.80	0.13	65,65,65,65	0
54	MG	2A	3540	1/1	0.80	0.12	47,47,47,47	0
54	MG	2B	3013	1/1	0.80	0.07	76,76,76,76	0
54	MG	1a	1832	1/1	0.80	0.11	72,72,72,72	0
54	MG	1a	1839	1/1	0.80	0.07	67,67,67,67	0
54	MG	2A	3380	1/1	0.80	0.15	35,35,35,35	0
54	MG	1a	1685	1/1	0.80	0.11	75,75,75,75	0
54	MG	1A	3416	1/1	0.80	0.27	33,33,33,33	0
54	MG	2a	1735	1/1	0.80	0.10	64,64,64,64	0
54	MG	2A	3577	1/1	0.80	0.08	57,57,57,57	0
54	MG	1A	3426	1/1	0.80	0.21	34,34,34,34	0
54	MG	2a	1631	1/1	0.81	0.11	77,77,77,77	0
54	MG	1A	3318	1/1	0.81	0.20	44,44,44,44	0
54	MG	2E	305	1/1	0.81	0.25	65,65,65,65	0
54	MG	1a	1768	1/1	0.81	0.10	71,71,71,71	0
54	MG	1A	3418	1/1	0.81	0.19	55,55,55,55	0
54	MG	1A	3942	1/1	0.81	0.09	59,59,59,59	0
54	MG	1A	3502	1/1	0.81	0.17	56,56,56,56	0
54	MG	1A	3331	1/1	0.81	0.12	75,75,75,75	0
54	MG	2a	1770	1/1	0.81	0.07	82,82,82,82	0
54	MG	1A	3067	1/1	0.81	0.13	60,60,60,60	0
54	MG	2a	1705	1/1	0.81	0.14	75,75,75,75	0
54	MG	1a	1795	1/1	0.81	0.08	71,71,71,71	0
54	MG	1a	1834	1/1	0.81	0.15	59,59,59,59	0
54	MG	2a	1618	1/1	0.81	0.09	75,75,75,75	0
54	MG	2A	3214	1/1	0.81	0.27	49,49,49,49	0
54	MG	2A	3582	1/1	0.81	0.33	70,70,70,70	0
54	MG	1A	3795	1/1	0.81	0.09	68,68,68,68	0
54	MG	2a	1785	1/1	0.81	0.10	76,76,76,76	0
54	MG	1A	3903	1/1	0.81	0.13	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3492	1/1	0.81	0.10	60,60,60,60	0
54	MG	1a	1705	1/1	0.81	0.16	56,56,56,56	0
54	MG	1O	8001	1/1	0.81	0.11	62,62,62,62	0
54	MG	1A	3481	1/1	0.81	0.18	57,57,57,57	0
54	MG	1A	3697	1/1	0.81	0.21	53,53,53,53	0
54	MG	2a	1675	1/1	0.81	0.20	69,69,69,69	0
54	MG	2A	3207	1/1	0.81	0.09	46,46,46,46	0
54	MG	2A	3534	1/1	0.81	0.63	78,78,78,78	0
54	MG	1a	1689	1/1	0.81	0.10	73,73,73,73	0
54	MG	2a	1693	1/1	0.81	0.14	88,88,88,88	0
54	MG	2a	1666	1/1	0.81	0.09	78,78,78,78	0
54	MG	1q	202	1/1	0.81	0.16	73,73,73,73	0
54	MG	1A	4005	1/1	0.81	0.09	97,97,97,97	0
54	MG	1D	313	1/1	0.81	0.16	52,52,52,52	0
54	MG	2O	202	1/1	0.81	0.12	94,94,94,94	0
54	MG	2a	1731	1/1	0.82	0.13	73,73,73,73	0
54	MG	1A	3756	1/1	0.82	0.17	47,47,47,47	0
54	MG	1A	3657	1/1	0.82	0.26	55,55,55,55	0
54	MG	2A	3608	1/1	0.82	0.08	64,64,64,64	0
54	MG	1A	3383	1/1	0.82	0.19	34,34,34,34	0
54	MG	2A	3614	1/1	0.82	0.14	42,42,42,42	0
54	MG	1G	3001	1/1	0.82	0.08	72,72,72,72	0
54	MG	1A	3549	1/1	0.82	0.11	63,63,63,63	0
54	MG	2D	302	1/1	0.82	0.20	52,52,52,52	0
54	MG	1a	1871	1/1	0.82	0.14	75,75,75,75	0
54	MG	1a	1815	1/1	0.82	0.12	75,75,75,75	0
54	MG	2A	3514	1/1	0.82	0.11	60,60,60,60	0
54	MG	2a	1623	1/1	0.82	0.17	73,73,73,73	0
54	MG	2A	3163	1/1	0.82	0.46	62,62,62,62	0
54	MG	2A	3644	1/1	0.82	0.08	58,58,58,58	0
54	MG	2A	3661	1/1	0.82	0.11	46,46,46,46	0
54	MG	1A	3638	1/1	0.82	0.13	35,35,35,35	0
54	MG	1A	3998	1/1	0.82	0.19	51,51,51,51	0
54	MG	2A	3675	1/1	0.82	0.05	61,61,61,61	0
54	MG	1W	3001	1/1	0.82	0.33	59,59,59,59	0
54	MG	2A	3209	1/1	0.82	0.18	63,63,63,63	0
54	MG	1A	3960	1/1	0.82	0.14	71,71,71,71	0
54	MG	2A	3058	1/1	0.82	0.21	58,58,58,58	0
54	MG	1g	203	1/1	0.82	0.19	78,78,78,78	0
54	MG	2a	1603	1/1	0.82	0.45	69,69,69,69	0
54	MG	1A	3112	1/1	0.82	0.25	67,67,67,67	0
54	MG	2A	3624	1/1	0.82	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1603	1/1	0.82	0.14	77,77,77,77	0
54	MG	1A	3666	1/1	0.82	0.11	64,64,64,64	0
54	MG	1A	3415	1/1	0.82	0.17	63,63,63,63	0
54	MG	2a	1783	1/1	0.82	0.06	62,62,62,62	0
54	MG	2A	3639	1/1	0.82	0.09	59,59,59,59	0
54	MG	2a	1620	1/1	0.82	0.11	77,77,77,77	0
54	MG	1a	1732	1/1	0.82	0.10	92,92,92,92	0
54	MG	1a	1813	1/1	0.82	0.12	81,81,81,81	0
54	MG	2a	1688	1/1	0.82	0.16	58,58,58,58	0
54	MG	1A	3010	1/1	0.82	0.13	49,49,49,49	0
54	MG	1A	3400	1/1	0.82	0.22	61,61,61,61	0
54	MG	1A	3531	1/1	0.82	0.15	66,66,66,66	0
54	MG	2A	3310	1/1	0.83	0.27	62,62,62,62	0
54	MG	2A	3457	1/1	0.83	0.13	62,62,62,62	0
54	MG	1B	223	1/1	0.83	0.08	69,69,69,69	0
54	MG	1I	103	1/1	0.83	0.14	60,60,60,60	0
54	MG	2A	3508	1/1	0.83	0.18	59,59,59,59	0
54	MG	1A	3672	1/1	0.83	0.07	68,68,68,68	0
54	MG	2A	3728	1/1	0.83	0.12	58,58,58,58	0
54	MG	2A	3547	1/1	0.83	0.21	63,63,63,63	0
54	MG	2a	1691	1/1	0.83	0.14	71,71,71,71	0
54	MG	1a	1874	1/1	0.83	0.11	66,66,66,66	0
54	MG	2A	3662	1/1	0.83	0.06	59,59,59,59	0
54	MG	2A	3247	1/1	0.83	0.19	55,55,55,55	0
54	MG	1a	1804	1/1	0.83	0.09	65,65,65,65	0
54	MG	2A	3667	1/1	0.83	0.15	49,49,49,49	0
54	MG	1G	3003	1/1	0.83	0.11	63,63,63,63	0
54	MG	1A	3190	1/1	0.83	0.14	61,61,61,61	0
54	MG	2a	1678	1/1	0.83	0.21	66,66,66,66	0
54	MG	1A	3768	1/1	0.83	0.17	67,67,67,67	0
54	MG	1A	3673	1/1	0.83	0.07	55,55,55,55	0
54	MG	1A	3293	1/1	0.83	0.12	50,50,50,50	0
54	MG	1B	211	1/1	0.83	0.16	69,69,69,69	0
54	MG	1A	3432	1/1	0.83	0.15	67,67,67,67	0
54	MG	2A	3363	1/1	0.83	0.10	64,64,64,64	0
54	MG	1A	3348	1/1	0.83	0.13	44,44,44,44	0
54	MG	2A	3146	1/1	0.83	0.18	61,61,61,61	0
54	MG	1A	3690	1/1	0.83	0.18	51,51,51,51	0
54	MG	2a	1644	1/1	0.83	0.18	75,75,75,75	0
54	MG	1B	224	1/1	0.83	0.12	44,44,44,44	0
54	MG	1A	3870	1/1	0.83	0.21	71,71,71,71	0
54	MG	1A	3987	1/1	0.83	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3784	1/1	0.83	0.11	36,36,36,36	0
54	MG	1A	3937	1/1	0.83	0.07	71,71,71,71	0
54	MG	1a	1797	1/1	0.83	0.07	74,74,74,74	0
54	MG	2a	1685	1/1	0.83	0.34	64,64,64,64	0
54	MG	2a	1636	1/1	0.84	0.11	64,64,64,64	0
54	MG	1A	3596	1/1	0.84	0.26	47,47,47,47	0
54	MG	2a	1724	1/1	0.84	0.14	82,82,82,82	0
54	MG	2A	3511	1/1	0.84	0.08	62,62,62,62	0
54	MG	1E	301	1/1	0.84	0.32	40,40,40,40	0
54	MG	2a	1714	1/1	0.84	0.09	69,69,69,69	0
54	MG	1B	227	1/1	0.84	0.11	76,76,76,76	0
54	MG	1e	201	1/1	0.84	0.16	65,65,65,65	0
54	MG	2A	3430	1/1	0.84	0.13	52,52,52,52	0
54	MG	1y	204	1/1	0.84	0.29	93,93,93,93	0
54	MG	1A	3261	1/1	0.84	0.13	64,64,64,64	0
55	MPD	2A	3747	8/8	0.84	0.23	37,47,59,61	0
54	MG	2A	3371	1/1	0.84	0.12	70,70,70,70	0
54	MG	2A	3446	1/1	0.84	0.07	58,58,58,58	0
54	MG	1A	3319	1/1	0.84	0.15	65,65,65,65	0
54	MG	2A	3202	1/1	0.84	0.16	49,49,49,49	0
54	MG	1B	215	1/1	0.84	0.12	59,59,59,59	0
54	MG	2B	3011	1/1	0.84	0.06	61,61,61,61	0
54	MG	1A	3601	1/1	0.84	0.25	38,38,38,38	0
54	MG	2A	3212	1/1	0.84	0.12	70,70,70,70	0
54	MG	1a	1730	1/1	0.84	0.12	62,62,62,62	0
54	MG	2A	3257	1/1	0.84	0.15	58,58,58,58	0
54	MG	2A	3714	1/1	0.84	0.08	56,56,56,56	0
54	MG	2A	3696	1/1	0.84	0.08	56,56,56,56	0
54	MG	1A	3969	1/1	0.84	0.24	61,61,61,61	0
54	MG	2A	3159	1/1	0.84	0.20	46,46,46,46	0
54	MG	1a	1696	1/1	0.84	0.20	68,68,68,68	0
54	MG	1A	3933	1/1	0.84	0.17	68,68,68,68	0
54	MG	2A	3035	1/1	0.84	0.13	67,67,67,67	0
54	MG	1A	3912	1/1	0.84	0.12	39,39,39,39	0
54	MG	1A	3459	1/1	0.84	0.11	55,55,55,55	0
54	MG	1a	1625	1/1	0.84	0.10	53,53,53,53	0
54	MG	2A	3519	1/1	0.84	0.22	60,60,60,60	0
54	MG	1A	3925	1/1	0.84	0.07	54,54,54,54	0
54	MG	1a	1613	1/1	0.84	0.17	71,71,71,71	0
54	MG	1A	3849	1/1	0.84	0.11	53,53,53,53	0
54	MG	1a	1777	1/1	0.84	0.11	55,55,55,55	0
54	MG	2B	3008	1/1	0.84	0.08	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1702	1/1	0.84	0.16	67,67,67,67	0
54	MG	1A	3721	1/1	0.84	0.11	64,64,64,64	0
54	MG	2A	3260	1/1	0.84	0.12	53,53,53,53	0
54	MG	1a	1822	1/1	0.84	0.13	68,68,68,68	0
54	MG	2a	1745	1/1	0.84	0.08	46,46,46,46	0
54	MG	1A	3292	1/1	0.84	0.14	58,58,58,58	0
54	MG	1A	3397	1/1	0.84	0.17	33,33,33,33	0
54	MG	2a	1622	1/1	0.84	0.15	74,74,74,74	0
54	MG	1A	4016	1/1	0.85	0.10	62,62,62,62	0
54	MG	1A	3212	1/1	0.85	0.18	48,48,48,48	0
54	MG	1A	3610	1/1	0.85	0.16	35,35,35,35	0
54	MG	1a	1814	1/1	0.85	0.06	67,67,67,67	0
54	MG	2A	3695	1/1	0.85	0.14	57,57,57,57	0
54	MG	2A	3302	1/1	0.85	0.15	57,57,57,57	0
54	MG	2a	1661	1/1	0.85	0.15	74,74,74,74	0
54	MG	2A	3329	1/1	0.85	0.18	60,60,60,60	0
54	MG	1A	3939	1/1	0.85	0.11	61,61,61,61	0
54	MG	1A	3739	1/1	0.85	0.09	45,45,45,45	0
54	MG	1A	3904	1/1	0.85	0.08	51,51,51,51	0
54	MG	2A	3142	1/1	0.85	0.09	47,47,47,47	0
54	MG	2A	3571	1/1	0.85	0.14	44,44,44,44	0
54	MG	2A	3690	1/1	0.85	0.06	63,63,63,63	0
54	MG	1A	3688	1/1	0.85	0.09	80,80,80,80	0
54	MG	2a	1763	1/1	0.85	0.13	51,51,51,51	0
54	MG	2A	3389	1/1	0.85	0.11	56,56,56,56	0
54	MG	1A	3591	1/1	0.85	0.10	55,55,55,55	0
54	MG	1A	4027	1/1	0.85	0.22	55,55,55,55	0
54	MG	1A	3843	1/1	0.85	0.19	53,53,53,53	0
54	MG	2a	1650	1/1	0.85	0.23	74,74,74,74	0
54	MG	2a	1633	1/1	0.85	0.11	69,69,69,69	0
54	MG	2a	1654	1/1	0.85	0.15	60,60,60,60	0
54	MG	2a	1720	1/1	0.85	0.09	63,63,63,63	0
54	MG	2a	1638	1/1	0.85	0.14	62,62,62,62	0
54	MG	2a	1637	1/1	0.85	0.10	92,92,92,92	0
54	MG	1A	3353	1/1	0.85	0.13	53,53,53,53	0
54	MG	2F	301	1/1	0.85	0.13	44,44,44,44	0
54	MG	1A	3288	1/1	0.85	0.42	57,57,57,57	0
54	MG	2a	1748	1/1	0.85	0.09	75,75,75,75	0
54	MG	2a	1676	1/1	0.85	0.23	62,62,62,62	0
54	MG	2a	1687	1/1	0.85	0.08	82,82,82,82	0
54	MG	1A	3407	1/1	0.85	0.19	66,66,66,66	0
54	MG	1A	3439	1/1	0.85	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1B	229	1/1	0.85	0.12	60,60,60,60	0
54	MG	1a	1840	1/1	0.85	0.17	58,58,58,58	0
54	MG	1a	1606	1/1	0.85	0.12	63,63,63,63	0
54	MG	2A	3166	1/1	0.85	0.16	61,61,61,61	0
54	MG	1A	3609	1/1	0.85	0.16	54,54,54,54	0
54	MG	1A	3803	1/1	0.85	0.15	50,50,50,50	0
54	MG	2a	1663	1/1	0.85	0.19	67,67,67,67	0
54	MG	2a	1719	1/1	0.85	0.10	76,76,76,76	0
54	MG	1a	1642	1/1	0.85	0.15	70,70,70,70	0
54	MG	2D	309	1/1	0.85	0.17	65,65,65,65	0
54	MG	2A	3565	1/1	0.85	0.21	57,57,57,57	0
54	MG	1a	1759	1/1	0.85	0.08	65,65,65,65	0
54	MG	2B	3003	1/1	0.85	0.21	71,71,71,71	0
54	MG	1A	4051	1/1	0.85	0.24	52,52,52,52	0
54	MG	1a	1752	1/1	0.85	0.10	73,73,73,73	0
54	MG	1A	3644	1/1	0.85	0.18	48,48,48,48	0
54	MG	2A	3118	1/1	0.85	0.22	45,45,45,45	0
54	MG	2A	3529	1/1	0.85	0.10	54,54,54,54	0
54	MG	1A	3090	1/1	0.85	0.24	55,55,55,55	0
54	MG	1a	1812	1/1	0.85	0.10	51,51,51,51	0
54	MG	2A	3213	1/1	0.85	0.14	60,60,60,60	0
54	MG	1A	3965	1/1	0.85	0.13	63,63,63,63	0
54	MG	2A	3034	1/1	0.85	0.16	49,49,49,49	0
54	MG	1A	3022	1/1	0.85	0.17	46,46,46,46	0
54	MG	1A	3973	1/1	0.85	0.16	44,44,44,44	0
54	MG	1A	3916	1/1	0.85	0.17	68,68,68,68	0
54	MG	1A	3527	1/1	0.86	0.15	32,32,32,32	0
54	MG	1a	1863	1/1	0.86	0.08	64,64,64,64	0
54	MG	2A	3191	1/1	0.86	0.10	53,53,53,53	0
54	MG	1A	3949	1/1	0.86	0.14	69,69,69,69	0
54	MG	1a	1866	1/1	0.86	0.10	69,69,69,69	0
54	MG	1A	3921	1/1	0.86	0.16	61,61,61,61	0
54	MG	1A	3611	1/1	0.86	0.13	54,54,54,54	0
54	MG	1A	3646	1/1	0.86	0.63	81,81,81,81	0
54	MG	2A	3040	1/1	0.86	0.18	58,58,58,58	0
54	MG	2A	3336	1/1	0.86	0.11	55,55,55,55	0
54	MG	1a	1719	1/1	0.86	0.11	94,94,94,94	0
54	MG	1A	3142	1/1	0.86	0.15	51,51,51,51	0
54	MG	2B	3005	1/1	0.86	0.22	60,60,60,60	0
54	MG	2A	3189	1/1	0.86	0.22	57,57,57,57	0
54	MG	2A	3572	1/1	0.86	0.15	52,52,52,52	0
54	MG	1A	3765	1/1	0.86	0.10	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2P	201	1/1	0.86	0.11	55,55,55,55	0
54	MG	1a	1789	1/1	0.86	0.08	67,67,67,67	0
54	MG	1a	1850	1/1	0.86	0.11	94,94,94,94	0
54	MG	2A	3055	1/1	0.86	0.25	54,54,54,54	0
54	MG	1A	3789	1/1	0.86	0.13	58,58,58,58	0
54	MG	1a	1680	1/1	0.86	0.09	69,69,69,69	0
54	MG	2B	3006	1/1	0.86	0.08	72,72,72,72	0
54	MG	1A	3284	1/1	0.86	0.12	59,59,59,59	0
54	MG	1A	3414	1/1	0.86	0.15	33,33,33,33	0
54	MG	1A	3035	1/1	0.86	0.26	57,57,57,57	0
54	MG	1a	1790	1/1	0.86	0.14	52,52,52,52	0
54	MG	2A	3266	1/1	0.86	0.17	55,55,55,55	0
54	MG	1a	1667	1/1	0.86	0.14	63,63,63,63	0
54	MG	2B	3014	1/1	0.86	0.12	65,65,65,65	0
54	MG	2a	1702	1/1	0.86	0.10	65,65,65,65	0
54	MG	2a	1740	1/1	0.86	0.10	80,80,80,80	0
54	MG	1A	3370	1/1	0.86	0.06	54,54,54,54	0
54	MG	2a	1671	1/1	0.86	0.21	70,70,70,70	0
54	MG	1A	3841	1/1	0.86	0.17	49,49,49,49	0
54	MG	2A	3275	1/1	0.86	0.10	58,58,58,58	0
54	MG	1a	1753	1/1	0.86	0.10	62,62,62,62	0
54	MG	2A	3704	1/1	0.86	0.06	48,48,48,48	0
54	MG	1A	3516	1/1	0.86	0.15	60,60,60,60	0
54	MG	2G	3001	1/1	0.86	0.07	76,76,76,76	0
54	MG	2A	3521	1/1	0.86	0.45	57,57,57,57	0
54	MG	1A	3282	1/1	0.86	0.15	60,60,60,60	0
55	MPD	2B	3020	8/8	0.86	0.17	47,70,77,79	0
54	MG	1a	1794	1/1	0.86	0.10	58,58,58,58	0
54	MG	2A	3153	1/1	0.86	0.14	48,48,48,48	0
54	MG	1a	1675	1/1	0.86	0.19	70,70,70,70	0
54	MG	2A	3144	1/1	0.86	0.21	53,53,53,53	0
54	MG	1A	3873	1/1	0.86	0.14	48,48,48,48	0
54	MG	1A	3002	1/1	0.86	0.12	54,54,54,54	0
54	MG	1a	1803	1/1	0.86	0.14	87,87,87,87	0
54	MG	1a	1784	1/1	0.86	0.09	66,66,66,66	0
54	MG	1a	1878	1/1	0.86	0.13	66,66,66,66	0
54	MG	2A	3235	1/1	0.86	0.36	48,48,48,48	0
54	MG	1A	3089	1/1	0.86	0.22	47,47,47,47	0
54	MG	2A	3252	1/1	0.86	0.17	54,54,54,54	0
54	MG	1n	502	1/1	0.86	0.10	46,46,46,46	0
54	MG	1a	1677	1/1	0.86	0.17	63,63,63,63	0
54	MG	1A	3480	1/1	0.86	0.22	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3458	1/1	0.86	0.11	57,57,57,57	0
54	MG	2G	3002	1/1	0.86	0.13	79,79,79,79	0
54	MG	2a	1617	1/1	0.86	0.12	65,65,65,65	0
54	MG	2A	3548	1/1	0.86	0.08	55,55,55,55	0
54	MG	2A	3204	1/1	0.86	0.19	66,66,66,66	0
54	MG	2A	3060	1/1	0.86	0.13	42,42,42,42	0
54	MG	2A	3650	1/1	0.86	0.06	61,61,61,61	0
54	MG	1A	3598	1/1	0.87	0.14	35,35,35,35	0
54	MG	2A	3050	1/1	0.87	0.13	54,54,54,54	0
54	MG	1B	216	1/1	0.87	0.35	58,58,58,58	0
54	MG	2A	3434	1/1	0.87	0.09	56,56,56,56	0
54	MG	1a	1684	1/1	0.87	0.34	73,73,73,73	0
54	MG	1F	305	1/1	0.87	0.30	66,66,66,66	0
54	MG	1V	203	1/1	0.87	0.12	63,63,63,63	0
54	MG	1l	102	1/1	0.87	0.08	49,49,49,49	0
54	MG	2a	1660	1/1	0.87	0.12	72,72,72,72	0
54	MG	2A	3428	1/1	0.87	0.09	57,57,57,57	0
54	MG	1W	3002	1/1	0.87	0.16	52,52,52,52	0
54	MG	2A	3333	1/1	0.87	0.15	38,38,38,38	0
54	MG	2a	1791	1/1	0.87	0.07	61,61,61,61	0
54	MG	2A	3320	1/1	0.87	0.13	47,47,47,47	0
54	MG	1A	3703	1/1	0.87	0.10	41,41,41,41	0
54	MG	1a	1820	1/1	0.87	0.10	76,76,76,76	0
54	MG	1A	3365	1/1	0.87	0.14	69,69,69,69	0
54	MG	1A	3627	1/1	0.87	0.23	42,42,42,42	0
54	MG	1A	3752	1/1	0.87	0.25	57,57,57,57	0
54	MG	2A	3366	1/1	0.87	0.07	53,53,53,53	0
54	MG	1A	3607	1/1	0.87	0.23	52,52,52,52	0
54	MG	1A	3814	1/1	0.87	0.12	60,60,60,60	0
54	MG	1a	1671	1/1	0.87	0.28	63,63,63,63	0
54	MG	1A	3451	1/1	0.87	0.10	48,48,48,48	0
54	MG	1A	3454	1/1	0.87	0.23	31,31,31,31	0
54	MG	2A	3164	1/1	0.87	0.37	58,58,58,58	0
54	MG	2A	3524	1/1	0.87	0.12	64,64,64,64	0
54	MG	2a	1658	1/1	0.87	0.14	60,60,60,60	0
54	MG	2A	3469	1/1	0.87	0.22	62,62,62,62	0
54	MG	1A	3219	1/1	0.87	0.14	65,65,65,65	0
54	MG	2A	3538	1/1	0.87	0.12	49,49,49,49	0
54	MG	2A	3475	1/1	0.87	0.09	62,62,62,62	0
54	MG	1A	3134	1/1	0.87	0.20	45,45,45,45	0
54	MG	2A	3372	1/1	0.87	0.17	51,51,51,51	0
54	MG	2A	3537	1/1	0.87	0.11	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3230	1/1	0.87	0.18	44,44,44,44	0
54	MG	1a	1837	1/1	0.87	0.07	74,74,74,74	0
54	MG	2A	3340	1/1	0.87	0.10	54,54,54,54	0
54	MG	1A	3324	1/1	0.87	0.19	61,61,61,61	0
54	MG	2A	3136	1/1	0.87	0.10	64,64,64,64	0
54	MG	2A	3345	1/1	0.87	0.13	35,35,35,35	0
54	MG	2A	3152	1/1	0.87	0.20	61,61,61,61	0
54	MG	2A	3306	1/1	0.87	0.12	56,56,56,56	0
54	MG	2A	3422	1/1	0.87	0.09	56,56,56,56	0
54	MG	2A	3664	1/1	0.87	0.05	61,61,61,61	0
54	MG	2A	3486	1/1	0.87	0.04	63,63,63,63	0
54	MG	1A	3321	1/1	0.87	0.12	50,50,50,50	0
54	MG	2A	3483	1/1	0.87	0.17	37,37,37,37	0
54	MG	2a	1757	1/1	0.87	0.09	49,49,49,49	0
54	MG	1a	1856	1/1	0.87	0.06	58,58,58,58	0
54	MG	2A	3059	1/1	0.87	0.15	45,45,45,45	0
54	MG	1A	3679	1/1	0.87	0.04	69,69,69,69	0
54	MG	1A	3926	1/1	0.87	0.12	65,65,65,65	0
54	MG	1a	1605	1/1	0.87	0.13	61,61,61,61	0
54	MG	2A	3416	1/1	0.87	0.18	61,61,61,61	0
54	MG	1A	3150	1/1	0.87	0.15	58,58,58,58	0
54	MG	2A	3346	1/1	0.87	0.14	55,55,55,55	0
54	MG	2A	3587	1/1	0.87	0.10	52,52,52,52	0
54	MG	1A	3846	1/1	0.87	0.13	47,47,47,47	0
54	MG	1a	1621	1/1	0.87	0.16	48,48,48,48	0
54	MG	1a	1622	1/1	0.87	0.07	47,47,47,47	0
54	MG	1a	1712	1/1	0.87	0.06	50,50,50,50	0
54	MG	1A	3581	1/1	0.87	0.10	67,67,67,67	0
54	MG	1A	3335	1/1	0.87	0.16	37,37,37,37	0
54	MG	2A	3197	1/1	0.87	0.14	47,47,47,47	0
54	MG	1A	4076	1/1	0.87	0.20	57,57,57,57	0
54	MG	1A	3434	1/1	0.87	0.14	72,72,72,72	0
54	MG	2A	3114	1/1	0.87	0.10	47,47,47,47	0
54	MG	2A	3751	1/1	0.87	0.22	48,48,48,48	0
54	MG	1A	3678	1/1	0.87	0.06	62,62,62,62	0
54	MG	1A	3339	1/1	0.87	0.11	54,54,54,54	0
54	MG	1A	3115	1/1	0.88	0.13	46,46,46,46	0
54	MG	2A	3515	1/1	0.88	0.22	34,34,34,34	0
54	MG	1A	3632	1/1	0.88	0.14	56,56,56,56	0
54	MG	1A	3199	1/1	0.88	0.19	70,70,70,70	0
54	MG	2a	1759	1/1	0.88	0.09	75,75,75,75	0
54	MG	1A	3285	1/1	0.88	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1665	1/1	0.88	0.08	67,67,67,67	0
54	MG	1A	3683	1/1	0.88	0.09	57,57,57,57	0
54	MG	2A	3358	1/1	0.88	0.11	69,69,69,69	0
54	MG	2A	3618	1/1	0.88	0.18	37,37,37,37	0
54	MG	1A	3166	1/1	0.88	0.24	61,61,61,61	0
54	MG	2A	3172	1/1	0.88	0.12	61,61,61,61	0
54	MG	2a	1779	1/1	0.88	0.08	78,78,78,78	0
54	MG	2A	3347	1/1	0.88	0.13	34,34,34,34	0
54	MG	1A	3737	1/1	0.88	0.12	57,57,57,57	0
54	MG	2A	3066	1/1	0.88	0.08	45,45,45,45	0
54	MG	1B	225	1/1	0.88	0.21	68,68,68,68	0
54	MG	1A	3761	1/1	0.88	0.14	58,58,58,58	0
54	MG	1A	3935	1/1	0.88	0.12	53,53,53,53	0
54	MG	2a	1655	1/1	0.88	0.16	69,69,69,69	0
54	MG	2a	1772	1/1	0.88	0.12	58,58,58,58	0
54	MG	2A	3730	1/1	0.88	0.17	56,56,56,56	0
54	MG	2A	3719	1/1	0.88	0.11	56,56,56,56	0
54	MG	2A	3476	1/1	0.88	0.08	55,55,55,55	0
54	MG	1A	3428	1/1	0.88	0.11	48,48,48,48	0
54	MG	2A	3474	1/1	0.88	0.15	65,65,65,65	0
54	MG	2a	1696	1/1	0.88	0.11	73,73,73,73	0
54	MG	2A	3236	1/1	0.88	0.11	49,49,49,49	0
54	MG	1a	1772	1/1	0.88	0.12	77,77,77,77	0
54	MG	1A	3560	1/1	0.88	0.12	57,57,57,57	0
54	MG	1A	3405	1/1	0.88	0.25	65,65,65,65	0
54	MG	2A	3707	1/1	0.88	0.10	39,39,39,39	0
54	MG	1A	3192	1/1	0.88	0.15	68,68,68,68	0
54	MG	18	101	1/1	0.88	0.05	60,60,60,60	0
54	MG	2A	3062	1/1	0.88	0.17	53,53,53,53	0
54	MG	1A	3958	1/1	0.88	0.08	63,63,63,63	0
54	MG	1a	1758	1/1	0.88	0.23	73,73,73,73	0
57	ZN	29	501	1/1	0.88	0.22	131,131,131,131	0
54	MG	1a	1823	1/1	0.88	0.11	75,75,75,75	0
54	MG	1A	3109	1/1	0.88	0.18	45,45,45,45	0
54	MG	1A	3930	1/1	0.88	0.16	60,60,60,60	0
54	MG	2a	1670	1/1	0.88	0.14	65,65,65,65	0
54	MG	1A	3399	1/1	0.88	0.15	54,54,54,54	0
54	MG	1A	3669	1/1	0.88	0.06	46,46,46,46	0
55	MPD	1T	8004	8/8	0.88	0.16	56,61,69,80	0
54	MG	1a	1830	1/1	0.88	0.28	84,84,84,84	0
54	MG	1A	3883	1/1	0.88	0.17	38,38,38,38	0
54	MG	2A	3687	1/1	0.88	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1849	1/1	0.88	0.13	66,66,66,66	0
54	MG	1A	3051	1/1	0.88	0.39	48,48,48,48	0
54	MG	1A	3033	1/1	0.88	0.23	44,44,44,44	0
54	MG	2D	308	1/1	0.88	0.12	31,31,31,31	0
54	MG	1A	3674	1/1	0.88	0.19	58,58,58,58	0
54	MG	2A	3693	1/1	0.88	0.11	57,57,57,57	0
54	MG	1B	219	1/1	0.88	0.18	44,44,44,44	0
54	MG	1A	3402	1/1	0.88	0.15	73,73,73,73	0
54	MG	2A	3267	1/1	0.88	0.07	60,60,60,60	0
54	MG	1A	3642	1/1	0.88	0.27	39,39,39,39	0
54	MG	1A	3441	1/1	0.88	0.18	64,64,64,64	0
54	MG	2a	1606	1/1	0.88	0.19	57,57,57,57	0
54	MG	2A	3042	1/1	0.88	0.19	47,47,47,47	0
54	MG	2A	3568	1/1	0.88	0.20	42,42,42,42	0
54	MG	1A	3060	1/1	0.88	0.16	49,49,49,49	0
54	MG	1a	1821	1/1	0.88	0.12	72,72,72,72	0
54	MG	1A	3225	1/1	0.88	0.13	49,49,49,49	0
54	MG	1q	201	1/1	0.88	0.24	55,55,55,55	0
54	MG	1A	3273	1/1	0.88	0.12	55,55,55,55	0
54	MG	1a	1800	1/1	0.88	0.19	70,70,70,70	0
54	MG	1A	3479	1/1	0.88	0.21	42,42,42,42	0
54	MG	1a	1602	1/1	0.88	0.09	73,73,73,73	0
54	MG	1A	3608	1/1	0.88	0.17	37,37,37,37	0
54	MG	2A	3218	1/1	0.88	0.19	60,60,60,60	0
54	MG	2A	3467	1/1	0.88	0.15	67,67,67,67	0
54	MG	2A	3182	1/1	0.88	0.13	49,49,49,49	0
54	MG	2A	3723	1/1	0.88	0.30	44,44,44,44	0
54	MG	2A	3157	1/1	0.88	0.74	68,68,68,68	0
54	MG	1A	4023	1/1	0.88	0.09	60,60,60,60	0
54	MG	2A	3487	1/1	0.88	0.15	73,73,73,73	0
54	MG	28	8001	1/1	0.88	0.12	66,66,66,66	0
54	MG	1A	3584	1/1	0.88	0.14	47,47,47,47	0
54	MG	2a	1711	1/1	0.88	0.08	79,79,79,79	0
54	MG	1A	3458	1/1	0.88	0.14	48,48,48,48	0
54	MG	1A	3695	1/1	0.88	0.11	51,51,51,51	0
54	MG	1A	3490	1/1	0.88	0.14	66,66,66,66	0
54	MG	2A	3226	1/1	0.88	0.20	69,69,69,69	0
54	MG	2A	3501	1/1	0.88	0.17	72,72,72,72	0
54	MG	1A	3129	1/1	0.88	0.14	49,49,49,49	0
54	MG	1A	3662	1/1	0.88	0.07	48,48,48,48	0
54	MG	1A	3689	1/1	0.88	0.09	71,71,71,71	0
54	MG	2a	1717	1/1	0.88	0.06	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3722	1/1	0.88	0.17	57,57,57,57	0
54	MG	2a	1608	1/1	0.88	0.17	69,69,69,69	0
54	MG	1A	3304	1/1	0.88	0.26	62,62,62,62	0
54	MG	2A	3245	1/1	0.88	0.13	56,56,56,56	0
54	MG	2A	3630	1/1	0.88	0.10	52,52,52,52	0
54	MG	1A	3835	1/1	0.88	0.13	47,47,47,47	0
54	MG	1B	203	1/1	0.88	0.09	70,70,70,70	0
54	MG	2A	3444	1/1	0.88	0.09	61,61,61,61	0
54	MG	1A	3900	1/1	0.88	0.14	29,29,29,29	0
54	MG	1A	3929	1/1	0.89	0.08	52,52,52,52	0
54	MG	2A	3427	1/1	0.89	0.07	51,51,51,51	0
54	MG	2a	1673	1/1	0.89	0.11	68,68,68,68	0
54	MG	2A	3083	1/1	0.89	0.08	69,69,69,69	0
54	MG	2A	3296	1/1	0.89	0.14	42,42,42,42	0
54	MG	2A	3277	1/1	0.89	0.14	58,58,58,58	0
54	MG	1A	3012	1/1	0.89	0.14	38,38,38,38	0
54	MG	2A	3678	1/1	0.89	0.07	54,54,54,54	0
54	MG	2A	3230	1/1	0.89	0.14	62,62,62,62	0
54	MG	2A	3132	1/1	0.89	0.09	60,60,60,60	0
54	MG	2A	3700	1/1	0.89	0.10	49,49,49,49	0
54	MG	1a	1731	1/1	0.89	0.11	54,54,54,54	0
54	MG	2A	3395	1/1	0.89	0.06	51,51,51,51	0
54	MG	1A	3565	1/1	0.89	0.15	50,50,50,50	0
54	MG	1A	3863	1/1	0.89	0.08	51,51,51,51	0
54	MG	1A	3548	1/1	0.89	0.11	57,57,57,57	0
54	MG	1a	1644	1/1	0.89	0.08	57,57,57,57	0
54	MG	1A	3635	1/1	0.89	0.08	59,59,59,59	0
54	MG	1a	1725	1/1	0.89	0.10	67,67,67,67	0
54	MG	1a	1756	1/1	0.89	0.15	57,57,57,57	0
54	MG	2A	3412	1/1	0.89	0.05	60,60,60,60	0
54	MG	2l	3001	1/1	0.89	0.24	64,64,64,64	0
54	MG	2A	3433	1/1	0.89	0.11	32,32,32,32	0
54	MG	2a	1725	1/1	0.89	0.06	64,64,64,64	0
54	MG	2A	3492	1/1	0.89	0.18	57,57,57,57	0
54	MG	1A	3557	1/1	0.89	0.08	61,61,61,61	0
54	MG	1A	3716	1/1	0.89	0.28	48,48,48,48	0
54	MG	1A	3014	1/1	0.89	0.14	58,58,58,58	0
54	MG	2A	3497	1/1	0.89	0.09	47,47,47,47	0
54	MG	1A	3563	1/1	0.89	0.23	53,53,53,53	0
54	MG	1A	3905	1/1	0.89	0.13	55,55,55,55	0
54	MG	1A	3974	1/1	0.89	0.16	75,75,75,75	0
54	MG	2A	3241	1/1	0.89	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3094	1/1	0.89	0.20	40,40,40,40	0
54	MG	2A	3143	1/1	0.89	0.09	40,40,40,40	0
54	MG	1A	3653	1/1	0.89	0.11	40,40,40,40	0
54	MG	2A	3527	1/1	0.89	0.07	66,66,66,66	0
54	MG	1A	3206	1/1	0.89	0.32	65,65,65,65	0
54	MG	1A	3465	1/1	0.89	0.08	59,59,59,59	0
54	MG	1A	3278	1/1	0.89	0.13	56,56,56,56	0
54	MG	2A	3725	1/1	0.89	0.14	61,61,61,61	0
54	MG	1a	1778	1/1	0.89	0.10	67,67,67,67	0
54	MG	2A	3348	1/1	0.89	0.10	62,62,62,62	0
54	MG	2A	3061	1/1	0.89	0.16	50,50,50,50	0
54	MG	1A	3213	1/1	0.89	0.25	63,63,63,63	0
54	MG	1T	8003	1/1	0.89	0.10	72,72,72,72	0
54	MG	1a	1782	1/1	0.89	0.12	75,75,75,75	0
54	MG	2A	3314	1/1	0.89	0.09	38,38,38,38	0
54	MG	1A	3073	1/1	0.89	0.12	38,38,38,38	0
54	MG	1A	3725	1/1	0.89	0.14	51,51,51,51	0
54	MG	1A	3154	1/1	0.89	0.12	67,67,67,67	0
54	MG	1a	1645	1/1	0.89	0.27	61,61,61,61	0
54	MG	1A	3718	1/1	0.89	0.19	47,47,47,47	0
54	MG	2A	3381	1/1	0.89	0.12	39,39,39,39	0
54	MG	1A	3877	1/1	0.89	0.20	40,40,40,40	0
54	MG	2j	8001	1/1	0.89	0.11	82,82,82,82	0
54	MG	1A	3995	1/1	0.89	0.16	44,44,44,44	0
54	MG	2A	3014	1/1	0.89	0.14	53,53,53,53	0
54	MG	2P	202	1/1	0.89	0.10	55,55,55,55	0
54	MG	2a	1733	1/1	0.89	0.19	83,83,83,83	0
54	MG	1A	3847	1/1	0.89	0.13	59,59,59,59	0
54	MG	1A	3997	1/1	0.89	0.19	58,58,58,58	0
54	MG	1A	3195	1/1	0.89	0.15	47,47,47,47	0
54	MG	1A	3205	1/1	0.89	0.30	57,57,57,57	0
54	MG	2a	1672	1/1	0.89	0.12	73,73,73,73	0
54	MG	1A	3684	1/1	0.89	0.19	39,39,39,39	0
54	MG	1A	3083	1/1	0.89	0.13	38,38,38,38	0
54	MG	2A	3073	1/1	0.89	0.18	49,49,49,49	0
54	MG	1A	3555	1/1	0.89	0.14	53,53,53,53	0
54	MG	1A	3694	1/1	0.89	0.22	69,69,69,69	0
54	MG	1A	3314	1/1	0.89	0.14	73,73,73,73	0
54	MG	1A	4026	1/1	0.89	0.11	46,46,46,46	0
54	MG	1A	3647	1/1	0.89	0.08	49,49,49,49	0
54	MG	1A	3731	1/1	0.89	0.16	38,38,38,38	0
54	MG	1A	3315	1/1	0.89	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1r	3001	1/1	0.89	0.14	65,65,65,65	0
54	MG	1A	3603	1/1	0.89	0.04	53,53,53,53	0
54	MG	1A	3102	1/1	0.89	0.14	48,48,48,48	0
54	MG	1a	1780	1/1	0.89	0.14	53,53,53,53	0
54	MG	1A	3224	1/1	0.89	0.09	69,69,69,69	0
54	MG	1A	3753	1/1	0.89	0.13	57,57,57,57	0
54	MG	2A	3413	1/1	0.89	0.21	59,59,59,59	0
54	MG	2A	3037	1/1	0.89	0.29	52,52,52,52	0
54	MG	1A	3305	1/1	0.89	0.17	54,54,54,54	0
54	MG	1a	1762	1/1	0.89	0.09	80,80,80,80	0
54	MG	2A	3273	1/1	0.89	0.06	44,44,44,44	0
54	MG	2a	1767	1/1	0.90	0.07	70,70,70,70	0
54	MG	2A	3317	1/1	0.90	0.10	37,37,37,37	0
54	MG	1A	3320	1/1	0.90	0.22	33,33,33,33	0
54	MG	1h	3002	1/1	0.90	0.18	58,58,58,58	0
54	MG	2A	3258	1/1	0.90	0.28	44,44,44,44	0
54	MG	1A	3961	1/1	0.90	0.09	45,45,45,45	0
54	MG	2A	3637	1/1	0.90	0.12	49,49,49,49	0
54	MG	1a	1681	1/1	0.90	0.15	61,61,61,61	0
54	MG	2B	3010	1/1	0.90	0.17	80,80,80,80	0
54	MG	1A	3781	1/1	0.90	0.08	48,48,48,48	0
54	MG	2A	3745	1/1	0.90	0.27	67,67,67,67	0
54	MG	1A	3724	1/1	0.90	0.06	66,66,66,66	0
54	MG	2A	3170	1/1	0.90	0.10	59,59,59,59	0
54	MG	1A	3501	1/1	0.90	0.09	69,69,69,69	0
54	MG	2A	3180	1/1	0.90	0.16	49,49,49,49	0
54	MG	1A	3429	1/1	0.90	0.20	57,57,57,57	0
54	MG	1B	206	1/1	0.90	0.10	51,51,51,51	0
54	MG	1A	3922	1/1	0.90	0.20	30,30,30,30	0
54	MG	2A	3080	1/1	0.90	0.07	50,50,50,50	0
54	MG	2A	3133	1/1	0.90	0.45	57,57,57,57	0
54	MG	1a	1649	1/1	0.90	0.19	58,58,58,58	0
54	MG	1D	312	1/1	0.90	0.11	54,54,54,54	0
54	MG	2a	1787	1/1	0.90	0.18	82,82,82,82	0
54	MG	1a	1637	1/1	0.90	0.26	68,68,68,68	0
54	MG	1B	218	1/1	0.90	0.09	48,48,48,48	0
54	MG	1A	3704	1/1	0.90	0.16	58,58,58,58	0
54	MG	1A	3494	1/1	0.90	0.18	41,41,41,41	0
54	MG	2A	3758	1/1	0.90	0.11	52,52,52,52	0
54	MG	1A	3124	1/1	0.90	0.14	45,45,45,45	0
54	MG	2A	3607	1/1	0.90	0.10	67,67,67,67	0
54	MG	1A	3419	1/1	0.90	0.25	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3802	1/1	0.90	0.09	47,47,47,47	0
54	MG	1A	3850	1/1	0.90	0.13	33,33,33,33	0
54	MG	2A	3350	1/1	0.90	0.11	43,43,43,43	0
54	MG	1a	1653	1/1	0.90	0.15	64,64,64,64	0
54	MG	2A	3689	1/1	0.90	0.05	45,45,45,45	0
54	MG	1A	3699	1/1	0.90	0.14	41,41,41,41	0
54	MG	2A	3631	1/1	0.90	0.04	64,64,64,64	0
54	MG	2A	3328	1/1	0.90	0.25	36,36,36,36	0
54	MG	1A	3058	1/1	0.90	0.21	49,49,49,49	0
54	MG	1a	1761	1/1	0.90	0.16	64,64,64,64	0
54	MG	1a	1738	1/1	0.90	0.12	64,64,64,64	0
54	MG	2a	1756	1/1	0.90	0.07	57,57,57,57	0
54	MG	2A	3049	1/1	0.90	0.11	50,50,50,50	0
54	MG	2A	3219	1/1	0.90	0.29	62,62,62,62	0
54	MG	2A	3706	1/1	0.90	0.13	51,51,51,51	0
54	MG	2A	3041	1/1	0.90	0.13	50,50,50,50	0
54	MG	2a	1713	1/1	0.90	0.09	61,61,61,61	0
54	MG	2A	3256	1/1	0.90	0.19	61,61,61,61	0
54	MG	1A	3437	1/1	0.90	0.12	41,41,41,41	0
54	MG	1A	3779	1/1	0.90	0.20	29,29,29,29	0
54	MG	1A	3670	1/1	0.90	0.05	64,64,64,64	0
54	MG	1A	3875	1/1	0.90	0.08	50,50,50,50	0
54	MG	1a	1807	1/1	0.90	0.06	73,73,73,73	0
54	MG	1A	3585	1/1	0.90	0.15	54,54,54,54	0
54	MG	1a	1720	1/1	0.90	0.10	65,65,65,65	0
54	MG	1A	3471	1/1	0.90	0.19	29,29,29,29	0
54	MG	2A	3097	1/1	0.90	0.09	57,57,57,57	0
54	MG	1A	3561	1/1	0.90	0.08	62,62,62,62	0
54	MG	1H	8001	1/1	0.90	0.19	62,62,62,62	0
54	MG	1A	3983	1/1	0.90	0.15	74,74,74,74	0
54	MG	2A	3702	1/1	0.90	0.16	55,55,55,55	0
54	MG	1A	3065	1/1	0.90	0.09	39,39,39,39	0
54	MG	1A	3341	1/1	0.90	0.12	46,46,46,46	0
54	MG	1A	3771	1/1	0.90	0.13	44,44,44,44	0
54	MG	2A	3674	1/1	0.90	0.18	25,25,25,25	0
54	MG	2A	3490	1/1	0.90	0.16	66,66,66,66	0
54	MG	1A	3062	1/1	0.90	0.27	46,46,46,46	0
54	MG	2A	3498	1/1	0.90	0.15	58,58,58,58	0
54	MG	2A	3124	1/1	0.90	0.16	66,66,66,66	0
54	MG	2D	304	1/1	0.90	0.16	36,36,36,36	0
54	MG	2A	3116	1/1	0.90	0.11	65,65,65,65	0
54	MG	1A	3254	1/1	0.90	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3026	1/1	0.90	0.14	45,45,45,45	0
54	MG	2a	1665	1/1	0.90	0.17	66,66,66,66	0
54	MG	1a	1760	1/1	0.90	0.10	63,63,63,63	0
54	MG	2A	3651	1/1	0.90	0.06	66,66,66,66	0
54	MG	1A	3346	1/1	0.90	0.14	35,35,35,35	0
54	MG	1a	1775	1/1	0.90	0.15	59,59,59,59	0
54	MG	2A	3113	1/1	0.90	0.26	57,57,57,57	0
54	MG	2f	3001	1/1	0.90	0.12	53,53,53,53	0
54	MG	1A	3963	1/1	0.90	0.14	67,67,67,67	0
54	MG	1A	3932	1/1	0.90	0.07	55,55,55,55	0
54	MG	1P	202	1/1	0.90	0.10	73,73,73,73	0
54	MG	2R	8001	1/1	0.90	0.19	52,52,52,52	0
54	MG	1B	214	1/1	0.90	0.15	42,42,42,42	0
54	MG	10	102	1/1	0.90	0.13	51,51,51,51	0
54	MG	1A	3705	1/1	0.90	0.19	67,67,67,67	0
54	MG	1A	3279	1/1	0.90	0.31	69,69,69,69	0
54	MG	1A	3484	1/1	0.90	0.14	41,41,41,41	0
54	MG	2A	3300	1/1	0.90	0.11	55,55,55,55	0
54	MG	2A	3718	1/1	0.90	0.18	67,67,67,67	0
54	MG	1a	1666	1/1	0.90	0.08	53,53,53,53	0
54	MG	2A	3557	1/1	0.90	0.06	52,52,52,52	0
54	MG	1A	3898	1/1	0.90	0.17	50,50,50,50	0
54	MG	1A	3750	1/1	0.90	0.25	33,33,33,33	0
54	MG	1T	8002	1/1	0.90	0.10	61,61,61,61	0
54	MG	1a	1881	1/1	0.90	0.07	68,68,68,68	0
54	MG	2A	3038	1/1	0.90	0.11	53,53,53,53	0
54	MG	1A	3328	1/1	0.90	0.28	19,19,19,19	0
54	MG	1A	3139	1/1	0.90	0.11	45,45,45,45	0
54	MG	2A	3105	1/1	0.90	0.19	55,55,55,55	0
54	MG	2A	3400	1/1	0.90	0.18	40,40,40,40	0
54	MG	2a	1616	1/1	0.90	0.10	48,48,48,48	0
54	MG	1a	1851	1/1	0.90	0.06	68,68,68,68	0
54	MG	1A	3698	1/1	0.91	0.15	51,51,51,51	0
54	MG	2A	3183	1/1	0.91	0.23	66,66,66,66	0
54	MG	1A	3079	1/1	0.91	0.19	40,40,40,40	0
54	MG	2A	3286	1/1	0.91	0.07	31,31,31,31	0
54	MG	2A	3208	1/1	0.91	0.24	48,48,48,48	0
54	MG	1A	3712	1/1	0.91	0.10	36,36,36,36	0
54	MG	1A	3210	1/1	0.91	0.29	58,58,58,58	0
54	MG	2a	1699	1/1	0.91	0.10	53,53,53,53	0
54	MG	2A	3585	1/1	0.91	0.15	38,38,38,38	0
54	MG	1A	3436	1/1	0.91	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1824	1/1	0.91	0.14	73,73,73,73	0
54	MG	2B	3019	1/1	0.91	0.15	51,51,51,51	0
54	MG	1A	3819	1/1	0.91	0.09	76,76,76,76	0
54	MG	2a	1722	1/1	0.91	0.16	64,64,64,64	0
54	MG	1A	3944	1/1	0.91	0.14	24,24,24,24	0
54	MG	1A	4004	1/1	0.91	0.08	56,56,56,56	0
54	MG	2B	3009	1/1	0.91	0.17	64,64,64,64	0
54	MG	1A	3664	1/1	0.91	0.07	60,60,60,60	0
54	MG	17	101	1/1	0.91	0.19	64,64,64,64	0
54	MG	2A	3406	1/1	0.91	0.14	42,42,42,42	0
54	MG	2A	3419	1/1	0.91	0.12	54,54,54,54	0
54	MG	1A	3928	1/1	0.91	0.17	58,58,58,58	0
54	MG	1A	3726	1/1	0.91	0.09	50,50,50,50	0
54	MG	1A	3081	1/1	0.91	0.30	46,46,46,46	0
54	MG	2a	1648	1/1	0.91	0.29	76,76,76,76	0
54	MG	1a	1609	1/1	0.91	0.11	57,57,57,57	0
54	MG	2A	3186	1/1	0.91	0.19	53,53,53,53	0
54	MG	2A	3454	1/1	0.91	0.05	58,58,58,58	0
54	MG	1A	3495	1/1	0.91	0.21	45,45,45,45	0
54	MG	2A	3134	1/1	0.91	0.17	49,49,49,49	0
54	MG	1a	1846	1/1	0.91	0.13	74,74,74,74	0
54	MG	2A	3264	1/1	0.91	0.17	59,59,59,59	0
54	MG	2A	3263	1/1	0.91	0.12	41,41,41,41	0
54	MG	1A	3887	1/1	0.91	0.16	56,56,56,56	0
54	MG	1A	3687	1/1	0.91	0.11	61,61,61,61	0
54	MG	2a	1728	1/1	0.91	0.23	77,77,77,77	0
54	MG	1A	3636	1/1	0.91	0.13	37,37,37,37	0
54	MG	2A	3703	1/1	0.91	0.08	59,59,59,59	0
54	MG	1A	3518	1/1	0.91	0.16	65,65,65,65	0
54	MG	1a	1854	1/1	0.91	0.05	52,52,52,52	0
54	MG	1A	3477	1/1	0.91	0.21	39,39,39,39	0
54	MG	2E	303	1/1	0.91	0.11	72,72,72,72	0
54	MG	1A	3869	1/1	0.91	0.08	50,50,50,50	0
54	MG	1A	3567	1/1	0.91	0.15	49,49,49,49	0
54	MG	2A	3701	1/1	0.91	0.10	63,63,63,63	0
54	MG	2a	1776	1/1	0.91	0.07	76,76,76,76	0
54	MG	1f	8001	1/1	0.91	0.14	52,52,52,52	0
54	MG	1a	1690	1/1	0.91	0.14	71,71,71,71	0
54	MG	2A	3282	1/1	0.91	0.07	52,52,52,52	0
54	MG	1A	3542	1/1	0.91	0.19	49,49,49,49	0
54	MG	1a	1808	1/1	0.91	0.12	67,67,67,67	0
54	MG	1E	305	1/1	0.91	0.17	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3727	1/1	0.91	0.18	42,42,42,42	0
54	MG	2A	3599	1/1	0.91	0.09	57,57,57,57	0
54	MG	2A	3732	1/1	0.91	0.25	47,47,47,47	0
54	MG	2A	3019	1/1	0.91	0.33	46,46,46,46	0
54	MG	1a	1617	1/1	0.91	0.10	50,50,50,50	0
54	MG	2A	3002	1/1	0.91	0.19	38,38,38,38	0
54	MG	2a	1736	1/1	0.91	0.10	67,67,67,67	0
54	MG	2A	3100	1/1	0.91	0.07	54,54,54,54	0
54	MG	1a	1748	1/1	0.91	0.07	58,58,58,58	0
54	MG	1A	3631	1/1	0.91	0.18	74,74,74,74	0
54	MG	2l	101	1/1	0.91	0.06	69,69,69,69	0
54	MG	1A	3263	1/1	0.91	0.23	49,49,49,49	0
54	MG	2A	3470	1/1	0.91	0.12	50,50,50,50	0
54	MG	1A	3191	1/1	0.91	0.20	55,55,55,55	0
57	ZN	2n	501	1/1	0.91	0.08	84,84,84,84	0
54	MG	1A	3456	1/1	0.91	0.18	62,62,62,62	0
54	MG	2A	3740	1/1	0.91	0.13	54,54,54,54	0
54	MG	2A	3161	1/1	0.91	0.11	51,51,51,51	0
54	MG	2a	1701	1/1	0.91	0.08	70,70,70,70	0
54	MG	1a	1620	1/1	0.91	0.13	48,48,48,48	0
54	MG	1H	8002	1/1	0.91	0.27	58,58,58,58	0
54	MG	1A	3138	1/1	0.91	0.13	60,60,60,60	0
54	MG	1A	3594	1/1	0.91	0.17	58,58,58,58	0
54	MG	1F	310	1/1	0.91	0.16	53,53,53,53	0
54	MG	2A	3045	1/1	0.91	0.18	41,41,41,41	0
54	MG	2a	1659	1/1	0.91	0.24	75,75,75,75	0
54	MG	1A	3651	1/1	0.91	0.16	58,58,58,58	0
54	MG	2A	3024	1/1	0.91	0.23	49,49,49,49	0
54	MG	2A	3099	1/1	0.91	0.14	53,53,53,53	0
54	MG	1A	3101	1/1	0.91	0.19	47,47,47,47	0
54	MG	1A	3663	1/1	0.91	0.26	37,37,37,37	0
54	MG	2A	3192	1/1	0.91	0.10	44,44,44,44	0
54	MG	1B	213	1/1	0.91	0.15	55,55,55,55	0
54	MG	1A	3815	1/1	0.91	0.11	47,47,47,47	0
54	MG	2A	3138	1/1	0.91	0.10	61,61,61,61	0
55	MPD	2A	3748	8/8	0.91	0.13	54,65,67,73	0
54	MG	2A	3562	1/1	0.91	0.06	50,50,50,50	0
54	MG	1a	1693	1/1	0.91	0.15	40,40,40,40	0
54	MG	2A	3610	1/1	0.91	0.13	44,44,44,44	0
54	MG	1A	3408	1/1	0.91	0.19	38,38,38,38	0
54	MG	2A	3666	1/1	0.91	0.15	54,54,54,54	0
54	MG	1A	3034	1/1	0.91	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3537	1/1	0.91	0.17	31,31,31,31	0
54	MG	1a	1663	1/1	0.91	0.20	58,58,58,58	0
54	MG	1A	3462	1/1	0.91	0.12	60,60,60,60	0
54	MG	1a	1743	1/1	0.91	0.09	53,53,53,53	0
54	MG	1A	3460	1/1	0.91	0.25	55,55,55,55	0
54	MG	1A	3037	1/1	0.91	0.21	39,39,39,39	0
54	MG	1A	3110	1/1	0.91	0.23	43,43,43,43	0
54	MG	1A	3938	1/1	0.91	0.15	56,56,56,56	0
54	MG	2A	3039	1/1	0.91	0.18	55,55,55,55	0
54	MG	2A	3265	1/1	0.91	0.17	55,55,55,55	0
54	MG	15	103	1/1	0.91	0.15	71,71,71,71	0
54	MG	2A	3151	1/1	0.91	0.07	48,48,48,48	0
54	MG	2A	3085	1/1	0.91	0.11	46,46,46,46	0
54	MG	1Q	203	1/1	0.91	0.17	50,50,50,50	0
54	MG	2A	3216	1/1	0.91	0.06	64,64,64,64	0
54	MG	1a	1607	1/1	0.91	0.19	54,54,54,54	0
54	MG	1A	3744	1/1	0.91	0.22	51,51,51,51	0
54	MG	1A	3251	1/1	0.91	0.12	52,52,52,52	0
54	MG	1y	202	1/1	0.91	0.08	59,59,59,59	0
54	MG	1a	1660	1/1	0.91	0.11	69,69,69,69	0
54	MG	2A	3339	1/1	0.91	0.13	36,36,36,36	0
54	MG	1A	4015	1/1	0.91	0.18	41,41,41,41	0
54	MG	1A	3170	1/1	0.91	0.14	38,38,38,38	0
54	MG	1A	4030	1/1	0.91	0.41	53,53,53,53	0
54	MG	1A	3126	1/1	0.91	0.17	44,44,44,44	0
54	MG	2A	3528	1/1	0.91	0.42	67,67,67,67	0
54	MG	13	101	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3736	1/1	0.92	0.12	54,54,54,54	0
54	MG	2A	3036	1/1	0.92	0.12	64,64,64,64	0
54	MG	2A	3573	1/1	0.92	0.06	50,50,50,50	0
54	MG	2A	3643	1/1	0.92	0.06	63,63,63,63	0
54	MG	1a	1624	1/1	0.92	0.14	52,52,52,52	0
54	MG	2A	3499	1/1	0.92	0.10	47,47,47,47	0
54	MG	1A	3283	1/1	0.92	0.17	60,60,60,60	0
54	MG	1a	1741	1/1	0.92	0.24	65,65,65,65	0
54	MG	1F	306	1/1	0.92	0.30	48,48,48,48	0
54	MG	2A	3411	1/1	0.92	0.10	62,62,62,62	0
54	MG	2A	3201	1/1	0.92	0.09	53,53,53,53	0
54	MG	1A	3343	1/1	0.92	0.15	31,31,31,31	0
54	MG	2A	3119	1/1	0.92	0.10	49,49,49,49	0
54	MG	1a	1679	1/1	0.92	0.23	55,55,55,55	0
54	MG	1a	1776	1/1	0.92	0.22	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3724	1/1	0.92	0.06	66,66,66,66	0
54	MG	2A	3555	1/1	0.92	0.11	52,52,52,52	0
54	MG	2A	3522	1/1	0.92	0.10	55,55,55,55	0
54	MG	2A	3755	1/1	0.92	0.43	52,52,52,52	0
54	MG	2a	1684	1/1	0.92	0.32	59,59,59,59	0
54	MG	19	101	1/1	0.92	0.27	62,62,62,62	0
54	MG	1A	3884	1/1	0.92	0.18	27,27,27,27	0
54	MG	1A	3622	1/1	0.92	0.23	53,53,53,53	0
54	MG	1A	3979	1/1	0.92	0.19	62,62,62,62	0
54	MG	1A	3357	1/1	0.92	0.18	51,51,51,51	0
54	MG	1A	3093	1/1	0.92	0.14	54,54,54,54	0
54	MG	1A	3797	1/1	0.92	0.11	65,65,65,65	0
54	MG	2A	3070	1/1	0.92	0.18	46,46,46,46	0
54	MG	2A	3620	1/1	0.92	0.15	42,42,42,42	0
54	MG	1A	3336	1/1	0.92	0.19	45,45,45,45	0
54	MG	1A	3128	1/1	0.92	0.33	65,65,65,65	0
54	MG	1A	4043	1/1	0.92	0.14	32,32,32,32	0
54	MG	1A	3918	1/1	0.92	0.07	52,52,52,52	0
54	MG	2A	3634	1/1	0.92	0.13	50,50,50,50	0
54	MG	2A	3224	1/1	0.92	0.23	49,49,49,49	0
54	MG	1a	1771	1/1	0.92	0.07	79,79,79,79	0
54	MG	1a	1766	1/1	0.92	0.11	71,71,71,71	0
54	MG	2A	3135	1/1	0.92	0.24	61,61,61,61	0
54	MG	1A	3382	1/1	0.92	0.15	32,32,32,32	0
54	MG	1A	3173	1/1	0.92	0.25	52,52,52,52	0
54	MG	2A	3606	1/1	0.92	0.08	48,48,48,48	0
54	MG	2A	3735	1/1	0.92	0.14	38,38,38,38	0
54	MG	2A	3194	1/1	0.92	0.13	53,53,53,53	0
54	MG	1A	3216	1/1	0.92	0.14	44,44,44,44	0
54	MG	1A	3629	1/1	0.92	0.11	68,68,68,68	0
54	MG	1a	1848	1/1	0.92	0.09	64,64,64,64	0
54	MG	2A	3154	1/1	0.92	0.15	45,45,45,45	0
54	MG	2A	3500	1/1	0.92	0.10	62,62,62,62	0
54	MG	1A	3493	1/1	0.92	0.19	53,53,53,53	0
54	MG	1A	3813	1/1	0.92	0.15	31,31,31,31	0
54	MG	2a	1764	1/1	0.92	0.08	64,64,64,64	0
54	MG	1a	1809	1/1	0.92	0.19	62,62,62,62	0
54	MG	1A	3425	1/1	0.92	0.20	57,57,57,57	0
54	MG	2A	3763	1/1	0.92	0.09	40,40,40,40	0
54	MG	1A	3174	1/1	0.92	0.15	57,57,57,57	0
54	MG	1A	3827	1/1	0.92	0.20	27,27,27,27	0
54	MG	2A	3280	1/1	0.92	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3506	1/1	0.92	0.23	36,36,36,36	0
54	MG	1A	3164	1/1	0.92	0.12	45,45,45,45	0
54	MG	2A	3289	1/1	0.92	0.11	69,69,69,69	0
54	MG	1A	3650	1/1	0.92	0.29	61,61,61,61	0
54	MG	1a	1831	1/1	0.92	0.13	67,67,67,67	0
54	MG	1a	1632	1/1	0.92	0.15	36,36,36,36	0
54	MG	2A	3594	1/1	0.92	0.17	46,46,46,46	0
54	MG	2A	3552	1/1	0.92	0.09	57,57,57,57	0
54	MG	1A	3475	1/1	0.92	0.27	40,40,40,40	0
54	MG	1E	306	1/1	0.92	0.17	68,68,68,68	0
54	MG	1A	3996	1/1	0.92	0.17	59,59,59,59	0
54	MG	1A	3424	1/1	0.92	0.09	46,46,46,46	0
54	MG	2A	3436	1/1	0.92	0.18	49,49,49,49	0
54	MG	1A	3837	1/1	0.92	0.17	29,29,29,29	0
54	MG	2A	3592	1/1	0.92	0.15	47,47,47,47	0
54	MG	1a	1638	1/1	0.92	0.16	61,61,61,61	0
54	MG	1A	3388	1/1	0.92	0.24	31,31,31,31	0
54	MG	1A	3119	1/1	0.92	0.37	47,47,47,47	0
54	MG	2a	1613	1/1	0.92	0.25	68,68,68,68	0
54	MG	2I	3001	1/1	0.92	0.09	52,52,52,52	0
54	MG	2A	3250	1/1	0.92	0.15	62,62,62,62	0
54	MG	1A	3668	1/1	0.92	0.26	52,52,52,52	0
54	MG	2a	1706	1/1	0.92	0.06	74,74,74,74	0
54	MG	2A	3750	1/1	0.92	0.28	48,48,48,48	0
54	MG	1a	1662	1/1	0.92	0.26	64,64,64,64	0
54	MG	2a	1739	1/1	0.92	0.06	79,79,79,79	0
54	MG	1A	3500	1/1	0.92	0.20	19,19,19,19	0
54	MG	1d	502	1/1	0.92	0.16	77,77,77,77	0
54	MG	2A	3176	1/1	0.92	0.16	45,45,45,45	0
54	MG	1A	3970	1/1	0.92	0.18	62,62,62,62	0
54	MG	2A	3480	1/1	0.92	0.18	53,53,53,53	0
54	MG	1a	1647	1/1	0.92	0.23	57,57,57,57	0
54	MG	1A	3762	1/1	0.92	0.14	52,52,52,52	0
54	MG	2A	3649	1/1	0.92	0.08	56,56,56,56	0
54	MG	1A	4033	1/1	0.92	0.36	47,47,47,47	0
54	MG	1a	1736	1/1	0.92	0.20	66,66,66,66	0
54	MG	1a	1799	1/1	0.92	0.06	65,65,65,65	0
54	MG	2A	3351	1/1	0.92	0.10	35,35,35,35	0
54	MG	1A	3158	1/1	0.92	0.10	49,49,49,49	0
54	MG	1A	3544	1/1	0.92	0.12	58,58,58,58	0
54	MG	1A	3198	1/1	0.92	0.27	56,56,56,56	0
54	MG	2a	1723	1/1	0.92	0.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3619	1/1	0.92	0.09	53,53,53,53	0
54	MG	1A	3538	1/1	0.92	0.14	36,36,36,36	0
54	MG	1A	3371	1/1	0.92	0.16	65,65,65,65	0
54	MG	2A	3301	1/1	0.92	0.12	48,48,48,48	0
54	MG	2A	3332	1/1	0.92	0.16	50,50,50,50	0
54	MG	2A	3448	1/1	0.92	0.12	66,66,66,66	0
54	MG	2A	3466	1/1	0.92	0.12	51,51,51,51	0
54	MG	2A	3726	1/1	0.92	0.14	58,58,58,58	0
54	MG	1a	1879	1/1	0.92	0.18	72,72,72,72	0
54	MG	1A	4014	1/1	0.92	0.07	33,33,33,33	0
54	MG	2A	3708	1/1	0.92	0.22	51,51,51,51	0
54	MG	2A	3057	1/1	0.92	0.21	63,63,63,63	0
54	MG	1A	3032	1/1	0.92	0.15	56,56,56,56	0
54	MG	2a	1652	1/1	0.92	0.24	57,57,57,57	0
54	MG	1A	3352	1/1	0.92	0.16	53,53,53,53	0
54	MG	1U	202	1/1	0.92	0.13	47,47,47,47	0
54	MG	1n	503	1/1	0.92	0.15	59,59,59,59	0
54	MG	1A	3177	1/1	0.92	0.29	52,52,52,52	0
54	MG	1a	1729	1/1	0.92	0.05	56,56,56,56	0
54	MG	2A	3648	1/1	0.92	0.09	48,48,48,48	0
54	MG	1A	3931	1/1	0.92	0.08	35,35,35,35	0
54	MG	2A	3559	1/1	0.92	0.08	55,55,55,55	0
54	MG	2A	3746	1/1	0.92	0.23	55,55,55,55	0
54	MG	2a	1765	1/1	0.92	0.23	68,68,68,68	0
54	MG	1A	3948	1/1	0.92	0.10	49,49,49,49	0
54	MG	2a	1647	1/1	0.92	0.31	67,67,67,67	0
54	MG	1a	1714	1/1	0.92	0.20	62,62,62,62	0
54	MG	2A	3579	1/1	0.92	0.12	56,56,56,56	0
54	MG	2a	1607	1/1	0.92	0.14	72,72,72,72	0
54	MG	1A	3559	1/1	0.92	0.11	46,46,46,46	0
54	MG	1Z	8001	1/1	0.92	0.17	64,64,64,64	0
54	MG	1A	3893	1/1	0.92	0.21	40,40,40,40	0
54	MG	11	101	1/1	0.92	0.34	66,66,66,66	0
54	MG	2A	3032	1/1	0.92	0.06	46,46,46,46	0
54	MG	2a	1751	1/1	0.92	0.10	65,65,65,65	0
54	MG	2A	3295	1/1	0.92	0.09	33,33,33,33	0
54	MG	2A	3178	1/1	0.92	0.13	59,59,59,59	0
54	MG	1A	3298	1/1	0.92	0.10	62,62,62,62	0
54	MG	2A	3705	1/1	0.92	0.17	57,57,57,57	0
54	MG	2A	3220	1/1	0.92	0.10	58,58,58,58	0
54	MG	1a	1683	1/1	0.92	0.19	58,58,58,58	0
54	MG	1A	3570	1/1	0.92	0.17	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	1682	1/1	0.92	0.12	51,51,51,51	0
54	MG	2A	3063	1/1	0.92	0.08	61,61,61,61	0
54	MG	1A	3413	1/1	0.92	0.17	68,68,68,68	0
54	MG	1A	3562	1/1	0.92	0.16	54,54,54,54	0
54	MG	1a	1698	1/1	0.92	0.20	60,60,60,60	0
54	MG	2A	3203	1/1	0.92	0.17	58,58,58,58	0
54	MG	2A	3489	1/1	0.92	0.15	33,33,33,33	0
54	MG	1A	3748	1/1	0.92	0.25	54,54,54,54	0
54	MG	2A	3385	1/1	0.92	0.24	43,43,43,43	0
54	MG	1a	1654	1/1	0.92	0.12	64,64,64,64	0
54	MG	1h	3001	1/1	0.92	0.18	65,65,65,65	0
54	MG	2A	3691	1/1	0.92	0.05	54,54,54,54	0
54	MG	2A	3591	1/1	0.93	0.13	43,43,43,43	0
54	MG	2a	1777	1/1	0.93	0.09	72,72,72,72	0
54	MG	2A	3087	1/1	0.93	0.20	47,47,47,47	0
54	MG	2a	1761	1/1	0.93	0.14	65,65,65,65	0
54	MG	2a	1674	1/1	0.93	0.11	74,74,74,74	0
54	MG	1a	1608	1/1	0.93	0.14	54,54,54,54	0
54	MG	1A	3711	1/1	0.93	0.09	40,40,40,40	0
54	MG	1a	1639	1/1	0.93	0.13	47,47,47,47	0
54	MG	1a	1781	1/1	0.93	0.14	62,62,62,62	0
54	MG	1A	3838	1/1	0.93	0.10	55,55,55,55	0
54	MG	2G	3003	1/1	0.93	0.09	65,65,65,65	0
54	MG	1A	3457	1/1	0.93	0.17	51,51,51,51	0
54	MG	2a	1732	1/1	0.93	0.07	62,62,62,62	0
54	MG	1a	1786	1/1	0.93	0.15	70,70,70,70	0
54	MG	10	103	1/1	0.93	0.11	53,53,53,53	0
54	MG	2a	1718	1/1	0.93	0.09	82,82,82,82	0
54	MG	1A	4049	1/1	0.93	0.15	41,41,41,41	0
54	MG	1a	1829	1/1	0.93	0.18	70,70,70,70	0
54	MG	2A	3262	1/1	0.93	0.06	58,58,58,58	0
54	MG	1A	3864	1/1	0.93	0.21	48,48,48,48	0
54	MG	1a	1721	1/1	0.93	0.09	71,71,71,71	0
54	MG	1A	3272	1/1	0.93	0.15	30,30,30,30	0
54	MG	1E	303	1/1	0.93	0.21	31,31,31,31	0
54	MG	1A	3709	1/1	0.93	0.07	53,53,53,53	0
54	MG	1a	1650	1/1	0.93	0.27	65,65,65,65	0
54	MG	2A	3683	1/1	0.93	0.11	51,51,51,51	0
54	MG	1a	1747	1/1	0.93	0.18	54,54,54,54	0
54	MG	1a	1855	1/1	0.93	0.04	59,59,59,59	0
54	MG	1a	1873	1/1	0.93	0.09	65,65,65,65	0
54	MG	2A	3352	1/1	0.93	0.12	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	20	102	1/1	0.93	0.10	60,60,60,60	0
54	MG	2A	3414	1/1	0.93	0.12	65,65,65,65	0
54	MG	1A	3363	1/1	0.93	0.18	33,33,33,33	0
54	MG	1A	3221	1/1	0.93	0.15	54,54,54,54	0
54	MG	1a	1707	1/1	0.93	0.10	74,74,74,74	0
54	MG	2A	3717	1/1	0.93	0.10	60,60,60,60	0
54	MG	1A	3982	1/1	0.93	0.17	62,62,62,62	0
54	MG	1A	3247	1/1	0.93	0.25	61,61,61,61	0
54	MG	1N	202	1/1	0.93	0.14	61,61,61,61	0
54	MG	2A	3442	1/1	0.93	0.13	51,51,51,51	0
54	MG	1A	3372	1/1	0.93	0.20	39,39,39,39	0
54	MG	2A	3549	1/1	0.93	0.13	51,51,51,51	0
54	MG	2A	3646	1/1	0.93	0.09	71,71,71,71	0
54	MG	2A	3566	1/1	0.93	0.16	63,63,63,63	0
54	MG	1B	212	1/1	0.93	0.11	59,59,59,59	0
54	MG	2A	3365	1/1	0.93	0.08	68,68,68,68	0
54	MG	1A	3940	1/1	0.93	0.07	43,43,43,43	0
54	MG	1A	3466	1/1	0.93	0.16	53,53,53,53	0
54	MG	1A	3955	1/1	0.93	0.11	60,60,60,60	0
54	MG	2A	3368	1/1	0.93	0.07	64,64,64,64	0
54	MG	2X	8001	1/1	0.93	0.09	47,47,47,47	0
54	MG	1a	1802	1/1	0.93	0.06	63,63,63,63	0
54	MG	1A	3828	1/1	0.93	0.16	27,27,27,27	0
54	MG	1a	1819	1/1	0.93	0.23	64,64,64,64	0
54	MG	1A	4048	1/1	0.93	0.15	35,35,35,35	0
54	MG	2a	1641	1/1	0.93	0.30	70,70,70,70	0
54	MG	1A	3812	1/1	0.93	0.14	46,46,46,46	0
57	ZN	1n	501	1/1	0.93	0.13	65,65,65,65	0
54	MG	2A	3342	1/1	0.93	0.13	45,45,45,45	0
54	MG	2A	3294	1/1	0.93	0.19	56,56,56,56	0
54	MG	1a	1658	1/1	0.93	0.25	61,61,61,61	0
54	MG	2A	3096	1/1	0.93	0.18	63,63,63,63	0
54	MG	1a	1629	1/1	0.93	0.20	65,65,65,65	0
54	MG	1A	3885	1/1	0.93	0.09	67,67,67,67	0
54	MG	2A	3071	1/1	0.93	0.17	52,52,52,52	0
54	MG	1a	1682	1/1	0.93	0.19	47,47,47,47	0
54	MG	2A	3228	1/1	0.93	0.13	64,64,64,64	0
54	MG	1a	1861	1/1	0.93	0.12	52,52,52,52	0
54	MG	2A	3279	1/1	0.93	0.22	37,37,37,37	0
54	MG	1A	3908	1/1	0.93	0.20	27,27,27,27	0
54	MG	2A	3601	1/1	0.93	0.07	50,50,50,50	0
54	MG	2A	3253	1/1	0.93	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3246	1/1	0.93	0.09	51,51,51,51	0
54	MG	1A	3467	1/1	0.93	0.24	43,43,43,43	0
54	MG	1a	1745	1/1	0.93	0.14	73,73,73,73	0
54	MG	15	102	1/1	0.93	0.08	55,55,55,55	0
54	MG	1i	3001	1/1	0.93	0.13	62,62,62,62	0
54	MG	1A	3677	1/1	0.93	0.10	54,54,54,54	0
54	MG	1a	1641	1/1	0.93	0.19	75,75,75,75	0
54	MG	2A	3657	1/1	0.93	0.10	40,40,40,40	0
54	MG	1D	311	1/1	0.93	0.08	69,69,69,69	0
54	MG	1A	4057	1/1	0.93	0.12	38,38,38,38	0
54	MG	2a	1680	1/1	0.93	0.14	75,75,75,75	0
54	MG	1A	3435	1/1	0.93	0.14	52,52,52,52	0
54	MG	2A	3225	1/1	0.93	0.12	54,54,54,54	0
54	MG	1A	4009	1/1	0.93	0.16	41,41,41,41	0
54	MG	1A	3999	1/1	0.93	0.18	39,39,39,39	0
54	MG	2A	3656	1/1	0.93	0.17	61,61,61,61	0
54	MG	1A	3297	1/1	0.93	0.10	71,71,71,71	0
54	MG	2A	3391	1/1	0.93	0.17	71,71,71,71	0
54	MG	1d	503	1/1	0.93	0.16	69,69,69,69	0
54	MG	2A	3744	1/1	0.93	0.14	40,40,40,40	0
54	MG	2A	3196	1/1	0.93	0.11	49,49,49,49	0
54	MG	2A	3185	1/1	0.93	0.20	50,50,50,50	0
54	MG	1A	3801	1/1	0.93	0.08	45,45,45,45	0
54	MG	1a	1717	1/1	0.93	0.06	64,64,64,64	0
54	MG	1A	3920	1/1	0.93	0.08	47,47,47,47	0
54	MG	2A	3276	1/1	0.93	0.13	40,40,40,40	0
54	MG	1A	4044	1/1	0.93	0.42	52,52,52,52	0
54	MG	1A	3389	1/1	0.93	0.24	35,35,35,35	0
54	MG	1A	3153	1/1	0.93	0.23	46,46,46,46	0
54	MG	1A	3313	1/1	0.93	0.39	70,70,70,70	0
54	MG	1A	3675	1/1	0.93	0.14	60,60,60,60	0
54	MG	1A	3821	1/1	0.93	0.19	36,36,36,36	0
54	MG	1d	505	1/1	0.93	0.14	60,60,60,60	0
54	MG	2A	3479	1/1	0.93	0.13	38,38,38,38	0
54	MG	1E	302	1/1	0.93	0.10	42,42,42,42	0
54	MG	1A	3665	1/1	0.93	0.16	60,60,60,60	0
54	MG	1A	3120	1/1	0.93	0.12	37,37,37,37	0
54	MG	1A	3167	1/1	0.93	0.20	53,53,53,53	0
54	MG	2A	3369	1/1	0.93	0.15	51,51,51,51	0
54	MG	2A	3477	1/1	0.93	0.10	49,49,49,49	0
54	MG	1A	3358	1/1	0.93	0.20	27,27,27,27	0
54	MG	2A	3227	1/1	0.93	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	4001	1/1	0.93	0.06	68,68,68,68	0
54	MG	2A	3410	1/1	0.93	0.11	57,57,57,57	0
54	MG	1A	3791	1/1	0.93	0.16	60,60,60,60	0
54	MG	1A	3868	1/1	0.93	0.09	39,39,39,39	0
54	MG	1A	3890	1/1	0.93	0.12	62,62,62,62	0
54	MG	1A	3165	1/1	0.93	0.15	37,37,37,37	0
54	MG	2A	3539	1/1	0.93	0.14	38,38,38,38	0
54	MG	1g	202	1/1	0.93	0.27	66,66,66,66	0
54	MG	2a	1668	1/1	0.93	0.16	77,77,77,77	0
54	MG	1A	3151	1/1	0.93	0.22	41,41,41,41	0
54	MG	2A	3313	1/1	0.93	0.17	52,52,52,52	0
54	MG	1a	1695	1/1	0.93	0.28	67,67,67,67	0
54	MG	2A	3523	1/1	0.93	0.07	51,51,51,51	0
54	MG	2a	1709	1/1	0.93	0.07	66,66,66,66	0
54	MG	1A	3187	1/1	0.93	0.19	56,56,56,56	0
54	MG	2A	3140	1/1	0.93	0.12	54,54,54,54	0
54	MG	1A	3943	1/1	0.93	0.18	38,38,38,38	0
54	MG	2a	1624	1/1	0.93	0.17	73,73,73,73	0
54	MG	1a	1706	1/1	0.93	0.12	47,47,47,47	0
54	MG	1a	1838	1/1	0.93	0.09	66,66,66,66	0
54	MG	1B	226	1/1	0.93	0.15	37,37,37,37	0
54	MG	2A	3394	1/1	0.93	0.17	33,33,33,33	0
54	MG	2D	303	1/1	0.93	0.42	44,44,44,44	0
54	MG	2A	3504	1/1	0.93	0.20	63,63,63,63	0
54	MG	1A	3623	1/1	0.93	0.22	29,29,29,29	0
54	MG	1A	3411	1/1	0.93	0.23	35,35,35,35	0
54	MG	2A	3156	1/1	0.93	0.14	36,36,36,36	0
54	MG	1A	3327	1/1	0.93	0.16	32,32,32,32	0
54	MG	1a	1699	1/1	0.93	0.23	73,73,73,73	0
54	MG	1A	3204	1/1	0.93	0.16	60,60,60,60	0
54	MG	1D	302	1/1	0.93	0.15	60,60,60,60	0
54	MG	1A	3604	1/1	0.93	0.19	59,59,59,59	0
54	MG	2A	3485	1/1	0.93	0.09	54,54,54,54	0
54	MG	1A	4022	1/1	0.93	0.09	55,55,55,55	0
54	MG	2a	1743	1/1	0.93	0.13	61,61,61,61	0
54	MG	10	105	1/1	0.93	0.11	65,65,65,65	0
54	MG	2a	1710	1/1	0.93	0.06	71,71,71,71	0
54	MG	2A	3425	1/1	0.93	0.18	55,55,55,55	0
54	MG	1A	4047	1/1	0.93	0.12	59,59,59,59	0
54	MG	2A	3148	1/1	0.93	0.25	51,51,51,51	0
54	MG	1a	1674	1/1	0.93	0.15	63,63,63,63	0
54	MG	2A	3546	1/1	0.93	0.09	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3540	1/1	0.93	0.12	52,52,52,52	0
54	MG	1D	304	1/1	0.93	0.16	61,61,61,61	0
54	MG	2A	3373	1/1	0.93	0.13	50,50,50,50	0
54	MG	1A	3038	1/1	0.93	0.31	60,60,60,60	0
54	MG	1A	3848	1/1	0.93	0.08	41,41,41,41	0
54	MG	1A	3099	1/1	0.93	0.09	59,59,59,59	0
54	MG	2A	3636	1/1	0.93	0.06	66,66,66,66	0
54	MG	1A	3201	1/1	0.93	0.12	47,47,47,47	0
54	MG	1A	3395	1/1	0.93	0.21	32,32,32,32	0
54	MG	1a	1853	1/1	0.93	0.11	54,54,54,54	0
54	MG	2a	1712	1/1	0.93	0.15	62,62,62,62	0
54	MG	1a	1774	1/1	0.93	0.10	68,68,68,68	0
54	MG	2A	3127	1/1	0.93	0.13	44,44,44,44	0
54	MG	1A	3901	1/1	0.93	0.13	46,46,46,46	0
54	MG	2A	3229	1/1	0.93	0.15	51,51,51,51	0
54	MG	1A	3390	1/1	0.93	0.17	42,42,42,42	0
54	MG	1e	204	1/1	0.93	0.08	62,62,62,62	0
54	MG	2A	3550	1/1	0.93	0.08	53,53,53,53	0
54	MG	1a	1852	1/1	0.93	0.08	52,52,52,52	0
54	MG	2A	3033	1/1	0.93	0.35	54,54,54,54	0
54	MG	2A	3377	1/1	0.93	0.10	57,57,57,57	0
54	MG	2A	3086	1/1	0.93	0.10	57,57,57,57	0
54	MG	1V	202	1/1	0.94	0.10	64,64,64,64	0
54	MG	1A	3159	1/1	0.94	0.19	53,53,53,53	0
54	MG	1A	4070	1/1	0.94	0.12	32,32,32,32	0
54	MG	1a	1627	1/1	0.94	0.16	54,54,54,54	0
54	MG	2A	3677	1/1	0.94	0.21	52,52,52,52	0
54	MG	1a	1643	1/1	0.94	0.12	62,62,62,62	0
54	MG	1B	220	1/1	0.94	0.15	34,34,34,34	0
54	MG	2A	3407	1/1	0.94	0.12	41,41,41,41	0
54	MG	1Q	202	1/1	0.94	0.16	55,55,55,55	0
54	MG	1A	3543	1/1	0.94	0.26	46,46,46,46	0
54	MG	1A	3394	1/1	0.94	0.20	26,26,26,26	0
54	MG	2a	1612	1/1	0.94	0.26	63,63,63,63	0
54	MG	1l	3002	1/1	0.94	0.10	72,72,72,72	0
54	MG	2A	3292	1/1	0.94	0.10	55,55,55,55	0
54	MG	2a	1746	1/1	0.94	0.09	56,56,56,56	0
54	MG	2A	3150	1/1	0.94	0.21	46,46,46,46	0
54	MG	2A	3596	1/1	0.94	0.08	58,58,58,58	0
56	ARG	1F	311	12/12	0.94	0.15	44,63,72,77	0
54	MG	1A	3751	1/1	0.94	0.22	27,27,27,27	0
54	MG	1A	3161	1/1	0.94	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1704	1/1	0.94	0.18	68,68,68,68	0
54	MG	2a	1697	1/1	0.94	0.09	66,66,66,66	0
54	MG	1A	3489	1/1	0.94	0.13	61,61,61,61	0
54	MG	1A	3984	1/1	0.94	0.14	59,59,59,59	0
54	MG	2a	1698	1/1	0.94	0.18	69,69,69,69	0
54	MG	2A	3612	1/1	0.94	0.18	33,33,33,33	0
54	MG	1a	1770	1/1	0.94	0.12	58,58,58,58	0
54	MG	2A	3025	1/1	0.94	0.14	44,44,44,44	0
54	MG	2A	3108	1/1	0.94	0.12	60,60,60,60	0
54	MG	2A	3319	1/1	0.94	0.13	42,42,42,42	0
54	MG	1a	1860	1/1	0.94	0.07	66,66,66,66	0
54	MG	1B	231	1/1	0.94	0.07	59,59,59,59	0
54	MG	1A	4000	1/1	0.94	0.16	78,78,78,78	0
54	MG	2A	3210	1/1	0.94	0.15	53,53,53,53	0
54	MG	2A	3122	1/1	0.94	0.11	44,44,44,44	0
54	MG	2A	3440	1/1	0.94	0.09	45,45,45,45	0
54	MG	1A	3545	1/1	0.94	0.30	64,64,64,64	0
54	MG	1A	3546	1/1	0.94	0.10	42,42,42,42	0
54	MG	2A	3072	1/1	0.94	0.31	36,36,36,36	0
54	MG	2A	3670	1/1	0.94	0.19	38,38,38,38	0
54	MG	1A	3661	1/1	0.94	0.07	46,46,46,46	0
54	MG	2A	3198	1/1	0.94	0.24	56,56,56,56	0
54	MG	1A	3310	1/1	0.94	0.15	45,45,45,45	0
54	MG	1A	3036	1/1	0.94	0.20	41,41,41,41	0
54	MG	1A	3189	1/1	0.94	0.23	44,44,44,44	0
54	MG	1a	1604	1/1	0.94	0.20	54,54,54,54	0
54	MG	1a	1615	1/1	0.94	0.21	28,28,28,28	0
54	MG	1A	3080	1/1	0.94	0.22	52,52,52,52	0
54	MG	2A	3420	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3681	1/1	0.94	0.17	29,29,29,29	0
54	MG	2A	3554	1/1	0.94	0.20	43,43,43,43	0
54	MG	2A	3580	1/1	0.94	0.16	39,39,39,39	0
54	MG	2A	3017	1/1	0.94	0.07	54,54,54,54	0
54	MG	1A	3578	1/1	0.94	0.30	58,58,58,58	0
54	MG	2A	3449	1/1	0.94	0.05	60,60,60,60	0
54	MG	1A	3980	1/1	0.94	0.15	58,58,58,58	0
54	MG	2a	1640	1/1	0.94	0.20	66,66,66,66	0
54	MG	1A	3945	1/1	0.94	0.12	37,37,37,37	0
54	MG	1A	3474	1/1	0.94	0.20	35,35,35,35	0
54	MG	1A	3742	1/1	0.94	0.21	47,47,47,47	0
54	MG	2A	3179	1/1	0.94	0.17	56,56,56,56	0
54	MG	2A	3471	1/1	0.94	0.19	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3334	1/1	0.94	0.19	31,31,31,31	0
54	MG	1a	1816	1/1	0.94	0.08	73,73,73,73	0
54	MG	1A	3453	1/1	0.94	0.14	40,40,40,40	0
54	MG	2A	3445	1/1	0.94	0.12	66,66,66,66	0
54	MG	2a	1694	1/1	0.94	0.14	50,50,50,50	0
54	MG	2A	3200	1/1	0.94	0.28	57,57,57,57	0
54	MG	1F	301	1/1	0.94	0.16	36,36,36,36	0
54	MG	1a	1691	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3818	1/1	0.94	0.15	47,47,47,47	0
54	MG	2A	3193	1/1	0.94	0.18	41,41,41,41	0
54	MG	1a	1858	1/1	0.94	0.13	54,54,54,54	0
54	MG	2A	3145	1/1	0.94	0.14	49,49,49,49	0
56	ARG	1B	230	12/12	0.94	0.17	29,41,51,51	0
54	MG	1A	3470	1/1	0.94	0.19	49,49,49,49	0
54	MG	1B	222	1/1	0.94	0.12	65,65,65,65	0
54	MG	2A	3052	1/1	0.94	0.17	43,43,43,43	0
54	MG	1a	1735	1/1	0.94	0.07	68,68,68,68	0
54	MG	1A	3472	1/1	0.94	0.17	36,36,36,36	0
54	MG	1A	3045	1/1	0.94	0.17	33,33,33,33	0
54	MG	1A	3145	1/1	0.94	0.12	43,43,43,43	0
54	MG	1A	3202	1/1	0.94	0.27	49,49,49,49	0
54	MG	1A	3385	1/1	0.94	0.24	40,40,40,40	0
54	MG	1y	203	1/1	0.94	0.12	61,61,61,61	0
54	MG	1a	1864	1/1	0.94	0.11	70,70,70,70	0
54	MG	2A	3261	1/1	0.94	0.17	47,47,47,47	0
54	MG	2A	3462	1/1	0.94	0.10	53,53,53,53	0
54	MG	2A	3517	1/1	0.94	0.07	57,57,57,57	0
54	MG	2A	3290	1/1	0.94	0.17	33,33,33,33	0
54	MG	2A	3353	1/1	0.94	0.15	44,44,44,44	0
54	MG	2A	3056	1/1	0.94	0.16	62,62,62,62	0
54	MG	2a	1609	1/1	0.94	0.11	74,74,74,74	0
54	MG	1A	3135	1/1	0.94	0.28	41,41,41,41	0
54	MG	2A	3355	1/1	0.94	0.13	49,49,49,49	0
54	MG	2A	3103	1/1	0.94	0.17	37,37,37,37	0
54	MG	1A	3262	1/1	0.94	0.18	60,60,60,60	0
54	MG	2A	3715	1/1	0.94	0.08	50,50,50,50	0
54	MG	1A	4074	1/1	0.94	0.12	43,43,43,43	0
54	MG	2A	3600	1/1	0.94	0.11	67,67,67,67	0
54	MG	2A	3759	1/1	0.94	0.24	46,46,46,46	0
54	MG	1A	3619	1/1	0.94	0.22	37,37,37,37	0
54	MG	1A	3059	1/1	0.94	0.26	26,26,26,26	0
54	MG	1a	1697	1/1	0.94	0.25	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3048	1/1	0.94	0.06	66,66,66,66	0
54	MG	28	8002	1/1	0.94	0.20	51,51,51,51	0
54	MG	1a	1737	1/1	0.94	0.16	54,54,54,54	0
54	MG	1A	3250	1/1	0.94	0.14	39,39,39,39	0
54	MG	2A	3491	1/1	0.94	0.19	51,51,51,51	0
54	MG	1A	3096	1/1	0.94	0.15	40,40,40,40	0
54	MG	2A	3482	1/1	0.94	0.18	36,36,36,36	0
54	MG	1A	3245	1/1	0.94	0.15	35,35,35,35	0
54	MG	2A	3443	1/1	0.94	0.11	41,41,41,41	0
54	MG	1A	3463	1/1	0.94	0.12	53,53,53,53	0
54	MG	1a	1668	1/1	0.94	0.10	59,59,59,59	0
54	MG	2a	1625	1/1	0.94	0.12	73,73,73,73	0
54	MG	1A	4050	1/1	0.94	0.21	29,29,29,29	0
54	MG	1a	1703	1/1	0.94	0.20	66,66,66,66	0
54	MG	1A	3587	1/1	0.94	0.17	50,50,50,50	0
54	MG	1A	3989	1/1	0.94	0.11	48,48,48,48	0
54	MG	1A	4064	1/1	0.94	0.26	40,40,40,40	0
54	MG	1A	3488	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3468	1/1	0.94	0.17	64,64,64,64	0
54	MG	17	102	1/1	0.94	0.14	63,63,63,63	0
54	MG	1e	203	1/1	0.94	0.25	58,58,58,58	0
54	MG	1a	1619	1/1	0.94	0.09	65,65,65,65	0
54	MG	1A	3822	1/1	0.94	0.16	34,34,34,34	0
54	MG	2A	3141	1/1	0.94	0.12	59,59,59,59	0
54	MG	1A	3155	1/1	0.94	0.11	54,54,54,54	0
54	MG	2A	3104	1/1	0.94	0.22	46,46,46,46	0
54	MG	2A	3239	1/1	0.94	0.32	49,49,49,49	0
54	MG	2A	3520	1/1	0.94	0.27	38,38,38,38	0
54	MG	2W	8001	1/1	0.94	0.14	50,50,50,50	0
54	MG	2A	3065	1/1	0.94	0.59	47,47,47,47	0
54	MG	1A	3728	1/1	0.94	0.12	68,68,68,68	0
54	MG	2A	3404	1/1	0.94	0.08	70,70,70,70	0
54	MG	2A	3632	1/1	0.94	0.04	72,72,72,72	0
54	MG	2a	1662	1/1	0.94	0.04	79,79,79,79	0
54	MG	1B	210	1/1	0.94	0.21	56,56,56,56	0
54	MG	1A	3881	1/1	0.94	0.22	28,28,28,28	0
54	MG	2A	3507	1/1	0.94	0.09	52,52,52,52	0
54	MG	1A	3252	1/1	0.94	0.21	59,59,59,59	0
54	MG	2A	3370	1/1	0.94	0.13	33,33,33,33	0
54	MG	1a	1765	1/1	0.94	0.18	48,48,48,48	0
54	MG	2a	1643	1/1	0.94	0.07	76,76,76,76	0
54	MG	2A	3009	1/1	0.94	0.18	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1656	1/1	0.94	0.16	37,37,37,37	0
54	MG	1A	3512	1/1	0.94	0.06	61,61,61,61	0
54	MG	2A	3647	1/1	0.94	0.18	58,58,58,58	0
54	MG	1a	1857	1/1	0.94	0.11	68,68,68,68	0
54	MG	1A	3654	1/1	0.94	0.12	34,34,34,34	0
54	MG	2A	3402	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	3440	1/1	0.94	0.11	42,42,42,42	0
54	MG	2A	3327	1/1	0.94	0.18	34,34,34,34	0
54	MG	1A	3676	1/1	0.94	0.09	71,71,71,71	0
54	MG	2A	3628	1/1	0.94	0.12	56,56,56,56	0
54	MG	1A	3648	1/1	0.94	0.16	29,29,29,29	0
54	MG	2A	3093	1/1	0.94	0.09	61,61,61,61	0
54	MG	2A	3120	1/1	0.94	0.19	55,55,55,55	0
54	MG	2A	3516	1/1	0.94	0.05	58,58,58,58	0
54	MG	1A	3200	1/1	0.94	0.32	63,63,63,63	0
54	MG	2A	3623	1/1	0.94	0.18	61,61,61,61	0
54	MG	2a	1630	1/1	0.94	0.13	71,71,71,71	0
54	MG	1A	3369	1/1	0.94	0.10	39,39,39,39	0
54	MG	1A	3057	1/1	0.94	0.22	53,53,53,53	0
54	MG	1a	1754	1/1	0.94	0.12	66,66,66,66	0
54	MG	1U	201	1/1	0.94	0.35	61,61,61,61	0
54	MG	1A	3878	1/1	0.94	0.29	65,65,65,65	0
54	MG	2a	1762	1/1	0.94	0.07	54,54,54,54	0
54	MG	2A	3125	1/1	0.94	0.17	44,44,44,44	0
54	MG	1A	3256	1/1	0.94	0.15	35,35,35,35	0
54	MG	2A	3051	1/1	0.94	0.19	57,57,57,57	0
54	MG	1A	3355	1/1	0.94	0.23	43,43,43,43	0
54	MG	1a	1757	1/1	0.94	0.10	71,71,71,71	0
54	MG	2a	1627	1/1	0.94	0.15	49,49,49,49	0
54	MG	2A	3259	1/1	0.94	0.11	51,51,51,51	0
54	MG	2N	8001	1/1	0.94	0.07	78,78,78,78	0
54	MG	2A	3386	1/1	0.94	0.18	45,45,45,45	0
54	MG	2A	3335	1/1	0.94	0.21	63,63,63,63	0
54	MG	1A	3237	1/1	0.94	0.18	36,36,36,36	0
54	MG	1a	1727	1/1	0.94	0.12	54,54,54,54	0
54	MG	1A	3723	1/1	0.94	0.12	44,44,44,44	0
54	MG	1A	3787	1/1	0.94	0.13	25,25,25,25	0
54	MG	1B	207	1/1	0.94	0.18	68,68,68,68	0
54	MG	2a	1653	1/1	0.94	0.18	62,62,62,62	0
54	MG	1A	3659	1/1	0.94	0.08	54,54,54,54	0
54	MG	1A	3880	1/1	0.94	0.21	39,39,39,39	0
54	MG	1A	3652	1/1	0.94	0.05	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2T	3001	1/1	0.94	0.12	65,65,65,65	0
54	MG	1a	1646	1/1	0.94	0.16	39,39,39,39	0
54	MG	1A	3361	1/1	0.94	0.16	47,47,47,47	0
54	MG	2A	3029	1/1	0.94	0.10	47,47,47,47	0
54	MG	2A	3541	1/1	0.94	0.14	43,43,43,43	0
54	MG	2a	1781	1/1	0.94	0.07	60,60,60,60	0
54	MG	1A	3186	1/1	0.94	0.31	43,43,43,43	0
54	MG	2A	3716	1/1	0.94	0.06	54,54,54,54	0
54	MG	1A	3618	1/1	0.94	0.23	32,32,32,32	0
54	MG	2a	1615	1/1	0.94	0.13	63,63,63,63	0
54	MG	1a	1630	1/1	0.94	0.11	64,64,64,64	0
54	MG	1a	1655	1/1	0.94	0.21	69,69,69,69	0
54	MG	1A	3696	1/1	0.95	0.23	38,38,38,38	0
54	MG	1a	1728	1/1	0.95	0.15	56,56,56,56	0
54	MG	1A	3232	1/1	0.95	0.16	42,42,42,42	0
54	MG	1A	3476	1/1	0.95	0.21	39,39,39,39	0
54	MG	2A	3672	1/1	0.95	0.13	39,39,39,39	0
54	MG	2A	3291	1/1	0.95	0.16	54,54,54,54	0
54	MG	1A	3851	1/1	0.95	0.12	44,44,44,44	0
54	MG	1A	3840	1/1	0.95	0.10	39,39,39,39	0
54	MG	1A	3734	1/1	0.95	0.07	41,41,41,41	0
54	MG	1A	3552	1/1	0.95	0.21	45,45,45,45	0
54	MG	2a	1621	1/1	0.95	0.30	56,56,56,56	0
54	MG	1A	4011	1/1	0.95	0.11	58,58,58,58	0
54	MG	2E	302	1/1	0.95	0.10	41,41,41,41	0
54	MG	2A	3461	1/1	0.95	0.18	52,52,52,52	0
54	MG	2A	3297	1/1	0.95	0.10	43,43,43,43	0
54	MG	2A	3232	1/1	0.95	0.11	52,52,52,52	0
54	MG	1d	504	1/1	0.95	0.21	67,67,67,67	0
54	MG	2a	1679	1/1	0.95	0.13	67,67,67,67	0
54	MG	1a	1867	1/1	0.95	0.11	47,47,47,47	0
54	MG	1l	104	1/1	0.95	0.10	41,41,41,41	0
54	MG	1A	3118	1/1	0.95	0.17	43,43,43,43	0
54	MG	2A	3344	1/1	0.95	0.14	42,42,42,42	0
54	MG	2A	3092	1/1	0.95	0.11	59,59,59,59	0
54	MG	1a	1755	1/1	0.95	0.17	58,58,58,58	0
54	MG	2A	3067	1/1	0.95	0.12	49,49,49,49	0
54	MG	2A	3405	1/1	0.95	0.15	53,53,53,53	0
54	MG	2A	3354	1/1	0.95	0.09	56,56,56,56	0
54	MG	1A	4067	1/1	0.95	0.18	42,42,42,42	0
54	MG	2a	1704	1/1	0.95	0.18	67,67,67,67	0
54	MG	1A	3404	1/1	0.95	0.10	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3624	1/1	0.95	0.15	60,60,60,60	0
54	MG	1A	3796	1/1	0.95	0.14	60,60,60,60	0
54	MG	1a	1611	1/1	0.95	0.13	38,38,38,38	0
54	MG	2a	1769	1/1	0.95	0.13	50,50,50,50	0
54	MG	1A	4020	1/1	0.95	0.22	63,63,63,63	0
54	MG	2A	3281	1/1	0.95	0.12	33,33,33,33	0
54	MG	1a	1652	1/1	0.95	0.18	44,44,44,44	0
54	MG	2a	1784	1/1	0.95	0.09	64,64,64,64	0
54	MG	1A	3040	1/1	0.95	0.19	39,39,39,39	0
54	MG	1a	1708	1/1	0.95	0.12	55,55,55,55	0
54	MG	1A	3746	1/1	0.95	0.14	59,59,59,59	0
54	MG	2A	3005	1/1	0.95	0.19	45,45,45,45	0
54	MG	1A	3116	1/1	0.95	0.28	49,49,49,49	0
54	MG	1A	3503	1/1	0.95	0.12	52,52,52,52	0
54	MG	2a	1651	1/1	0.95	0.29	67,67,67,67	0
54	MG	1a	1811	1/1	0.95	0.10	78,78,78,78	0
54	MG	2A	3399	1/1	0.95	0.15	61,61,61,61	0
54	MG	2A	3106	1/1	0.95	0.25	56,56,56,56	0
54	MG	1A	3897	1/1	0.95	0.25	44,44,44,44	0
54	MG	1D	308	1/1	0.95	0.09	45,45,45,45	0
54	MG	2e	201	1/1	0.95	0.15	71,71,71,71	0
54	MG	2a	1628	1/1	0.95	0.09	66,66,66,66	0
54	MG	2A	3137	1/1	0.95	0.09	57,57,57,57	0
54	MG	1a	1723	1/1	0.95	0.12	64,64,64,64	0
54	MG	1a	1633	1/1	0.95	0.24	67,67,67,67	0
54	MG	1a	1672	1/1	0.95	0.18	58,58,58,58	0
54	MG	2A	3278	1/1	0.95	0.12	50,50,50,50	0
54	MG	1A	3417	1/1	0.95	0.27	40,40,40,40	0
54	MG	1A	3839	1/1	0.95	0.29	60,60,60,60	0
54	MG	1A	3421	1/1	0.95	0.24	24,24,24,24	0
54	MG	1A	3806	1/1	0.95	0.15	62,62,62,62	0
54	MG	1A	3236	1/1	0.95	0.14	59,59,59,59	0
54	MG	1A	3231	1/1	0.95	0.13	44,44,44,44	0
54	MG	1A	3910	1/1	0.95	0.10	42,42,42,42	0
54	MG	1a	1610	1/1	0.95	0.20	45,45,45,45	0
54	MG	2A	3531	1/1	0.95	0.07	62,62,62,62	0
54	MG	1A	3354	1/1	0.95	0.08	63,63,63,63	0
54	MG	1A	3338	1/1	0.95	0.18	46,46,46,46	0
54	MG	1a	1636	1/1	0.95	0.09	47,47,47,47	0
54	MG	1Q	204	1/1	0.95	0.21	55,55,55,55	0
54	MG	2A	3558	1/1	0.95	0.07	32,32,32,32	0
54	MG	2A	3168	1/1	0.95	0.36	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3842	1/1	0.95	0.17	41,41,41,41	0
54	MG	1A	3520	1/1	0.95	0.17	32,32,32,32	0
54	MG	2t	3001	1/1	0.95	0.17	52,52,52,52	0
54	MG	2A	3307	1/1	0.95	0.12	53,53,53,53	0
54	MG	2A	3326	1/1	0.95	0.21	30,30,30,30	0
54	MG	1A	3447	1/1	0.95	0.10	53,53,53,53	0
54	MG	2A	3269	1/1	0.95	0.19	38,38,38,38	0
54	MG	1A	3586	1/1	0.95	0.19	55,55,55,55	0
54	MG	26	502	1/1	0.95	0.16	68,68,68,68	0
54	MG	1a	1877	1/1	0.95	0.08	55,55,55,55	0
54	MG	1A	3180	1/1	0.95	0.18	48,48,48,48	0
54	MG	2a	1669	1/1	0.95	0.17	77,77,77,77	0
54	MG	2a	1742	1/1	0.95	0.06	69,69,69,69	0
54	MG	1A	3229	1/1	0.95	0.09	47,47,47,47	0
54	MG	1A	3778	1/1	0.95	0.14	34,34,34,34	0
54	MG	1A	3048	1/1	0.95	0.14	28,28,28,28	0
54	MG	2A	3012	1/1	0.95	0.15	39,39,39,39	0
54	MG	2a	1741	1/1	0.95	0.10	82,82,82,82	0
54	MG	1B	204	1/1	0.95	0.37	65,65,65,65	0
54	MG	1A	3015	1/1	0.95	0.14	38,38,38,38	0
54	MG	1X	8001	1/1	0.95	0.18	43,43,43,43	0
54	MG	1A	3486	1/1	0.95	0.16	31,31,31,31	0
54	MG	1A	3735	1/1	0.95	0.09	39,39,39,39	0
54	MG	1A	4035	1/1	0.95	0.20	27,27,27,27	0
54	MG	2A	3089	1/1	0.95	0.12	33,33,33,33	0
54	MG	2A	3359	1/1	0.95	0.16	40,40,40,40	0
54	MG	1A	3401	1/1	0.95	0.14	32,32,32,32	0
54	MG	1A	3131	1/1	0.95	0.09	46,46,46,46	0
54	MG	1A	3117	1/1	0.95	0.14	39,39,39,39	0
54	MG	1A	3785	1/1	0.95	0.12	58,58,58,58	0
54	MG	2a	1768	1/1	0.95	0.09	52,52,52,52	0
54	MG	2A	3243	1/1	0.95	0.38	46,46,46,46	0
54	MG	2A	3075	1/1	0.95	0.37	46,46,46,46	0
54	MG	2B	3002	1/1	0.95	0.13	72,72,72,72	0
54	MG	2a	1753	1/1	0.95	0.08	74,74,74,74	0
54	MG	1l	3001	1/1	0.95	0.33	62,62,62,62	0
54	MG	2A	3435	1/1	0.95	0.06	43,43,43,43	0
54	MG	1A	3350	1/1	0.95	0.23	37,37,37,37	0
57	ZN	25	101	1/1	0.95	0.15	64,64,64,64	0
54	MG	1A	3188	1/1	0.95	0.14	40,40,40,40	0
54	MG	2A	3272	1/1	0.95	0.13	46,46,46,46	0
54	MG	2a	1677	1/1	0.95	0.07	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3655	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3307	1/1	0.95	0.13	46,46,46,46	0
54	MG	2A	3112	1/1	0.95	0.17	50,50,50,50	0
54	MG	1A	3345	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	3547	1/1	0.95	0.15	41,41,41,41	0
54	MG	1N	203	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3064	1/1	0.95	0.19	44,44,44,44	0
54	MG	1A	3602	1/1	0.95	0.25	32,32,32,32	0
54	MG	2A	3424	1/1	0.95	0.16	61,61,61,61	0
54	MG	2A	3472	1/1	0.95	0.07	65,65,65,65	0
54	MG	2A	3496	1/1	0.95	0.10	41,41,41,41	0
54	MG	2a	1760	1/1	0.95	0.08	63,63,63,63	0
54	MG	1a	1842	1/1	0.95	0.12	64,64,64,64	0
55	MPD	1A	4028	8/8	0.95	0.15	39,59,65,70	0
54	MG	2A	3682	1/1	0.95	0.06	40,40,40,40	0
54	MG	1A	3981	1/1	0.95	0.14	58,58,58,58	0
54	MG	2a	1683	1/1	0.95	0.15	69,69,69,69	0
54	MG	2A	3098	1/1	0.95	0.14	53,53,53,53	0
54	MG	1A	3257	1/1	0.95	0.37	51,51,51,51	0
54	MG	1A	3783	1/1	0.95	0.18	37,37,37,37	0
54	MG	1A	3777	1/1	0.95	0.16	40,40,40,40	0
54	MG	1A	3130	1/1	0.95	0.24	55,55,55,55	0
54	MG	2A	3315	1/1	0.95	0.10	57,57,57,57	0
54	MG	2a	1734	1/1	0.95	0.06	64,64,64,64	0
54	MG	2A	3331	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3656	1/1	0.95	0.18	26,26,26,26	0
54	MG	1A	3127	1/1	0.95	0.32	57,57,57,57	0
54	MG	1A	3176	1/1	0.95	0.26	46,46,46,46	0
54	MG	2a	1695	1/1	0.95	0.15	67,67,67,67	0
54	MG	2A	3398	1/1	0.95	0.19	56,56,56,56	0
54	MG	1A	3258	1/1	0.95	0.21	40,40,40,40	0
54	MG	2A	3287	1/1	0.95	0.11	48,48,48,48	0
54	MG	1A	3554	1/1	0.95	0.12	58,58,58,58	0
54	MG	2A	3090	1/1	0.95	0.11	63,63,63,63	0
54	MG	1A	3100	1/1	0.95	0.23	50,50,50,50	0
54	MG	1A	3125	1/1	0.95	0.17	49,49,49,49	0
54	MG	1A	3782	1/1	0.95	0.14	35,35,35,35	0
54	MG	2a	1766	1/1	0.95	0.04	63,63,63,63	0
54	MG	2A	3753	1/1	0.95	0.29	39,39,39,39	0
54	MG	1A	3767	1/1	0.95	0.12	43,43,43,43	0
54	MG	1A	3183	1/1	0.95	0.25	41,41,41,41	0
54	MG	1A	3215	1/1	0.95	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3274	1/1	0.95	0.12	74,74,74,74	0
54	MG	1A	3743	1/1	0.95	0.19	45,45,45,45	0
54	MG	2A	3536	1/1	0.95	0.06	63,63,63,63	0
54	MG	1A	3478	1/1	0.95	0.21	36,36,36,36	0
54	MG	1A	3030	1/1	0.95	0.11	33,33,33,33	0
54	MG	1A	3714	1/1	0.95	0.14	45,45,45,45	0
54	MG	2A	3403	1/1	0.95	0.19	36,36,36,36	0
54	MG	2A	3016	1/1	0.95	0.15	59,59,59,59	0
54	MG	1A	3242	1/1	0.95	0.15	40,40,40,40	0
54	MG	1A	3504	1/1	0.95	0.28	26,26,26,26	0
54	MG	1A	3384	1/1	0.95	0.19	43,43,43,43	0
54	MG	1A	3934	1/1	0.95	0.12	35,35,35,35	0
54	MG	1A	3867	1/1	0.95	0.27	32,32,32,32	0
54	MG	1a	1635	1/1	0.95	0.14	37,37,37,37	0
54	MG	1a	1657	1/1	0.95	0.19	53,53,53,53	0
54	MG	2a	1639	1/1	0.95	0.10	73,73,73,73	0
54	MG	2A	3374	1/1	0.95	0.11	57,57,57,57	0
54	MG	1A	3160	1/1	0.95	0.34	44,44,44,44	0
54	MG	1A	3820	1/1	0.95	0.20	31,31,31,31	0
54	MG	1A	3691	1/1	0.95	0.12	54,54,54,54	0
54	MG	1A	3701	1/1	0.95	0.27	68,68,68,68	0
54	MG	1A	3255	1/1	0.95	0.25	45,45,45,45	0
54	MG	1A	3311	1/1	0.95	0.12	46,46,46,46	0
54	MG	1A	3738	1/1	0.95	0.17	34,34,34,34	0
54	MG	1A	3757	1/1	0.95	0.15	50,50,50,50	0
54	MG	1A	3614	1/1	0.95	0.12	38,38,38,38	0
54	MG	1A	3522	1/1	0.95	0.12	61,61,61,61	0
54	MG	1a	1640	1/1	0.95	0.15	61,61,61,61	0
54	MG	2A	3308	1/1	0.95	0.16	56,56,56,56	0
54	MG	2A	3284	1/1	0.95	0.12	41,41,41,41	0
54	MG	1N	201	1/1	0.95	0.11	44,44,44,44	0
54	MG	1A	3754	1/1	0.95	0.28	59,59,59,59	0
54	MG	2A	3293	1/1	0.95	0.10	42,42,42,42	0
54	MG	2A	3532	1/1	0.95	0.18	47,47,47,47	0
54	MG	1F	302	1/1	0.95	0.23	40,40,40,40	0
54	MG	1A	3876	1/1	0.95	0.16	37,37,37,37	0
54	MG	1A	3954	1/1	0.95	0.16	24,24,24,24	0
54	MG	1A	3483	1/1	0.96	0.21	31,31,31,31	0
54	MG	1a	1651	1/1	0.96	0.17	38,38,38,38	0
54	MG	1A	3103	1/1	0.96	0.20	44,44,44,44	0
54	MG	1a	1844	1/1	0.96	0.12	54,54,54,54	0
54	MG	1A	3637	1/1	0.96	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3217	1/1	0.96	0.16	61,61,61,61	0
54	MG	2A	3506	1/1	0.96	0.09	59,59,59,59	0
54	MG	1A	3182	1/1	0.96	0.16	61,61,61,61	0
58	SF4	1d	501	8/8	0.96	0.14	64,70,74,95	0
54	MG	2A	3525	1/1	0.96	0.11	51,51,51,51	0
54	MG	2A	3357	1/1	0.96	0.14	41,41,41,41	0
54	MG	2a	1716	1/1	0.96	0.05	64,64,64,64	0
54	MG	1a	1845	1/1	0.96	0.20	68,68,68,68	0
54	MG	2A	3175	1/1	0.96	0.09	52,52,52,52	0
54	MG	2A	3382	1/1	0.96	0.10	58,58,58,58	0
54	MG	1A	3773	1/1	0.96	0.12	31,31,31,31	0
54	MG	2a	1782	1/1	0.96	0.10	65,65,65,65	0
54	MG	1A	3505	1/1	0.96	0.21	28,28,28,28	0
54	MG	1A	3270	1/1	0.96	0.21	32,32,32,32	0
54	MG	1A	3075	1/1	0.96	0.12	41,41,41,41	0
54	MG	1A	4069	1/1	0.96	0.23	40,40,40,40	0
54	MG	1A	3551	1/1	0.96	0.19	50,50,50,50	0
54	MG	2A	3309	1/1	0.96	0.15	39,39,39,39	0
54	MG	1A	3143	1/1	0.96	0.15	44,44,44,44	0
54	MG	2a	1727	1/1	0.96	0.09	69,69,69,69	0
54	MG	1A	3172	1/1	0.96	0.13	48,48,48,48	0
54	MG	1A	3946	1/1	0.96	0.20	56,56,56,56	0
54	MG	2A	3711	1/1	0.96	0.07	50,50,50,50	0
54	MG	1B	209	1/1	0.96	0.15	39,39,39,39	0
54	MG	2A	3673	1/1	0.96	0.15	38,38,38,38	0
54	MG	1A	3444	1/1	0.96	0.18	61,61,61,61	0
54	MG	2A	3713	1/1	0.96	0.10	57,57,57,57	0
54	MG	1a	1810	1/1	0.96	0.15	60,60,60,60	0
54	MG	2A	3165	1/1	0.96	0.12	64,64,64,64	0
54	MG	1a	1833	1/1	0.96	0.15	48,48,48,48	0
54	MG	1A	3169	1/1	0.96	0.11	53,53,53,53	0
54	MG	2A	3460	1/1	0.96	0.20	54,54,54,54	0
54	MG	2A	3447	1/1	0.96	0.20	48,48,48,48	0
54	MG	2a	1700	1/1	0.96	0.23	47,47,47,47	0
54	MG	1A	3111	1/1	0.96	0.12	38,38,38,38	0
54	MG	1a	1661	1/1	0.96	0.30	44,44,44,44	0
54	MG	1A	3001	1/1	0.96	0.21	33,33,33,33	0
54	MG	2A	3761	1/1	0.96	0.19	37,37,37,37	0
54	MG	1A	4021	1/1	0.96	0.14	34,34,34,34	0
54	MG	2A	3421	1/1	0.96	0.14	69,69,69,69	0
54	MG	2A	3694	1/1	0.96	0.13	41,41,41,41	0
54	MG	1A	3147	1/1	0.96	0.21	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3004	1/1	0.96	0.16	44,44,44,44	0
54	MG	1A	3515	1/1	0.96	0.18	34,34,34,34	0
54	MG	1A	3056	1/1	0.96	0.11	47,47,47,47	0
54	MG	1A	3793	1/1	0.96	0.13	55,55,55,55	0
54	MG	1y	201	1/1	0.96	0.10	72,72,72,72	0
54	MG	1A	3809	1/1	0.96	0.18	46,46,46,46	0
54	MG	1A	3392	1/1	0.96	0.22	27,27,27,27	0
54	MG	2A	3115	1/1	0.96	0.07	50,50,50,50	0
54	MG	1a	1716	1/1	0.96	0.27	74,74,74,74	0
54	MG	2a	1632	1/1	0.96	0.23	59,59,59,59	0
54	MG	2E	304	1/1	0.96	0.12	35,35,35,35	0
54	MG	1A	3798	1/1	0.96	0.07	71,71,71,71	0
54	MG	2A	3010	1/1	0.96	0.20	60,60,60,60	0
54	MG	2A	3181	1/1	0.96	0.08	46,46,46,46	0
54	MG	2A	3102	1/1	0.96	0.17	49,49,49,49	0
54	MG	2T	3003	1/1	0.96	0.09	68,68,68,68	0
54	MG	2a	1708	1/1	0.96	0.10	55,55,55,55	0
54	MG	1a	1715	1/1	0.96	0.08	65,65,65,65	0
54	MG	2A	3415	1/1	0.96	0.21	49,49,49,49	0
54	MG	2A	3741	1/1	0.96	0.28	50,50,50,50	0
54	MG	2Q	3001	1/1	0.96	0.12	44,44,44,44	0
54	MG	1a	1612	1/1	0.96	0.22	62,62,62,62	0
54	MG	1A	3994	1/1	0.96	0.20	38,38,38,38	0
54	MG	1a	1805	1/1	0.96	0.11	68,68,68,68	0
54	MG	1A	3157	1/1	0.96	0.22	39,39,39,39	0
54	MG	2A	3493	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3894	1/1	0.96	0.13	62,62,62,62	0
54	MG	1A	3844	1/1	0.96	0.14	58,58,58,58	0
54	MG	1A	3473	1/1	0.96	0.17	33,33,33,33	0
54	MG	1A	3816	1/1	0.96	0.09	32,32,32,32	0
54	MG	1A	3800	1/1	0.96	0.17	38,38,38,38	0
54	MG	1A	3291	1/1	0.96	0.18	43,43,43,43	0
54	MG	1A	3733	1/1	0.96	0.11	55,55,55,55	0
54	MG	1A	3859	1/1	0.96	0.12	33,33,33,33	0
54	MG	1A	4002	1/1	0.96	0.16	68,68,68,68	0
54	MG	1a	1688	1/1	0.96	0.16	70,70,70,70	0
54	MG	2A	3107	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	4046	1/1	0.96	0.21	29,29,29,29	0
54	MG	1A	3055	1/1	0.96	0.29	42,42,42,42	0
54	MG	2A	3743	1/1	0.96	0.12	63,63,63,63	0
54	MG	1A	3715	1/1	0.96	0.20	48,48,48,48	0
54	MG	1A	3845	1/1	0.96	0.21	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1806	1/1	0.96	0.11	52,52,52,52	0
54	MG	2A	3046	1/1	0.96	0.13	48,48,48,48	0
54	MG	1A	3049	1/1	0.96	0.24	55,55,55,55	0
54	MG	2a	1790	1/1	0.96	0.08	61,61,61,61	0
54	MG	2a	1602	1/1	0.96	0.08	58,58,58,58	0
54	MG	1A	3265	1/1	0.96	0.12	40,40,40,40	0
54	MG	2A	3338	1/1	0.96	0.15	33,33,33,33	0
54	MG	1A	3853	1/1	0.96	0.10	40,40,40,40	0
54	MG	1A	3008	1/1	0.96	0.17	40,40,40,40	0
54	MG	2A	3396	1/1	0.96	0.13	50,50,50,50	0
54	MG	1A	4013	1/1	0.96	0.11	43,43,43,43	0
54	MG	1D	310	1/1	0.96	0.20	52,52,52,52	0
54	MG	2a	1793	1/1	0.96	0.18	51,51,51,51	0
54	MG	2A	3215	1/1	0.96	0.11	54,54,54,54	0
54	MG	2A	3249	1/1	0.96	0.15	49,49,49,49	0
54	MG	1A	3387	1/1	0.96	0.21	25,25,25,25	0
54	MG	1A	3039	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3362	1/1	0.96	0.17	39,39,39,39	0
54	MG	1a	1634	1/1	0.96	0.12	61,61,61,61	0
54	MG	1A	3368	1/1	0.96	0.13	24,24,24,24	0
54	MG	1R	202	1/1	0.96	0.10	50,50,50,50	0
54	MG	2A	3121	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3613	1/1	0.96	0.25	42,42,42,42	0
54	MG	1A	3780	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3804	1/1	0.96	0.18	37,37,37,37	0
54	MG	1a	1828	1/1	0.96	0.07	55,55,55,55	0
54	MG	1A	3854	1/1	0.96	0.10	42,42,42,42	0
54	MG	2A	3147	1/1	0.96	0.09	47,47,47,47	0
54	MG	1t	3001	1/1	0.96	0.07	49,49,49,49	0
54	MG	1a	1825	1/1	0.96	0.08	77,77,77,77	0
54	MG	1A	3107	1/1	0.96	0.19	38,38,38,38	0
54	MG	1A	3076	1/1	0.96	0.12	44,44,44,44	0
54	MG	2A	3736	1/1	0.96	0.18	50,50,50,50	0
54	MG	2A	3611	1/1	0.96	0.12	34,34,34,34	0
54	MG	2A	3738	1/1	0.96	0.10	46,46,46,46	0
54	MG	1A	4010	1/1	0.96	0.18	34,34,34,34	0
54	MG	1A	3322	1/1	0.96	0.20	30,30,30,30	0
54	MG	2A	3322	1/1	0.96	0.13	40,40,40,40	0
54	MG	1A	3755	1/1	0.96	0.14	47,47,47,47	0
54	MG	1A	3740	1/1	0.96	0.19	22,22,22,22	0
54	MG	2A	3160	1/1	0.96	0.23	44,44,44,44	0
54	MG	1A	3024	1/1	0.96	0.27	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3233	1/1	0.96	0.14	58,58,58,58	0
54	MG	2A	3762	1/1	0.96	0.16	53,53,53,53	0
54	MG	1a	1626	1/1	0.96	0.10	43,43,43,43	0
54	MG	1A	3197	1/1	0.96	0.12	52,52,52,52	0
54	MG	1D	303	1/1	0.96	0.23	36,36,36,36	0
54	MG	2A	3084	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	4053	1/1	0.96	0.18	45,45,45,45	0
54	MG	1a	1862	1/1	0.96	0.07	64,64,64,64	0
54	MG	1A	3380	1/1	0.96	0.19	26,26,26,26	0
54	MG	2A	3321	1/1	0.96	0.15	33,33,33,33	0
54	MG	2A	3376	1/1	0.96	0.07	58,58,58,58	0
54	MG	1a	1827	1/1	0.96	0.15	73,73,73,73	0
54	MG	1A	3047	1/1	0.96	0.35	63,63,63,63	0
54	MG	1A	3491	1/1	0.96	0.23	24,24,24,24	0
55	MPD	18	102	8/8	0.96	0.23	30,34,40,47	0
54	MG	2T	3002	1/1	0.96	0.08	69,69,69,69	0
54	MG	1A	3235	1/1	0.96	0.23	41,41,41,41	0
54	MG	2A	3158	1/1	0.96	0.10	44,44,44,44	0
54	MG	1A	3386	1/1	0.96	0.16	41,41,41,41	0
54	MG	1A	3403	1/1	0.96	0.18	25,25,25,25	0
54	MG	1A	4068	1/1	0.96	0.32	43,43,43,43	0
54	MG	1A	3914	1/1	0.96	0.11	49,49,49,49	0
54	MG	2A	3195	1/1	0.96	0.14	66,66,66,66	0
54	MG	1a	1742	1/1	0.96	0.20	55,55,55,55	0
54	MG	2a	1634	1/1	0.96	0.17	37,37,37,37	0
54	MG	1A	3301	1/1	0.96	0.27	48,48,48,48	0
54	MG	1A	3976	1/1	0.96	0.13	50,50,50,50	0
54	MG	1A	3446	1/1	0.96	0.21	30,30,30,30	0
54	MG	1A	3993	1/1	0.96	0.41	54,54,54,54	0
54	MG	1A	3302	1/1	0.96	0.19	34,34,34,34	0
54	MG	1A	3168	1/1	0.96	0.15	32,32,32,32	0
54	MG	2A	3126	1/1	0.96	0.17	28,28,28,28	0
54	MG	2a	1730	1/1	0.96	0.14	55,55,55,55	0
54	MG	2A	3533	1/1	0.96	0.14	58,58,58,58	0
54	MG	2A	3199	1/1	0.96	0.18	56,56,56,56	0
54	MG	2A	3613	1/1	0.96	0.13	49,49,49,49	0
54	MG	1V	201	1/1	0.96	0.17	55,55,55,55	0
54	MG	1A	3309	1/1	0.96	0.10	47,47,47,47	0
54	MG	1A	3108	1/1	0.96	0.15	41,41,41,41	0
54	MG	1A	3427	1/1	0.96	0.18	39,39,39,39	0
54	MG	2A	3271	1/1	0.96	0.34	47,47,47,47	0
54	MG	2A	3686	1/1	0.96	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1648	1/1	0.96	0.23	56,56,56,56	0
54	MG	1a	1618	1/1	0.96	0.17	65,65,65,65	0
54	MG	2A	3654	1/1	0.96	0.04	56,56,56,56	0
54	MG	1A	3347	1/1	0.96	0.20	24,24,24,24	0
54	MG	1a	1724	1/1	0.96	0.15	36,36,36,36	0
54	MG	2A	3583	1/1	0.96	0.07	34,34,34,34	0
54	MG	2D	307	1/1	0.96	0.12	37,37,37,37	0
54	MG	2A	3752	1/1	0.96	0.18	46,46,46,46	0
54	MG	1A	3281	1/1	0.96	0.12	39,39,39,39	0
54	MG	1A	3660	1/1	0.96	0.21	23,23,23,23	0
54	MG	2A	3047	1/1	0.96	0.08	46,46,46,46	0
54	MG	1A	3482	1/1	0.96	0.19	30,30,30,30	0
54	MG	2A	3409	1/1	0.96	0.16	44,44,44,44	0
54	MG	1A	3381	1/1	0.96	0.21	24,24,24,24	0
54	MG	1A	3811	1/1	0.96	0.17	32,32,32,32	0
54	MG	2A	3437	1/1	0.96	0.18	52,52,52,52	0
54	MG	2A	3605	1/1	0.96	0.11	36,36,36,36	0
54	MG	1A	3054	1/1	0.96	0.21	34,34,34,34	0
54	MG	2a	1738	1/1	0.96	0.10	71,71,71,71	0
54	MG	2a	1690	1/1	0.96	0.06	71,71,71,71	0
54	MG	2B	3017	1/1	0.96	0.09	68,68,68,68	0
54	MG	1A	3136	1/1	0.96	0.17	39,39,39,39	0
54	MG	2A	3109	1/1	0.96	0.10	47,47,47,47	0
54	MG	1A	3207	1/1	0.96	0.07	60,60,60,60	0
54	MG	1A	3640	1/1	0.96	0.23	71,71,71,71	0
54	MG	1A	3317	1/1	0.96	0.27	45,45,45,45	0
54	MG	2A	3641	1/1	0.96	0.13	49,49,49,49	0
54	MG	1a	1678	1/1	0.96	0.16	64,64,64,64	0
54	MG	1A	4071	1/1	0.96	0.14	39,39,39,39	0
54	MG	2A	3439	1/1	0.96	0.05	46,46,46,46	0
54	MG	1D	309	1/1	0.96	0.12	40,40,40,40	0
54	MG	1A	3823	1/1	0.96	0.21	36,36,36,36	0
54	MG	1A	3430	1/1	0.96	0.17	56,56,56,56	0
54	MG	1A	3952	1/1	0.97	0.13	33,33,33,33	0
54	MG	1A	3227	1/1	0.97	0.31	37,37,37,37	0
54	MG	1A	3776	1/1	0.97	0.22	21,21,21,21	0
54	MG	2A	3222	1/1	0.97	0.23	53,53,53,53	0
54	MG	1A	3469	1/1	0.97	0.23	25,25,25,25	0
54	MG	2A	3710	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3410	1/1	0.97	0.14	36,36,36,36	0
54	MG	1A	3769	1/1	0.97	0.20	57,57,57,57	0
54	MG	2a	1773	1/1	0.97	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3304	1/1	0.97	0.22	37,37,37,37	0
54	MG	1A	4072	1/1	0.97	0.17	36,36,36,36	0
54	MG	2A	3617	1/1	0.97	0.10	23,23,23,23	0
54	MG	1A	4032	1/1	0.97	0.21	35,35,35,35	0
54	MG	2A	3303	1/1	0.97	0.21	61,61,61,61	0
54	MG	1A	3253	1/1	0.97	0.26	34,34,34,34	0
54	MG	1A	3234	1/1	0.97	0.15	37,37,37,37	0
54	MG	2A	3621	1/1	0.97	0.15	56,56,56,56	0
54	MG	1a	1847	1/1	0.97	0.10	42,42,42,42	0
54	MG	1A	3326	1/1	0.97	0.20	33,33,33,33	0
54	MG	1A	3941	1/1	0.97	0.12	66,66,66,66	0
54	MG	1a	1763	1/1	0.97	0.15	59,59,59,59	0
54	MG	2A	3128	1/1	0.97	0.20	45,45,45,45	0
54	MG	2A	3044	1/1	0.97	0.09	44,44,44,44	0
54	MG	1A	3599	1/1	0.97	0.10	50,50,50,50	0
54	MG	1A	3246	1/1	0.97	0.18	54,54,54,54	0
54	MG	2a	1657	1/1	0.97	0.11	52,52,52,52	0
54	MG	2O	201	1/1	0.97	0.16	58,58,58,58	0
54	MG	1A	3741	1/1	0.97	0.17	56,56,56,56	0
54	MG	2A	3101	1/1	0.97	0.11	34,34,34,34	0
54	MG	1A	3532	1/1	0.97	0.11	61,61,61,61	0
54	MG	1A	3006	1/1	0.97	0.16	30,30,30,30	0
54	MG	1A	3829	1/1	0.97	0.10	25,25,25,25	0
54	MG	2A	3177	1/1	0.97	0.25	39,39,39,39	0
54	MG	1o	3001	1/1	0.97	0.26	65,65,65,65	0
54	MG	1A	3630	1/1	0.97	0.12	41,41,41,41	0
54	MG	1A	3720	1/1	0.97	0.20	33,33,33,33	0
54	MG	1A	3095	1/1	0.97	0.34	45,45,45,45	0
54	MG	1A	3228	1/1	0.97	0.31	41,41,41,41	0
54	MG	1A	3391	1/1	0.97	0.20	49,49,49,49	0
54	MG	1a	1826	1/1	0.97	0.06	70,70,70,70	0
54	MG	1A	4060	1/1	0.97	0.30	32,32,32,32	0
54	MG	1A	3915	1/1	0.97	0.20	34,34,34,34	0
54	MG	1A	3105	1/1	0.97	0.09	57,57,57,57	0
54	MG	2A	3211	1/1	0.97	0.09	56,56,56,56	0
54	MG	1A	3713	1/1	0.97	0.13	33,33,33,33	0
54	MG	1T	8001	1/1	0.97	0.18	60,60,60,60	0
54	MG	2a	1703	1/1	0.97	0.14	69,69,69,69	0
54	MG	1a	1711	1/1	0.97	0.09	69,69,69,69	0
54	MG	1A	3879	1/1	0.97	0.13	38,38,38,38	0
54	MG	1A	3178	1/1	0.97	0.15	38,38,38,38	0
54	MG	2A	3255	1/1	0.97	0.24	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3734	1/1	0.97	0.19	41,41,41,41	0
54	MG	1A	3536	1/1	0.97	0.18	33,33,33,33	0
54	MG	2A	3757	1/1	0.97	0.18	64,64,64,64	0
54	MG	1R	201	1/1	0.97	0.22	53,53,53,53	0
54	MG	1A	3133	1/1	0.97	0.15	42,42,42,42	0
54	MG	1A	3269	1/1	0.97	0.14	53,53,53,53	0
54	MG	1A	3194	1/1	0.97	0.29	42,42,42,42	0
54	MG	1A	3856	1/1	0.97	0.11	33,33,33,33	0
54	MG	2A	3268	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3860	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	3026	1/1	0.97	0.28	34,34,34,34	0
54	MG	1A	3218	1/1	0.97	0.37	48,48,48,48	0
54	MG	1A	4065	1/1	0.97	0.21	49,49,49,49	0
54	MG	1A	3121	1/1	0.97	0.17	35,35,35,35	0
54	MG	2A	3453	1/1	0.97	0.17	52,52,52,52	0
54	MG	1A	3831	1/1	0.97	0.11	53,53,53,53	0
54	MG	2A	3173	1/1	0.97	0.10	55,55,55,55	0
54	MG	2A	3003	1/1	0.97	0.09	51,51,51,51	0
54	MG	2A	3760	1/1	0.97	0.41	40,40,40,40	0
54	MG	2A	3031	1/1	0.97	0.19	27,27,27,27	0
54	MG	2A	3721	1/1	0.97	0.28	59,59,59,59	0
54	MG	1A	3977	1/1	0.97	0.18	24,24,24,24	0
54	MG	1A	3276	1/1	0.97	0.14	29,29,29,29	0
54	MG	1a	1713	1/1	0.97	0.10	44,44,44,44	0
54	MG	1A	3509	1/1	0.97	0.11	62,62,62,62	0
54	MG	1A	3445	1/1	0.97	0.20	31,31,31,31	0
54	MG	2A	3589	1/1	0.97	0.06	54,54,54,54	0
54	MG	1A	3730	1/1	0.97	0.15	53,53,53,53	0
54	MG	1A	3992	1/1	0.97	0.17	19,19,19,19	0
54	MG	2A	3604	1/1	0.97	0.18	35,35,35,35	0
54	MG	1A	3438	1/1	0.97	0.16	27,27,27,27	0
54	MG	1A	3146	1/1	0.97	0.22	28,28,28,28	0
54	MG	1A	3296	1/1	0.97	0.16	31,31,31,31	0
54	MG	2A	3330	1/1	0.97	0.18	31,31,31,31	0
54	MG	2W	8002	1/1	0.97	0.12	60,60,60,60	0
54	MG	2F	302	1/1	0.97	0.18	41,41,41,41	0
54	MG	1A	3907	1/1	0.97	0.13	13,13,13,13	0
54	MG	1A	3865	1/1	0.97	0.15	35,35,35,35	0
54	MG	1A	3523	1/1	0.97	0.17	49,49,49,49	0
54	MG	1A	3329	1/1	0.97	0.23	39,39,39,39	0
54	MG	2A	3742	1/1	0.97	0.19	56,56,56,56	0
54	MG	1A	3193	1/1	0.97	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3063	1/1	0.97	0.18	31,31,31,31	0
54	MG	2A	3077	1/1	0.97	0.23	48,48,48,48	0
54	MG	1A	3114	1/1	0.97	0.17	33,33,33,33	0
54	MG	1A	3517	1/1	0.97	0.24	22,22,22,22	0
54	MG	2A	3285	1/1	0.97	0.15	32,32,32,32	0
54	MG	2A	3088	1/1	0.97	0.39	47,47,47,47	0
54	MG	1A	4063	1/1	0.97	0.15	41,41,41,41	0
54	MG	1A	3267	1/1	0.97	0.10	82,82,82,82	0
54	MG	1A	3633	1/1	0.97	0.23	46,46,46,46	0
54	MG	2A	3270	1/1	0.97	0.13	41,41,41,41	0
54	MG	1A	3808	1/1	0.97	0.23	55,55,55,55	0
54	MG	1A	3175	1/1	0.97	0.15	43,43,43,43	0
54	MG	2A	3274	1/1	0.97	0.06	53,53,53,53	0
54	MG	2A	3248	1/1	0.97	0.26	43,43,43,43	0
54	MG	1A	3226	1/1	0.97	0.30	42,42,42,42	0
54	MG	1A	3442	1/1	0.97	0.15	61,61,61,61	0
54	MG	1A	3214	1/1	0.97	0.22	42,42,42,42	0
54	MG	2A	3652	1/1	0.97	0.16	38,38,38,38	0
57	ZN	1Y	501	1/1	0.97	0.22	56,56,56,56	0
54	MG	1A	3906	1/1	0.97	0.23	38,38,38,38	0
54	MG	1A	3260	1/1	0.97	0.17	44,44,44,44	0
54	MG	1A	3913	1/1	0.97	0.16	22,22,22,22	0
54	MG	2a	1611	1/1	0.97	0.10	41,41,41,41	0
54	MG	2A	3079	1/1	0.97	0.19	44,44,44,44	0
54	MG	1A	4058	1/1	0.97	0.15	37,37,37,37	0
54	MG	2A	3567	1/1	0.97	0.07	46,46,46,46	0
54	MG	1A	3094	1/1	0.97	0.16	37,37,37,37	0
54	MG	1A	3217	1/1	0.97	0.34	49,49,49,49	0
54	MG	1A	3564	1/1	0.97	0.22	26,26,26,26	0
54	MG	1A	3899	1/1	0.97	0.15	47,47,47,47	0
54	MG	2A	3131	1/1	0.97	0.19	39,39,39,39	0
54	MG	1A	3569	1/1	0.97	0.09	37,37,37,37	0
54	MG	1A	3303	1/1	0.97	0.13	31,31,31,31	0
54	MG	1a	1750	1/1	0.97	0.08	69,69,69,69	0
54	MG	13	102	1/1	0.97	0.08	49,49,49,49	0
54	MG	2A	3318	1/1	0.97	0.17	37,37,37,37	0
54	MG	2A	3432	1/1	0.97	0.11	35,35,35,35	0
54	MG	1A	3412	1/1	0.97	0.24	27,27,27,27	0
54	MG	2A	3022	1/1	0.97	0.35	44,44,44,44	0
54	MG	2A	3110	1/1	0.97	0.19	28,28,28,28	0
54	MG	1A	3122	1/1	0.97	0.13	37,37,37,37	0
54	MG	1a	1835	1/1	0.97	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3188	1/1	0.97	0.08	57,57,57,57	0
54	MG	1a	1740	1/1	0.97	0.24	69,69,69,69	0
54	MG	1A	3702	1/1	0.97	0.13	43,43,43,43	0
54	MG	2A	3581	1/1	0.97	0.14	48,48,48,48	0
54	MG	2A	3739	1/1	0.97	0.05	52,52,52,52	0
54	MG	2B	3016	1/1	0.97	0.13	67,67,67,67	0
54	MG	1A	3449	1/1	0.97	0.13	54,54,54,54	0
54	MG	2A	3653	1/1	0.97	0.12	38,38,38,38	0
54	MG	1a	1692	1/1	0.97	0.13	44,44,44,44	0
54	MG	2a	1642	1/1	0.97	0.10	80,80,80,80	0
54	MG	1A	3007	1/1	0.97	0.24	35,35,35,35	0
54	MG	1A	3986	1/1	0.97	0.15	19,19,19,19	0
54	MG	2A	3117	1/1	0.97	0.14	52,52,52,52	0
54	MG	2A	3669	1/1	0.97	0.12	38,38,38,38	0
54	MG	1A	4062	1/1	0.97	0.14	37,37,37,37	0
54	MG	1a	1734	1/1	0.97	0.15	47,47,47,47	0
54	MG	1A	3535	1/1	0.97	0.16	26,26,26,26	0
54	MG	2A	3221	1/1	0.97	0.25	45,45,45,45	0
54	MG	1A	3378	1/1	0.97	0.25	36,36,36,36	0
54	MG	2A	3028	1/1	0.97	0.12	33,33,33,33	0
54	MG	1a	1792	1/1	0.97	0.11	62,62,62,62	0
54	MG	2A	3149	1/1	0.97	0.15	28,28,28,28	0
54	MG	2A	3590	1/1	0.97	0.05	49,49,49,49	0
54	MG	1a	1876	1/1	0.97	0.24	41,41,41,41	0
54	MG	1A	3852	1/1	0.97	0.09	46,46,46,46	0
54	MG	1A	3682	1/1	0.97	0.14	59,59,59,59	0
54	MG	1D	306	1/1	0.97	0.20	46,46,46,46	0
54	MG	2A	3356	1/1	0.97	0.07	48,48,48,48	0
54	MG	2A	3676	1/1	0.97	0.09	48,48,48,48	0
54	MG	1a	1669	1/1	0.97	0.08	70,70,70,70	0
54	MG	1A	3707	1/1	0.97	0.12	43,43,43,43	0
54	MG	1A	3097	1/1	0.97	0.18	42,42,42,42	0
54	MG	1A	3061	1/1	0.97	0.17	49,49,49,49	0
54	MG	2A	3378	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3289	1/1	0.97	0.16	31,31,31,31	0
54	MG	1A	3911	1/1	0.97	0.16	28,28,28,28	0
54	MG	2A	3343	1/1	0.97	0.07	56,56,56,56	0
54	MG	2A	3756	1/1	0.97	0.52	52,52,52,52	0
54	MG	2A	3324	1/1	0.97	0.10	44,44,44,44	0
54	MG	1A	4075	1/1	0.97	0.15	39,39,39,39	0
54	MG	2r	101	1/1	0.97	0.08	68,68,68,68	0
54	MG	19	103	1/1	0.97	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3342	1/1	0.97	0.12	57,57,57,57	0
54	MG	1A	3364	1/1	0.97	0.17	33,33,33,33	0
54	MG	1A	3617	1/1	0.97	0.19	24,24,24,24	0
54	MG	1A	3162	1/1	0.97	0.21	40,40,40,40	0
54	MG	1A	3406	1/1	0.97	0.17	30,30,30,30	0
54	MG	1A	3287	1/1	0.97	0.18	39,39,39,39	0
54	MG	1G	3004	1/1	0.97	0.12	45,45,45,45	0
54	MG	1A	3700	1/1	0.97	0.17	41,41,41,41	0
54	MG	1A	3572	1/1	0.97	0.20	30,30,30,30	0
54	MG	1A	3550	1/1	0.97	0.16	57,57,57,57	0
54	MG	1A	3349	1/1	0.97	0.19	30,30,30,30	0
54	MG	2A	3450	1/1	0.97	0.10	58,58,58,58	0
54	MG	1A	3909	1/1	0.97	0.20	28,28,28,28	0
54	MG	1A	3807	1/1	0.97	0.12	52,52,52,52	0
54	MG	1A	4056	1/1	0.97	0.28	41,41,41,41	0
54	MG	1A	3628	1/1	0.97	0.23	20,20,20,20	0
54	MG	1A	3373	1/1	0.97	0.12	52,52,52,52	0
54	MG	1A	3082	1/1	0.97	0.34	53,53,53,53	0
54	MG	2A	3078	1/1	0.97	0.14	56,56,56,56	0
54	MG	1A	3068	1/1	0.97	0.26	49,49,49,49	0
54	MG	1a	1726	1/1	0.97	0.14	65,65,65,65	0
54	MG	2A	3167	1/1	0.97	0.18	41,41,41,41	0
54	MG	2A	3362	1/1	0.97	0.13	34,34,34,34	0
54	MG	1A	3074	1/1	0.97	0.20	36,36,36,36	0
54	MG	1a	1623	1/1	0.97	0.10	43,43,43,43	0
54	MG	1A	3052	1/1	0.97	0.28	44,44,44,44	0
54	MG	1A	3448	1/1	0.97	0.12	67,67,67,67	0
54	MG	1a	1628	1/1	0.97	0.12	37,37,37,37	0
54	MG	1A	3857	1/1	0.97	0.16	23,23,23,23	0
54	MG	2A	3021	1/1	0.97	0.13	31,31,31,31	0
54	MG	2A	3401	1/1	0.97	0.10	43,43,43,43	0
54	MG	1e	202	1/1	0.97	0.27	58,58,58,58	0
54	MG	1A	3337	1/1	0.97	0.17	35,35,35,35	0
54	MG	1A	3104	1/1	0.97	0.32	41,41,41,41	0
54	MG	1D	314	1/1	0.98	0.19	72,72,72,72	0
54	MG	2a	1619	1/1	0.98	0.13	48,48,48,48	0
54	MG	1A	3223	1/1	0.98	0.15	32,32,32,32	0
54	MG	2A	3595	1/1	0.98	0.16	33,33,33,33	0
54	MG	1A	3013	1/1	0.98	0.22	17,17,17,17	0
54	MG	1A	3085	1/1	0.98	0.30	38,38,38,38	0
54	MG	2A	3139	1/1	0.98	0.21	28,28,28,28	0
54	MG	1A	3211	1/1	0.98	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3361	1/1	0.98	0.13	34,34,34,34	0
54	MG	1A	3396	1/1	0.98	0.17	26,26,26,26	0
54	MG	2A	3316	1/1	0.98	0.12	40,40,40,40	0
54	MG	1A	3340	1/1	0.98	0.19	25,25,25,25	0
54	MG	1a	1709	1/1	0.98	0.14	39,39,39,39	0
54	MG	1A	3452	1/1	0.98	0.16	56,56,56,56	0
54	MG	1A	4029	1/1	0.98	0.15	49,49,49,49	0
54	MG	1A	3379	1/1	0.98	0.15	27,27,27,27	0
54	MG	1A	3050	1/1	0.98	0.24	44,44,44,44	0
54	MG	2A	3364	1/1	0.98	0.14	49,49,49,49	0
54	MG	1A	4045	1/1	0.98	0.17	36,36,36,36	0
54	MG	1A	3605	1/1	0.98	0.18	40,40,40,40	0
54	MG	2a	1775	1/1	0.98	0.12	57,57,57,57	0
54	MG	1A	3244	1/1	0.98	0.34	36,36,36,36	0
54	MG	2A	3660	1/1	0.98	0.16	47,47,47,47	0
54	MG	2A	3754	1/1	0.98	0.34	46,46,46,46	0
54	MG	1A	3749	1/1	0.98	0.13	27,27,27,27	0
54	MG	2A	3699	1/1	0.98	0.16	44,44,44,44	0
54	MG	1A	3043	1/1	0.98	0.24	17,17,17,17	0
54	MG	1A	3017	1/1	0.98	0.20	37,37,37,37	0
54	MG	1A	3760	1/1	0.98	0.12	34,34,34,34	0
54	MG	1A	4059	1/1	0.98	0.22	28,28,28,28	0
54	MG	1A	3239	1/1	0.98	0.27	43,43,43,43	0
54	MG	1A	3106	1/1	0.98	0.18	30,30,30,30	0
54	MG	1A	3091	1/1	0.98	0.17	42,42,42,42	0
54	MG	1A	3508	1/1	0.98	0.14	46,46,46,46	0
54	MG	2A	3698	1/1	0.98	0.15	39,39,39,39	0
54	MG	1A	3510	1/1	0.98	0.19	31,31,31,31	0
54	MG	1A	3268	1/1	0.98	0.17	45,45,45,45	0
54	MG	1A	3243	1/1	0.98	0.16	33,33,33,33	0
54	MG	1A	3086	1/1	0.98	0.34	45,45,45,45	0
54	MG	1A	3398	1/1	0.98	0.20	22,22,22,22	0
54	MG	1A	3686	1/1	0.98	0.09	50,50,50,50	0
54	MG	2A	3205	1/1	0.98	0.15	66,66,66,66	0
54	MG	2A	3341	1/1	0.98	0.13	36,36,36,36	0
54	MG	2A	3299	1/1	0.98	0.08	35,35,35,35	0
54	MG	1F	308	1/1	0.98	0.17	41,41,41,41	0
54	MG	2A	3238	1/1	0.98	0.27	47,47,47,47	0
54	MG	2A	3423	1/1	0.98	0.08	33,33,33,33	0
54	MG	1A	3817	1/1	0.98	0.10	45,45,45,45	0
54	MG	1A	3896	1/1	0.98	0.10	49,49,49,49	0
54	MG	2A	3007	1/1	0.98	0.16	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3290	1/1	0.98	0.22	36,36,36,36	0
54	MG	2A	3390	1/1	0.98	0.11	31,31,31,31	0
54	MG	2A	3311	1/1	0.98	0.14	49,49,49,49	0
54	MG	1A	3088	1/1	0.98	0.14	47,47,47,47	0
54	MG	1A	3919	1/1	0.98	0.24	35,35,35,35	0
54	MG	1A	3132	1/1	0.98	0.16	39,39,39,39	0
54	MG	1A	4018	1/1	0.98	0.11	44,44,44,44	0
54	MG	1A	3892	1/1	0.98	0.14	38,38,38,38	0
54	MG	1A	3356	1/1	0.98	0.18	11,11,11,11	0
54	MG	1A	3021	1/1	0.98	0.19	34,34,34,34	0
54	MG	1A	3031	1/1	0.98	0.20	24,24,24,24	0
54	MG	1A	3271	1/1	0.98	0.19	37,37,37,37	0
54	MG	1A	3461	1/1	0.98	0.16	44,44,44,44	0
54	MG	2A	3417	1/1	0.98	0.20	52,52,52,52	0
54	MG	1A	3533	1/1	0.98	0.11	27,27,27,27	0
54	MG	1a	1739	1/1	0.98	0.16	60,60,60,60	0
54	MG	1A	3422	1/1	0.98	0.20	32,32,32,32	0
54	MG	1A	3333	1/1	0.98	0.16	47,47,47,47	0
54	MG	2A	3076	1/1	0.98	0.20	51,51,51,51	0
54	MG	2E	301	1/1	0.98	0.06	50,50,50,50	0
54	MG	1A	3005	1/1	0.98	0.26	24,24,24,24	0
54	MG	1A	3917	1/1	0.98	0.16	15,15,15,15	0
54	MG	2A	3091	1/1	0.98	0.15	34,34,34,34	0
54	MG	1A	3046	1/1	0.98	0.28	13,13,13,13	0
54	MG	1A	3053	1/1	0.98	0.13	36,36,36,36	0
54	MG	1A	3722	1/1	0.98	0.14	32,32,32,32	0
54	MG	1A	3923	1/1	0.98	0.06	43,43,43,43	0
54	MG	1a	1686	1/1	0.98	0.29	64,64,64,64	0
54	MG	2A	3392	1/1	0.98	0.12	65,65,65,65	0
54	MG	2A	3184	1/1	0.98	0.15	45,45,45,45	0
54	MG	1A	3078	1/1	0.98	0.23	38,38,38,38	0
54	MG	1A	3966	1/1	0.98	0.10	48,48,48,48	0
54	MG	1A	3028	1/1	0.98	0.19	28,28,28,28	0
54	MG	1A	4066	1/1	0.98	0.16	38,38,38,38	0
54	MG	1A	3521	1/1	0.98	0.15	31,31,31,31	0
54	MG	1A	3487	1/1	0.98	0.14	25,25,25,25	0
54	MG	1A	3300	1/1	0.98	0.21	12,12,12,12	0
54	MG	1A	3359	1/1	0.98	0.27	11,11,11,11	0
54	MG	1A	3526	1/1	0.98	0.09	48,48,48,48	0
54	MG	2a	1780	1/1	0.98	0.13	66,66,66,66	0
54	MG	1a	1701	1/1	0.98	0.20	64,64,64,64	0
54	MG	1A	3524	1/1	0.98	0.17	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3832	1/1	0.98	0.14	50,50,50,50	0
54	MG	2A	3155	1/1	0.98	0.20	52,52,52,52	0
54	MG	2A	3008	1/1	0.98	0.11	30,30,30,30	0
54	MG	1A	3330	1/1	0.98	0.20	33,33,33,33	0
54	MG	2A	3379	1/1	0.98	0.16	30,30,30,30	0
54	MG	1A	3259	1/1	0.98	0.16	40,40,40,40	0
54	MG	2A	3027	1/1	0.98	0.15	45,45,45,45	0
54	MG	2a	1726	1/1	0.98	0.18	57,57,57,57	0
54	MG	1A	3951	1/1	0.98	0.14	31,31,31,31	0
54	MG	1A	3041	1/1	0.98	0.19	54,54,54,54	0
54	MG	1A	3393	1/1	0.98	0.24	26,26,26,26	0
54	MG	2F	303	1/1	0.98	0.26	43,43,43,43	0
54	MG	1A	3334	1/1	0.98	0.20	37,37,37,37	0
54	MG	1A	3184	1/1	0.98	0.13	35,35,35,35	0
54	MG	1A	3071	1/1	0.98	0.15	32,32,32,32	0
54	MG	1A	3280	1/1	0.98	0.20	48,48,48,48	0
54	MG	2A	3004	1/1	0.98	0.17	26,26,26,26	0
54	MG	1A	3824	1/1	0.98	0.19	33,33,33,33	0
54	MG	1A	4042	1/1	0.98	0.16	36,36,36,36	0
54	MG	2A	3615	1/1	0.98	0.12	34,34,34,34	0
54	MG	1a	1769	1/1	0.98	0.06	58,58,58,58	0
54	MG	1a	1779	1/1	0.98	0.13	56,56,56,56	0
54	MG	1D	307	1/1	0.98	0.24	17,17,17,17	0
54	MG	2A	3006	1/1	0.98	0.10	46,46,46,46	0
54	MG	1A	3016	1/1	0.98	0.26	42,42,42,42	0
54	MG	1a	1687	1/1	0.98	0.11	52,52,52,52	0
54	MG	1A	3774	1/1	0.98	0.14	43,43,43,43	0
54	MG	2A	3169	1/1	0.98	0.10	41,41,41,41	0
54	MG	1A	3658	1/1	0.98	0.18	19,19,19,19	0
54	MG	1B	205	1/1	0.98	0.25	39,39,39,39	0
54	MG	1A	4036	1/1	0.98	0.20	35,35,35,35	0
54	MG	1A	4034	1/1	0.98	0.12	31,31,31,31	0
54	MG	1A	3323	1/1	0.98	0.20	28,28,28,28	0
54	MG	2A	3459	1/1	0.98	0.16	49,49,49,49	0
54	MG	2A	3069	1/1	0.98	0.21	44,44,44,44	0
54	MG	1A	3947	1/1	0.98	0.14	50,50,50,50	0
54	MG	2A	3397	1/1	0.98	0.16	36,36,36,36	0
54	MG	2D	305	1/1	0.98	0.24	49,49,49,49	0
54	MG	1A	3266	1/1	0.98	0.15	28,28,28,28	0
54	MG	1A	3029	1/1	0.98	0.18	40,40,40,40	0
54	MG	2V	201	1/1	0.98	0.21	60,60,60,60	0
54	MG	2A	3564	1/1	0.98	0.08	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3248	1/1	0.98	0.35	58,58,58,58	0
54	MG	1A	3113	1/1	0.98	0.14	34,34,34,34	0
54	MG	1A	3978	1/1	0.98	0.19	29,29,29,29	0
54	MG	1A	3717	1/1	0.98	0.26	39,39,39,39	0
54	MG	1A	3886	1/1	0.98	0.12	29,29,29,29	0
54	MG	1A	3072	1/1	0.98	0.20	37,37,37,37	0
54	MG	1a	1710	1/1	0.98	0.20	38,38,38,38	0
54	MG	1A	3264	1/1	0.98	0.23	29,29,29,29	0
54	MG	2A	3441	1/1	0.98	0.10	70,70,70,70	0
54	MG	1A	3729	1/1	0.98	0.21	27,27,27,27	0
54	MG	1a	1601	1/1	0.98	0.12	57,57,57,57	0
54	MG	2A	3242	1/1	0.98	0.26	48,48,48,48	0
54	MG	2A	3337	1/1	0.98	0.12	32,32,32,32	0
54	MG	1A	4039	1/1	0.98	0.24	41,41,41,41	0
54	MG	2A	3043	1/1	0.98	0.14	23,23,23,23	0
54	MG	1A	3070	1/1	0.98	0.23	43,43,43,43	0
54	MG	1A	3123	1/1	0.98	0.25	23,23,23,23	0
54	MG	1A	3582	1/1	0.98	0.15	50,50,50,50	0
54	MG	2A	3054	1/1	0.98	0.11	44,44,44,44	0
54	MG	1a	1798	1/1	0.98	0.10	48,48,48,48	0
54	MG	1A	3003	1/1	0.98	0.27	24,24,24,24	0
54	MG	1A	4008	1/1	0.98	0.24	33,33,33,33	0
54	MG	2a	1758	1/1	0.98	0.15	50,50,50,50	0
54	MG	1A	3895	1/1	0.98	0.15	35,35,35,35	0
54	MG	1A	3220	1/1	0.98	0.17	39,39,39,39	0
54	MG	2A	3749	1/1	0.98	0.23	39,39,39,39	0
58	SF4	2d	501	8/8	0.98	0.12	61,78,84,104	0
54	MG	1A	3588	1/1	0.98	0.20	21,21,21,21	0
54	MG	1D	301	1/1	0.98	0.17	37,37,37,37	0
57	ZN	26	501	1/1	0.98	0.18	60,60,60,60	0
54	MG	1A	3069	1/1	0.98	0.12	37,37,37,37	0
54	MG	2A	3543	1/1	0.98	0.09	42,42,42,42	0
54	MG	2A	3510	1/1	0.98	0.16	47,47,47,47	0
54	MG	2A	3298	1/1	0.98	0.11	33,33,33,33	0
54	MG	1A	3306	1/1	0.98	0.18	29,29,29,29	0
54	MG	1A	4054	1/1	0.98	0.13	44,44,44,44	0
54	MG	1A	3181	1/1	0.98	0.12	36,36,36,36	0
54	MG	1A	3575	1/1	0.98	0.18	33,33,33,33	0
54	MG	2A	3733	1/1	0.98	0.19	33,33,33,33	0
54	MG	1A	3710	1/1	0.98	0.15	55,55,55,55	0
54	MG	2A	3602	1/1	0.98	0.13	32,32,32,32	0
54	MG	1F	303	1/1	0.98	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3222	1/1	0.98	0.17	36,36,36,36	0
54	MG	2A	3015	1/1	0.98	0.25	36,36,36,36	0
54	MG	2A	3393	1/1	0.98	0.14	43,43,43,43	0
54	MG	1A	4061	1/1	0.98	0.23	37,37,37,37	0
54	MG	1A	3042	1/1	0.98	0.22	24,24,24,24	0
54	MG	2A	3064	1/1	0.98	0.14	38,38,38,38	0
54	MG	1A	4052	1/1	0.98	0.19	45,45,45,45	0
54	MG	1A	3316	1/1	0.98	0.17	39,39,39,39	0
54	MG	1A	3241	1/1	0.98	0.17	37,37,37,37	0
54	MG	1A	4040	1/1	0.98	0.11	37,37,37,37	0
54	MG	1A	3968	1/1	0.98	0.11	44,44,44,44	0
54	MG	1A	3790	1/1	0.98	0.13	21,21,21,21	0
54	MG	1A	3764	1/1	0.98	0.20	29,29,29,29	0
54	MG	1A	4038	1/1	0.98	0.17	37,37,37,37	0
54	MG	1A	4031	1/1	0.98	0.32	38,38,38,38	0
54	MG	1A	3541	1/1	0.98	0.18	27,27,27,27	0
54	MG	1A	3667	1/1	0.98	0.21	47,47,47,47	0
54	MG	1B	228	1/1	0.98	0.13	65,65,65,65	0
54	MG	1A	3953	1/1	0.98	0.21	19,19,19,19	0
54	MG	1A	3140	1/1	0.98	0.22	31,31,31,31	0
54	MG	2A	3518	1/1	0.99	0.15	35,35,35,35	0
54	MG	1A	4073	1/1	0.99	0.19	40,40,40,40	0
54	MG	1A	3325	1/1	0.99	0.21	21,21,21,21	0
54	MG	1A	3009	1/1	0.99	0.18	26,26,26,26	0
54	MG	1A	3376	1/1	0.99	0.15	45,45,45,45	0
54	MG	1A	3498	1/1	0.99	0.12	50,50,50,50	0
54	MG	1A	3539	1/1	0.99	0.17	36,36,36,36	0
54	MG	1A	3308	1/1	0.99	0.22	46,46,46,46	0
54	MG	1A	3233	1/1	0.99	0.16	37,37,37,37	0
54	MG	1A	4041	1/1	0.99	0.22	37,37,37,37	0
54	MG	1A	3238	1/1	0.99	0.20	38,38,38,38	0
54	MG	1A	3185	1/1	0.99	0.18	37,37,37,37	0
54	MG	1A	3286	1/1	0.99	0.12	41,41,41,41	0
54	MG	1A	3156	1/1	0.99	0.26	30,30,30,30	0
54	MG	1B	201	1/1	0.99	0.17	44,44,44,44	0
54	MG	2A	3030	1/1	0.99	0.23	39,39,39,39	0
54	MG	2A	3095	1/1	0.99	0.20	38,38,38,38	0
54	MG	1D	305	1/1	0.99	0.26	38,38,38,38	0
54	MG	1A	4055	1/1	0.99	0.15	42,42,42,42	0
54	MG	2A	3018	1/1	0.99	0.27	35,35,35,35	0
54	MG	2A	3130	1/1	0.99	0.24	42,42,42,42	0
54	MG	1A	3209	1/1	0.99	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3240	1/1	0.99	0.14	34,34,34,34	0
54	MG	2A	3560	1/1	0.99	0.17	23,23,23,23	0
54	MG	1A	3077	1/1	0.99	0.26	53,53,53,53	0
54	MG	1A	3671	1/1	0.99	0.18	36,36,36,36	0
54	MG	1a	1722	1/1	0.99	0.14	40,40,40,40	0
54	MG	2A	3494	1/1	0.99	0.17	27,27,27,27	0
54	MG	1A	3351	1/1	0.99	0.17	24,24,24,24	0
54	MG	1A	3606	1/1	0.99	0.19	32,32,32,32	0
54	MG	1A	3098	1/1	0.99	0.24	12,12,12,12	0
54	MG	1A	3020	1/1	0.99	0.20	39,39,39,39	0
54	MG	2A	3013	1/1	0.99	0.21	24,24,24,24	0
54	MG	1A	3148	1/1	0.99	0.17	33,33,33,33	0
54	MG	1A	3872	1/1	0.99	0.12	42,42,42,42	0
54	MG	1A	3019	1/1	0.99	0.20	30,30,30,30	0
54	MG	2A	3011	1/1	0.99	0.14	28,28,28,28	0
54	MG	27	3001	1/1	0.99	0.18	43,43,43,43	0
54	MG	1A	3423	1/1	0.99	0.18	16,16,16,16	0
54	MG	2A	3731	1/1	0.99	0.24	23,23,23,23	0
54	MG	1A	3137	1/1	0.99	0.24	42,42,42,42	0
54	MG	2A	3451	1/1	0.99	0.20	39,39,39,39	0
54	MG	1a	1733	1/1	0.99	0.15	34,34,34,34	0
54	MG	1A	3834	1/1	0.99	0.12	45,45,45,45	0
54	MG	1Q	201	1/1	0.99	0.22	33,33,33,33	0
54	MG	1A	3972	1/1	0.99	0.18	26,26,26,26	0
54	MG	1A	3275	1/1	0.99	0.21	41,41,41,41	0
54	MG	1A	3179	1/1	0.99	0.15	34,34,34,34	0
54	MG	2A	3123	1/1	0.99	0.44	48,48,48,48	0
54	MG	2A	3503	1/1	0.99	0.21	35,35,35,35	0
54	MG	1A	3420	1/1	0.99	0.25	24,24,24,24	0
54	MG	2A	3542	1/1	0.99	0.18	34,34,34,34	0
54	MG	1A	3874	1/1	0.99	0.17	24,24,24,24	0
54	MG	1A	3574	1/1	0.99	0.22	31,31,31,31	0
57	ZN	15	101	1/1	0.99	0.16	50,50,50,50	0
54	MG	1A	3025	1/1	0.99	0.21	40,40,40,40	0
54	MG	1A	3299	1/1	0.99	0.23	22,22,22,22	0
57	ZN	19	102	1/1	0.99	0.19	37,37,37,37	0
54	MG	1A	3645	1/1	0.99	0.20	30,30,30,30	0
54	MG	1A	3277	1/1	0.99	0.20	29,29,29,29	0
54	MG	1A	3366	1/1	0.99	0.11	46,46,46,46	0
54	MG	1A	3044	1/1	0.99	0.20	32,32,32,32	0
54	MG	1A	3556	1/1	0.99	0.19	39,39,39,39	0
54	MG	2A	3452	1/1	0.99	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	4037	1/1	0.99	0.19	32,32,32,32	0
54	MG	1A	3208	1/1	0.99	0.21	42,42,42,42	0
54	MG	2A	3305	1/1	0.99	0.19	19,19,19,19	0
54	MG	1A	3163	1/1	0.99	0.28	34,34,34,34	0
54	MG	2A	3283	1/1	0.99	0.21	19,19,19,19	0
54	MG	1A	3971	1/1	0.99	0.19	31,31,31,31	0
54	MG	2A	3574	1/1	0.99	0.13	30,30,30,30	0
54	MG	2A	3456	1/1	0.99	0.18	24,24,24,24	0
54	MG	1P	201	1/1	0.99	0.10	26,26,26,26	0
54	MG	1A	3332	1/1	0.99	0.22	28,28,28,28	0
54	MG	1a	1616	1/1	0.99	0.18	48,48,48,48	0
54	MG	1A	4007	1/1	0.99	0.25	17,17,17,17	0
54	MG	1A	3249	1/1	0.99	0.18	35,35,35,35	0
54	MG	2A	3053	1/1	0.99	0.13	39,39,39,39	0
54	MG	1A	3514	1/1	0.99	0.20	23,23,23,23	0
54	MG	1A	4012	1/1	0.99	0.21	23,23,23,23	0
54	MG	1a	1796	1/1	0.99	0.06	68,68,68,68	0
54	MG	2A	3111	1/1	0.99	0.11	54,54,54,54	0
54	MG	2A	3020	1/1	0.99	0.20	44,44,44,44	0
54	MG	1A	3826	1/1	0.99	0.16	8,8,8,8	0
54	MG	2A	3074	1/1	0.99	0.17	23,23,23,23	0
54	MG	2A	3429	1/1	0.99	0.13	36,36,36,36	0
54	MG	1A	4024	1/1	0.99	0.34	36,36,36,36	0
54	MG	1A	3144	1/1	0.99	0.17	41,41,41,41	0
54	MG	1A	3023	1/1	0.99	0.16	34,34,34,34	0
54	MG	1A	3792	1/1	0.99	0.18	26,26,26,26	0
54	MG	1A	3092	1/1	0.99	0.15	35,35,35,35	0
54	MG	1A	3871	1/1	0.99	0.08	45,45,45,45	0
54	MG	1A	3240	1/1	0.99	0.27	38,38,38,38	0
54	MG	1A	3087	1/1	0.99	0.28	34,34,34,34	0
54	MG	1F	304	1/1	0.99	0.16	33,33,33,33	0
54	MG	1g	201	1/1	0.99	0.12	62,62,62,62	0
54	MG	1A	3018	1/1	0.99	0.20	33,33,33,33	0
54	MG	2A	3254	1/1	0.99	0.33	39,39,39,39	0
57	ZN	16	501	1/1	0.99	0.22	39,39,39,39	0
54	MG	1A	3693	1/1	0.99	0.36	54,54,54,54	0
54	MG	1A	3732	1/1	0.99	0.18	32,32,32,32	0
54	MG	1A	3626	1/1	0.99	0.18	30,30,30,30	0
54	MG	1A	3141	1/1	1.00	0.31	36,36,36,36	0
54	MG	1A	3149	1/1	1.00	0.21	28,28,28,28	0
54	MG	1A	3433	1/1	1.00	0.23	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.