wwPDB X-ray Structure Validation Summary Report (i)

Jan 5, 2024 – 12:12 am GMT

PDB ID	:	5FDV
Title	:	Crystal structure of the Pyrrhocoricin antimicrobial peptide bound to the Thermus thermophilus 70S ribosome
Authors	:	Seefeldt, A.C.; Graf, M.; Perebaskine, N.; Nguyen, F.; Arenz, S.; Mardirossian, M.; Scocchi, M.; Wilson, D.N.; Innis, C.A.
Deposited on	:	2015-12-16
Resolution	:	2.80 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

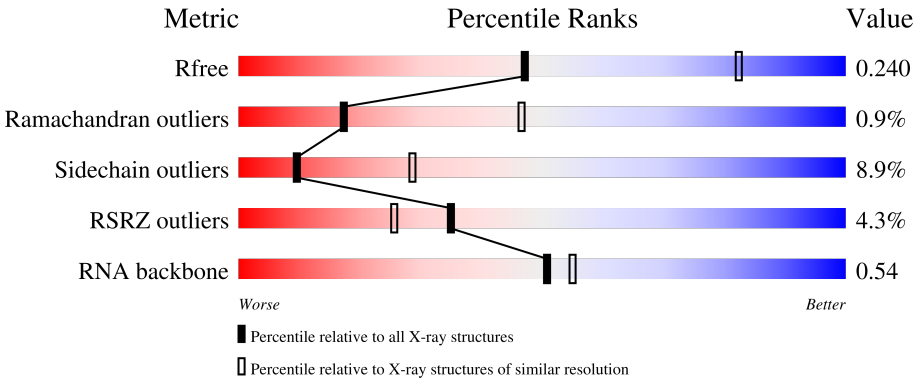
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	5% 35% 54% 10% .
1	2A	2915	6% 54% 38% 7% .
2	1B	120	49% 50% .
2	2B	120	71% 29%

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Mol	Chain	Length	Quality of chain
3	1D	275	92% 8%
3	2D	275	91% 9%
4	1E	204	91% 8%
4	2E	204	91% 9%
5	1F	203	87% 13%
5	2F	203	91% 9%
6	1G	181	92% 7%
6	2G	181	8% 93% 7%
7	1H	174	93% 7%
7	2H	174	16% 92% 7%
8	1I	147	88% 11%
8	2I	147	3% 90% 8%
9	1N	140	88% 12%
9	2N	140	90% 10%
10	1O	122	92% 7%
10	2O	122	93% 7%
11	1P	149	94% 6%
11	2P	149	93% 7%
12	1Q	141	94% 6%
12	2Q	141	94% 6%
13	1R	118	87% 11%
13	2R	118	87% 13%
14	1S	110	88% 11%
14	2S	110	3% 91% 9%
15	1T	131	92% 8%

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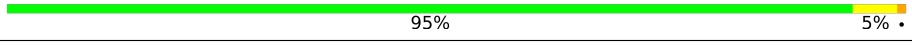
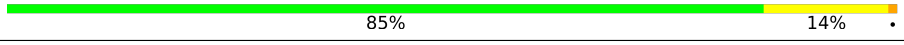
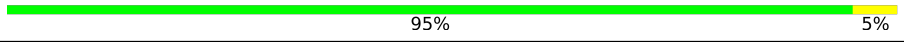
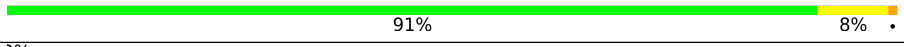
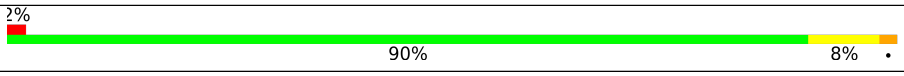
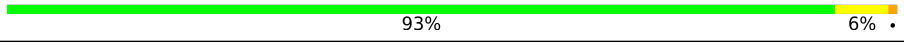
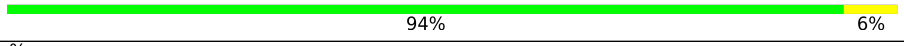
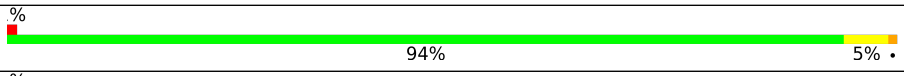
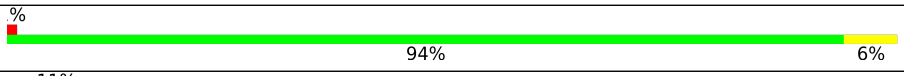
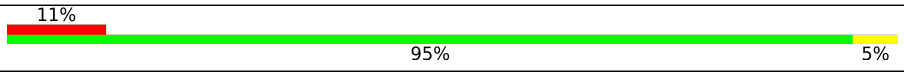
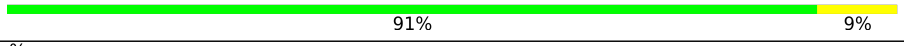
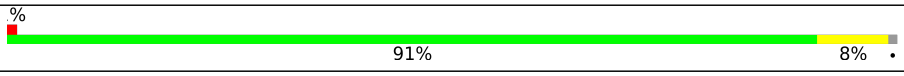
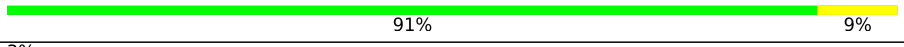
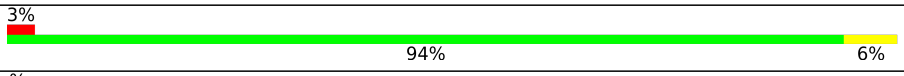
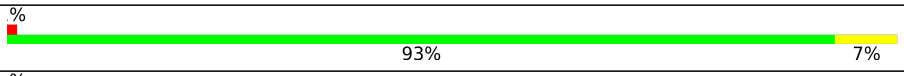
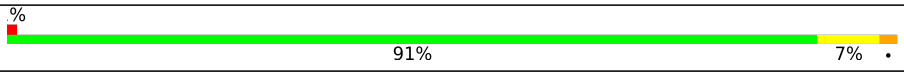
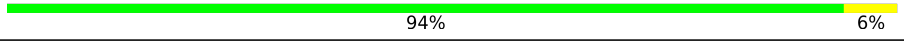
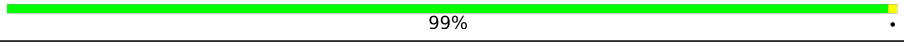
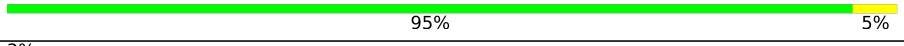
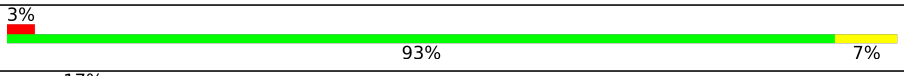
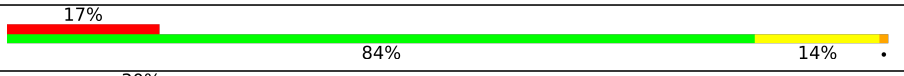
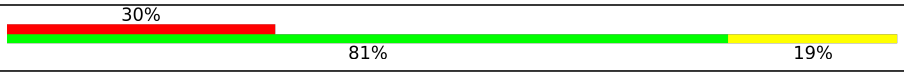
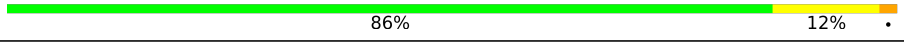
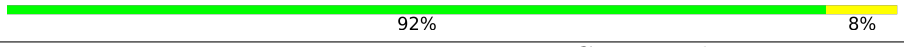
Mol	Chain	Length	Quality of chain
15	2T	131	
16	1U	116	
16	2U	116	
17	1V	101	
17	2V	101	
18	1W	112	
18	2W	112	
19	1X	95	
19	2X	95	
20	1Y	107	
20	2Y	107	
21	1Z	203	
21	2Z	203	
22	10	77	
22	20	77	
23	11	97	
23	21	97	
24	12	70	
24	22	70	
25	13	59	
25	23	59	
26	14	69	
26	24	69	
27	15	59	
27	25	59	

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Mol	Chain	Length	Quality of chain
28	16	53	83% 17%
28	26	53	92% 8%
29	17	48	92% 6%
29	27	48	96%
30	18	64	84% 16%
30	28	64	92% 8%
31	19	37	92% 5%
31	29	37	3% 100%
32	1a	1521	4% 52% 38% 8%
32	2a	1521	4% 57% 35% 8%
33	1x	97	% 95% 5%
33	2x	97	41% 89% 10%
34	1b	231	8% 84% 14%
34	2b	231	6% 87% 12%
35	1c	206	6% 98%
35	2c	206	8% 91% 9%
36	1d	208	% 91% 9%
36	2d	208	% 91% 9%
37	1e	148	93% 7%
37	2e	148	94% 6%
38	1f	100	96%
38	2f	100	94% 6%
39	1g	155	3% 95% 5%
39	2g	155	9% 94% 6%
40	1h	137	% 94% 6%

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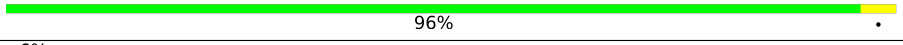
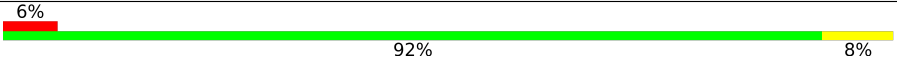
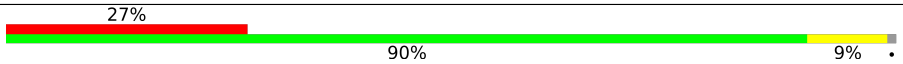
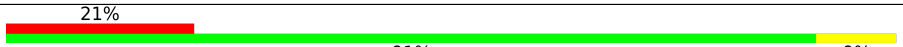
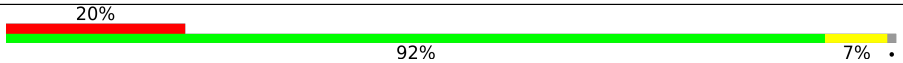
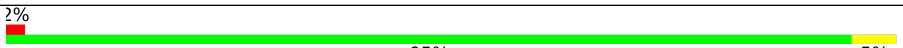
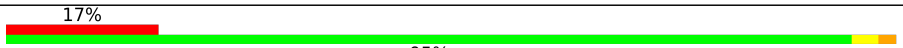
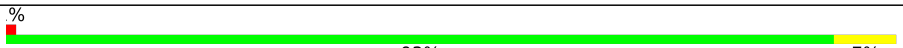
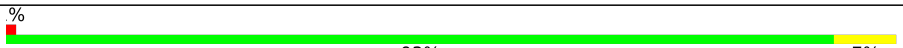
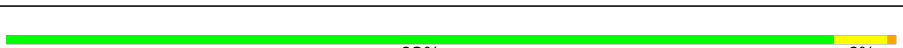
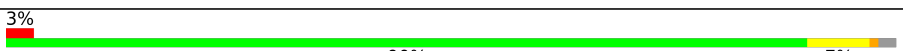
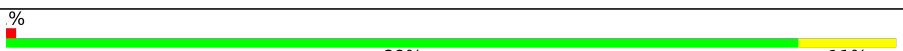
Mol	Chain	Length	Quality of chain
40	2h	137	
41	1i	127	
41	2i	127	
42	1j	97	
42	2j	97	
43	1k	114	
43	2k	114	
44	1l	122	
44	2l	122	
45	1m	116	
45	2m	116	
46	1n	60	
46	2n	60	
47	1o	88	
47	2o	88	
48	1p	82	
48	2p	82	
49	1q	99	
49	2q	99	
50	1r	68	
50	2r	68	
51	1s	83	
51	2s	83	
52	1t	98	
52	2t	98	

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Mol	Chain	Length	Quality of chain
53	1u	23	22% 87% 13%
53	2u	23	39% 96%
54	1y	16	12% 94% 6%
54	2y	16	31% 88% 12%

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
55	MG	1A	3062	-	-	-	X
55	MG	1A	3095	-	-	-	X
55	MG	1A	3174	-	-	-	X
55	MG	1A	3213	-	-	-	X
55	MG	1A	3219	-	-	-	X
55	MG	1A	3254	-	-	-	X
55	MG	1A	3514	-	-	-	X
55	MG	1A	3700	-	-	-	X
55	MG	1A	3724	-	-	-	X
55	MG	1A	3757	-	-	-	X
55	MG	1A	3758	-	-	-	X
55	MG	1A	3898	-	-	-	X
55	MG	1A	3904	-	-	-	X
55	MG	1D	303	-	-	-	X
55	MG	1a	3038	-	-	-	X
55	MG	1a	3039	-	-	-	X
55	MG	1a	3049	-	-	-	X
55	MG	1a	3057	-	-	-	X
55	MG	1a	3058	-	-	-	X
55	MG	1a	3063	-	-	-	X
55	MG	1a	3074	-	-	-	X
55	MG	1a	3077	-	-	-	X
55	MG	1a	3078	-	-	-	X
55	MG	1a	3136	-	-	-	X
55	MG	28	101	-	-	-	X
55	MG	2A	3011	-	-	-	X
55	MG	2A	3028	-	-	-	X
55	MG	2A	3041	-	-	-	X
55	MG	2A	3042	-	-	-	X
55	MG	2A	3049	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2A	3109	-	-	-	X
55	MG	2A	3128	-	-	-	X
55	MG	2A	3131	-	-	-	X
55	MG	2A	3132	-	-	-	X
55	MG	2A	3133	-	-	-	X
55	MG	2A	3136	-	-	-	X
55	MG	2A	3138	-	-	-	X
55	MG	2A	3141	-	-	-	X
55	MG	2A	3151	-	-	-	X
55	MG	2A	3183	-	-	-	X
55	MG	2A	3188	-	-	-	X
55	MG	2A	3255	-	-	-	X
55	MG	2A	3411	-	-	-	X
55	MG	2A	3416	-	-	-	X
55	MG	2A	3454	-	-	-	X
55	MG	2A	3475	-	-	-	X
55	MG	2A	3506	-	-	-	X
55	MG	2A	3513	-	-	-	X
55	MG	2A	3533	-	-	-	X
55	MG	2A	3549	-	-	-	X
55	MG	2A	3554	-	-	-	X
55	MG	2A	3555	-	-	-	X
55	MG	2A	3562	-	-	-	X
55	MG	2A	3631	-	-	-	X
55	MG	2A	3727	-	-	-	X
55	MG	2A	3752	-	-	-	X
55	MG	2A	3765	-	-	-	X
55	MG	2A	3791	-	-	-	X
55	MG	2A	3795	-	-	-	X
55	MG	2A	3811	-	-	-	X
55	MG	2A	3813	-	-	-	X
55	MG	2A	3815	-	-	-	X
55	MG	2D	304	-	-	-	X
55	MG	2N	201	-	-	-	X
55	MG	2Q	204	-	-	-	X
55	MG	2X	102	-	-	-	X
55	MG	2a	1603	-	-	-	X
55	MG	2a	1620	-	-	-	X
55	MG	2a	1641	-	-	-	X
55	MG	2a	1654	-	-	-	X
55	MG	2a	1733	-	-	-	X
55	MG	2a	1741	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2l	201	-	-	-	X
55	MG	2n	502	-	-	-	X
58	A	2A	3816	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 293583 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
			61862	27535	11569	19886	2872			
1	2A	2867	Total	C	N	O	P	0	0	0
			61751	27486	11547	19852	2866			

- 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
			2575	1145	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2571	1146	476	831	118			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 33 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	2x	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			
33	1x	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
34	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
35	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
36	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
37	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
38	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
39	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
40	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
41	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	2j	96	Total 710	C 442	N 137	O 131	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1k	114	Total 834	C 520	N 156	O 155	S 3	0	0	0
43	2k	114	Total 833	C 519	N 156	O 155	S 3	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1l	122	Total 932	C 586	N 185	O 159	S 2	0	0	0
44	2l	122	Total 932	C 586	N 185	O 159	S 2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1m	116	Total 914	C 564	N 189	O 159	S 2	0	0	0
45	2m	114	Total 895	C 550	N 186	O 157	S 2	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1n	60	Total 492	C 312	N 104	O 72	S 4	0	0	0
46	2n	60	Total 492	C 312	N 104	O 72	S 4	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1o	88	Total 728	C 456	N 144	O 126	S 2	0	0	0
47	2o	88	Total 728	C 456	N 144	O 126	S 2	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
48	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
49	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
50	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
51	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
52	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

- Molecule 53 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	1u	23	Total 199	C 122	N 48	O 29	0	0	0
53	2u	23	Total 199	C 122	N 48	O 29	0	0	0

- Molecule 54 is a protein called Pyrrhocoricin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	1y	16	Total 120	C 79	N 20	O 21	0	0	0
54	2y	16	Total 120	C 79	N 20	O 21	0	0	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1A	945	Total 945	Mg 945	0	0
55	1B	26	Total 26	Mg 26	0	0
55	1D	14	Total 14	Mg 14	0	0
55	1E	5	Total 5	Mg 5	0	0
55	1F	12	Total 12	Mg 12	0	0
55	1G	3	Total 3	Mg 3	0	0
55	1H	2	Total 2	Mg 2	0	0
55	1N	4	Total 4	Mg 4	0	0
55	1P	2	Total 2	Mg 2	0	0
55	1Q	4	Total 4	Mg 4	0	0
55	1R	3	Total 3	Mg 3	0	0
55	1U	3	Total 3	Mg 3	0	0
55	1V	1	Total 1	Mg 1	0	0
55	1W	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1X	1	Total Mg 1 1	0	0
55	1Y	1	Total Mg 1 1	0	0
55	10	7	Total Mg 7 7	0	0
55	11	3	Total Mg 3 3	0	0
55	13	1	Total Mg 1 1	0	0
55	15	4	Total Mg 4 4	0	0
55	17	2	Total Mg 2 2	0	0
55	18	3	Total Mg 3 3	0	0
55	19	2	Total Mg 2 2	0	0
55	1a	226	Total Mg 226 226	0	0
55	1b	1	Total Mg 1 1	0	0
55	1d	5	Total Mg 5 5	0	0
55	1e	1	Total Mg 1 1	0	0
55	1f	1	Total Mg 1 1	0	0
55	1g	1	Total Mg 1 1	0	0
55	1h	2	Total Mg 2 2	0	0
55	1k	1	Total Mg 1 1	0	0
55	1l	1	Total Mg 1 1	0	0
55	1o	1	Total Mg 1 1	0	0
55	1t	1	Total Mg 1 1	0	0
55	1y	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	2A	837	Total Mg 837 837	0	0
55	2B	18	Total Mg 18 18	0	0
55	2D	10	Total Mg 10 10	0	0
55	2E	4	Total Mg 4 4	0	0
55	2F	9	Total Mg 9 9	0	0
55	2G	3	Total Mg 3 3	0	0
55	2H	1	Total Mg 1 1	0	0
55	2N	1	Total Mg 1 1	0	0
55	2P	2	Total Mg 2 2	0	0
55	2Q	5	Total Mg 5 5	0	0
55	2R	2	Total Mg 2 2	0	0
55	2S	1	Total Mg 1 1	0	0
55	2U	2	Total Mg 2 2	0	0
55	2V	3	Total Mg 3 3	0	0
55	2W	1	Total Mg 1 1	0	0
55	2X	3	Total Mg 3 3	0	0
55	20	5	Total Mg 5 5	0	0
55	21	2	Total Mg 2 2	0	0
55	25	3	Total Mg 3 3	0	0
55	27	2	Total Mg 2 2	0	0
55	28	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	2a	197	Total Mg 197 197	0	0
55	2b	1	Total Mg 1 1	0	0
55	2d	3	Total Mg 3 3	0	0
55	2e	2	Total Mg 2 2	0	0
55	2f	1	Total Mg 1 1	0	0
55	2g	1	Total Mg 1 1	0	0
55	2h	2	Total Mg 2 2	0	0
55	2l	2	Total Mg 2 2	0	0
55	2n	1	Total Mg 1 1	0	0
55	2o	1	Total Mg 1 1	0	0
55	2q	1	Total Mg 1 1	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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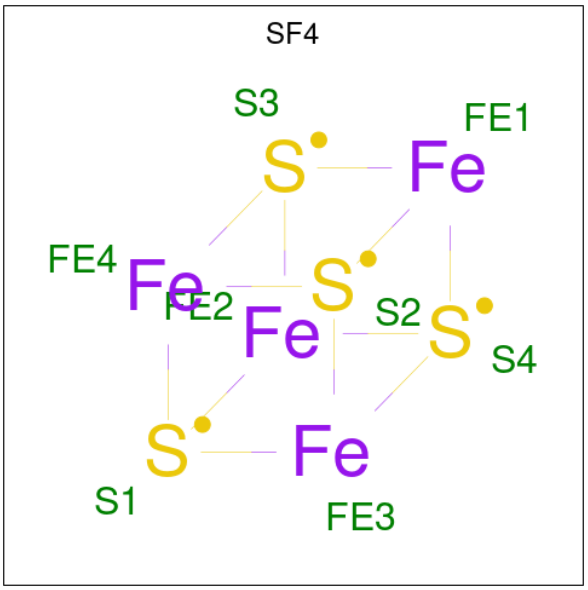
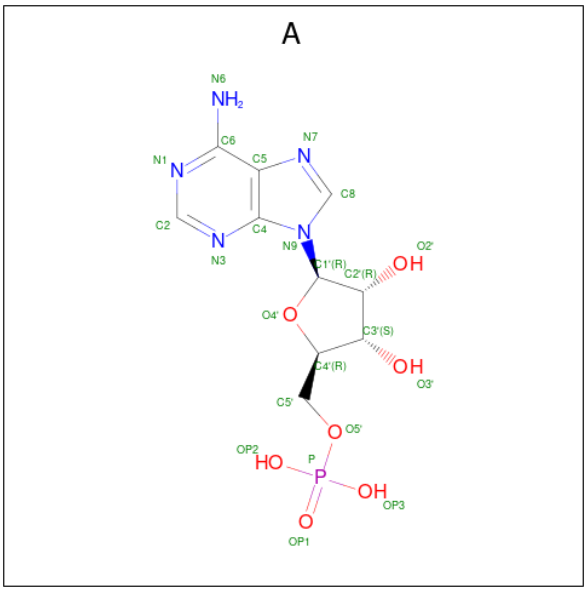
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	25	1	Total Zn 1 1	0	0
56	26	1	Total Zn 1 1	0	0
56	29	1	Total Zn 1 1	0	0
56	2n	1	Total Zn 1 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 58 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	2A	1	Total P 1 1	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1740	Total O 1740 1740	0	0
59	1B	43	Total O 43 43	0	0
59	1D	16	Total O 16 16	0	0
59	1E	17	Total O 17 17	0	0
59	1F	9	Total O 9 9	0	0
59	1G	2	Total O 2 2	0	0
59	1H	3	Total O 3 3	0	0
59	1N	8	Total O 8 8	0	0
59	1P	13	Total O 13 13	0	0
59	1Q	7	Total O 7 7	0	0
59	1R	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1T	5	Total O 5 5	0	0
59	1U	5	Total O 5 5	0	0
59	1V	3	Total O 3 3	0	0
59	1W	2	Total O 2 2	0	0
59	1X	4	Total O 4 4	0	0
59	1Y	4	Total O 4 4	0	0
59	10	5	Total O 5 5	0	0
59	11	3	Total O 3 3	0	0
59	13	1	Total O 1 1	0	0
59	15	2	Total O 2 2	0	0
59	16	2	Total O 2 2	0	0
59	17	2	Total O 2 2	0	0
59	18	9	Total O 9 9	0	0
59	19	2	Total O 2 2	0	0
59	1a	395	Total O 395 395	0	0
59	1d	10	Total O 10 10	0	0
59	1e	2	Total O 2 2	0	0
59	1f	1	Total O 1 1	0	0
59	1h	1	Total O 1 1	0	0
59	1j	1	Total O 1 1	0	0
59	1l	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1m	2	Total O 2 2	0	0
59	1n	1	Total O 1 1	0	0
59	1p	1	Total O 1 1	0	0
59	1q	1	Total O 1 1	0	0
59	1t	1	Total O 1 1	0	0
59	1y	2	Total O 2 2	0	0
59	2A	1667	Total O 1667 1667	0	0
59	2B	35	Total O 35 35	0	0
59	2D	14	Total O 14 14	0	0
59	2E	16	Total O 16 16	0	0
59	2F	11	Total O 11 11	0	0
59	2G	2	Total O 2 2	0	0
59	2H	2	Total O 2 2	0	0
59	2N	2	Total O 2 2	0	0
59	2P	11	Total O 11 11	0	0
59	2Q	4	Total O 4 4	0	0
59	2R	4	Total O 4 4	0	0
59	2T	2	Total O 2 2	0	0
59	2U	2	Total O 2 2	0	0
59	2V	2	Total O 2 2	0	0
59	2W	2	Total O 2 2	0	0

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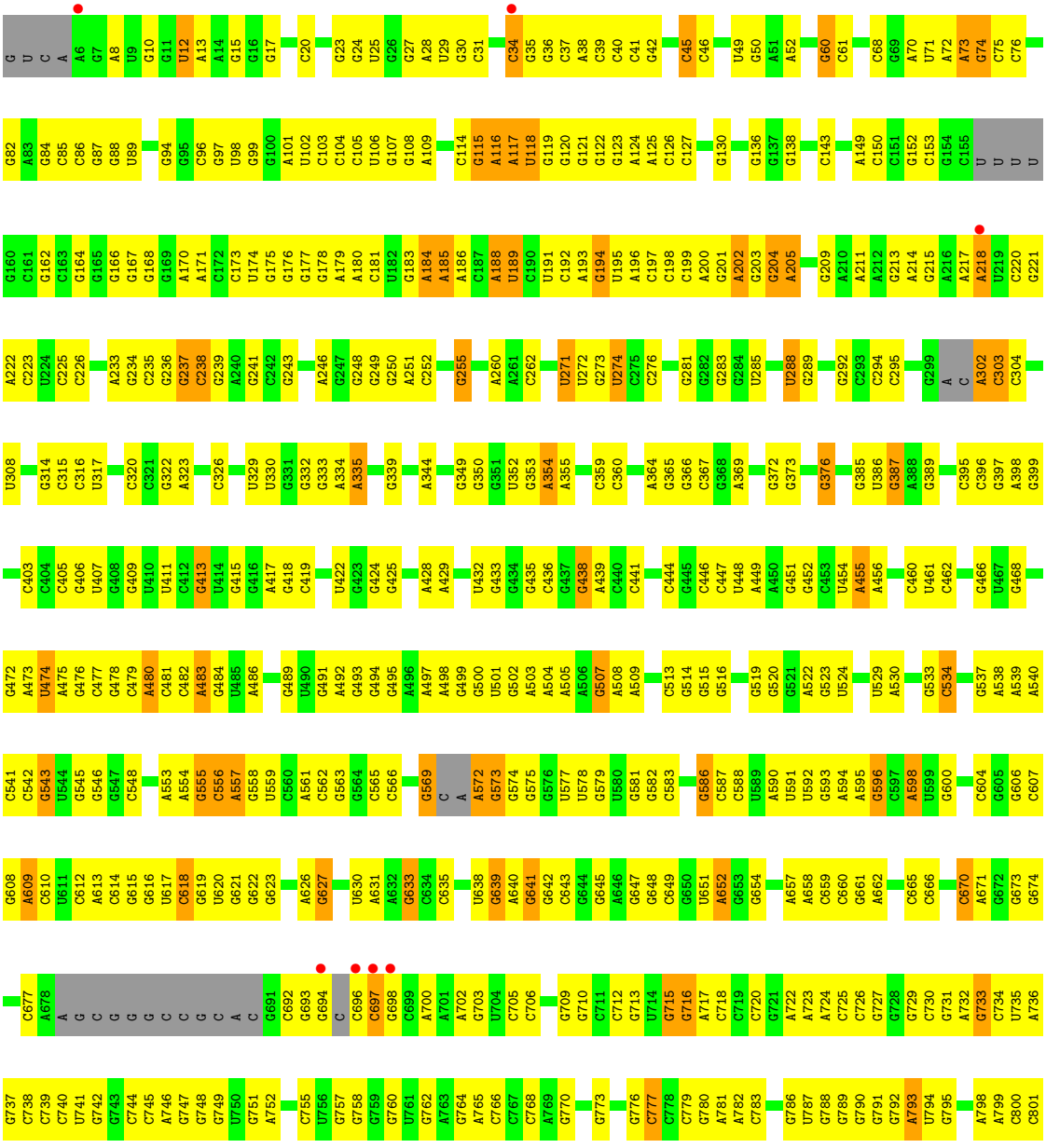
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2X	5	Total O 5 5	0	0
59	2Y	3	Total O 3 3	0	0
59	20	7	Total O 7 7	0	0
59	21	2	Total O 2 2	0	0
59	23	2	Total O 2 2	0	0
59	25	1	Total O 1 1	0	0
59	26	2	Total O 2 2	0	0
59	27	1	Total O 1 1	0	0
59	28	6	Total O 6 6	0	0
59	2a	387	Total O 387 387	0	0
59	2c	1	Total O 1 1	0	0
59	2d	6	Total O 6 6	0	0
59	2e	4	Total O 4 4	0	0
59	2f	1	Total O 1 1	0	0
59	2h	1	Total O 1 1	0	0
59	2j	1	Total O 1 1	0	0
59	2l	3	Total O 3 3	0	0
59	2m	2	Total O 2 2	0	0
59	2o	1	Total O 1 1	0	0
59	2t	1	Total O 1 1	0	0
59	2y	1	Total O 1 1	0	0

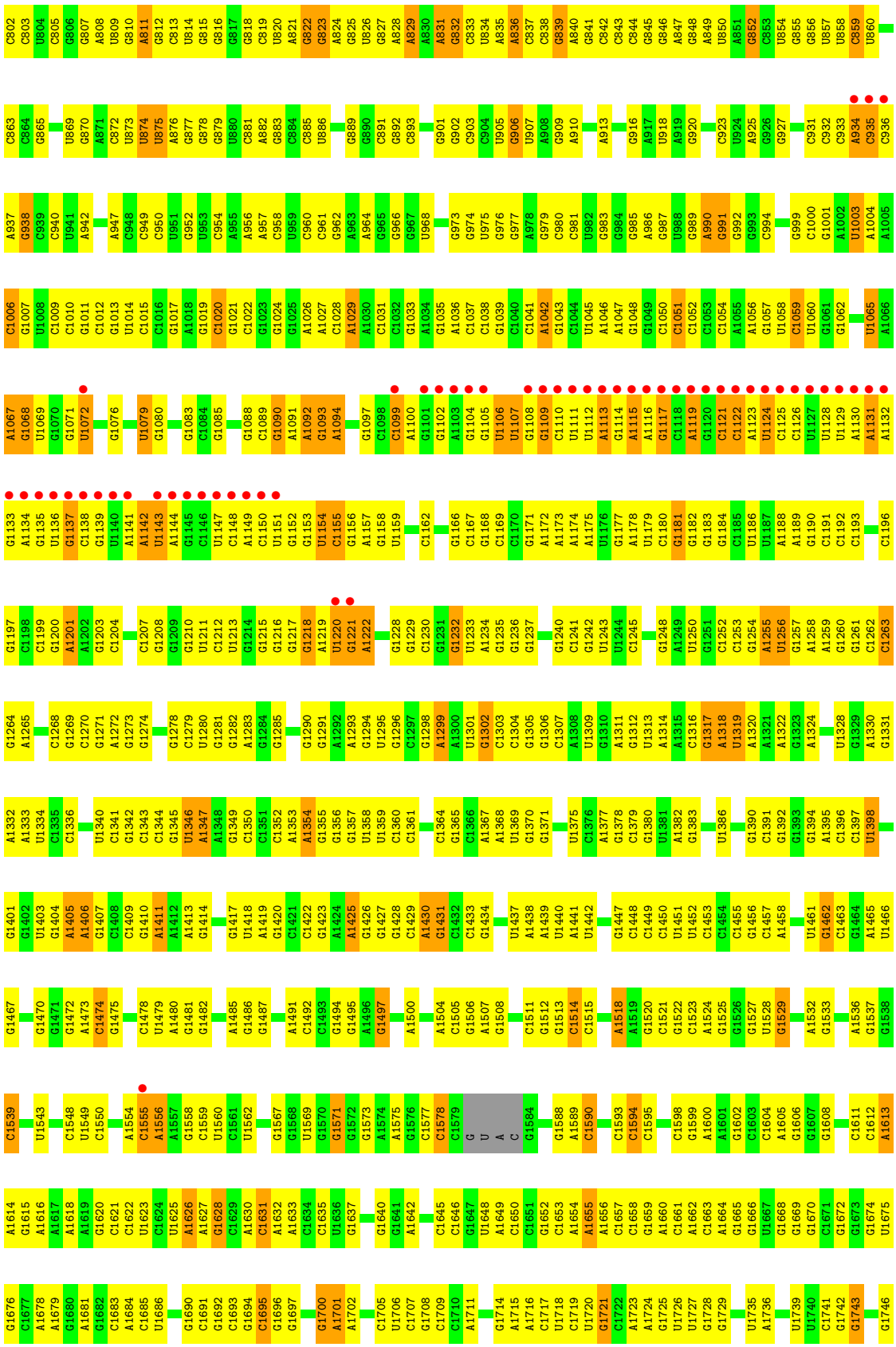
3 Residue-property plots (i)

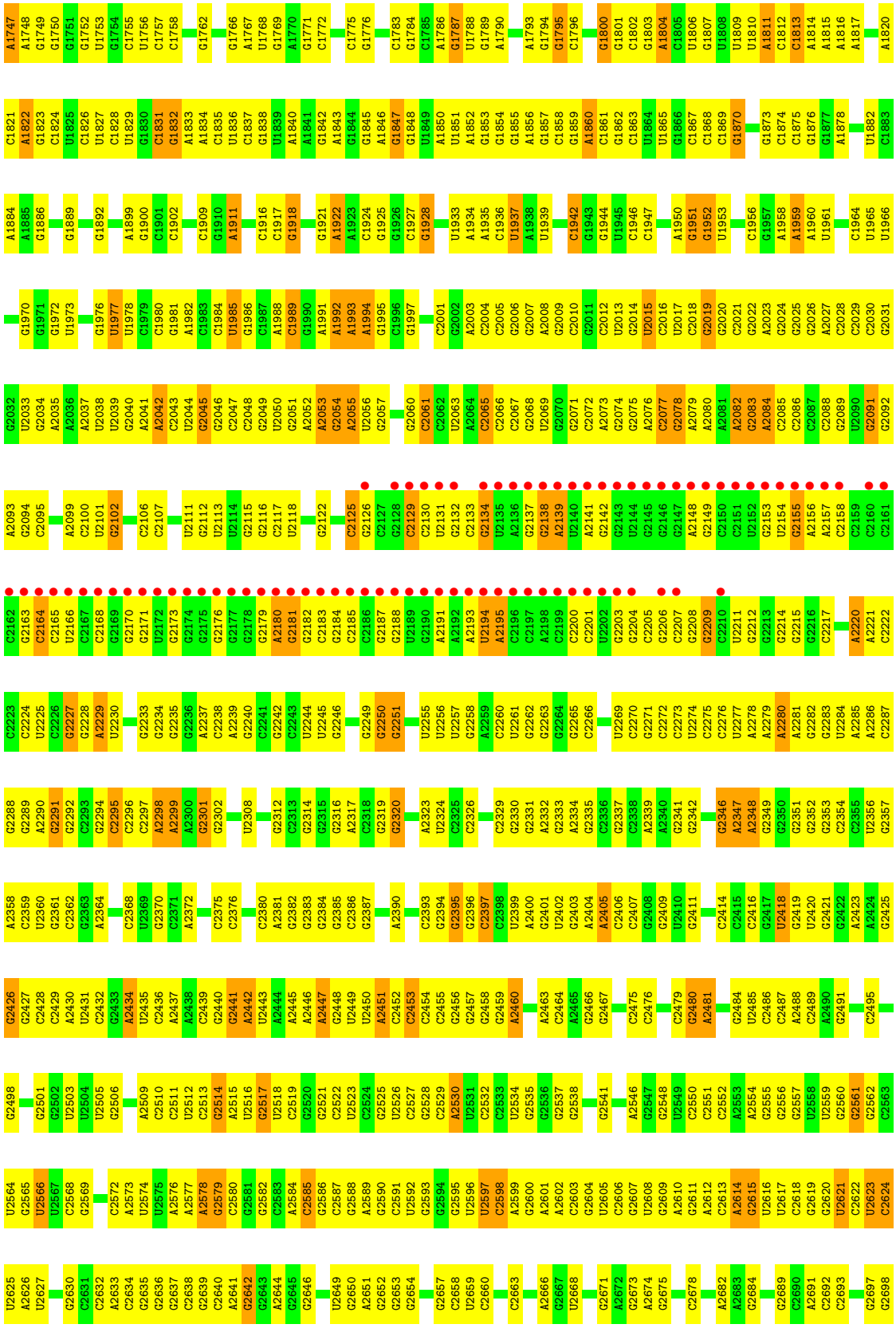
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

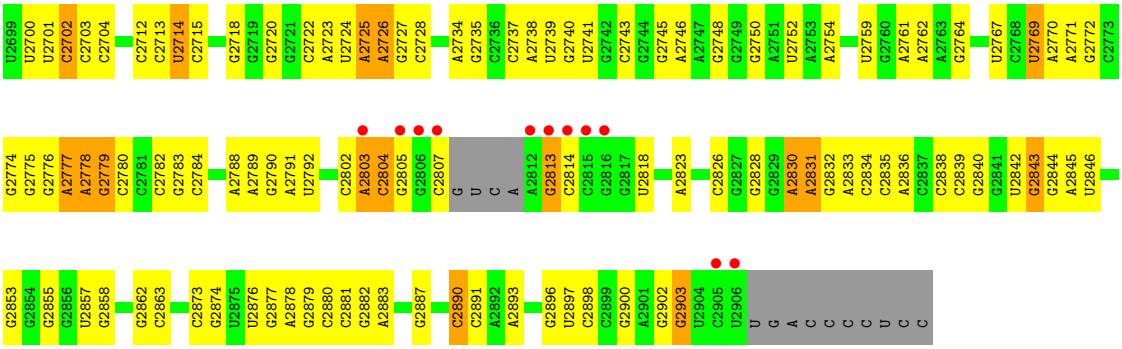
- Molecule 1: 23S ribosomal RNA

Chain 1A:



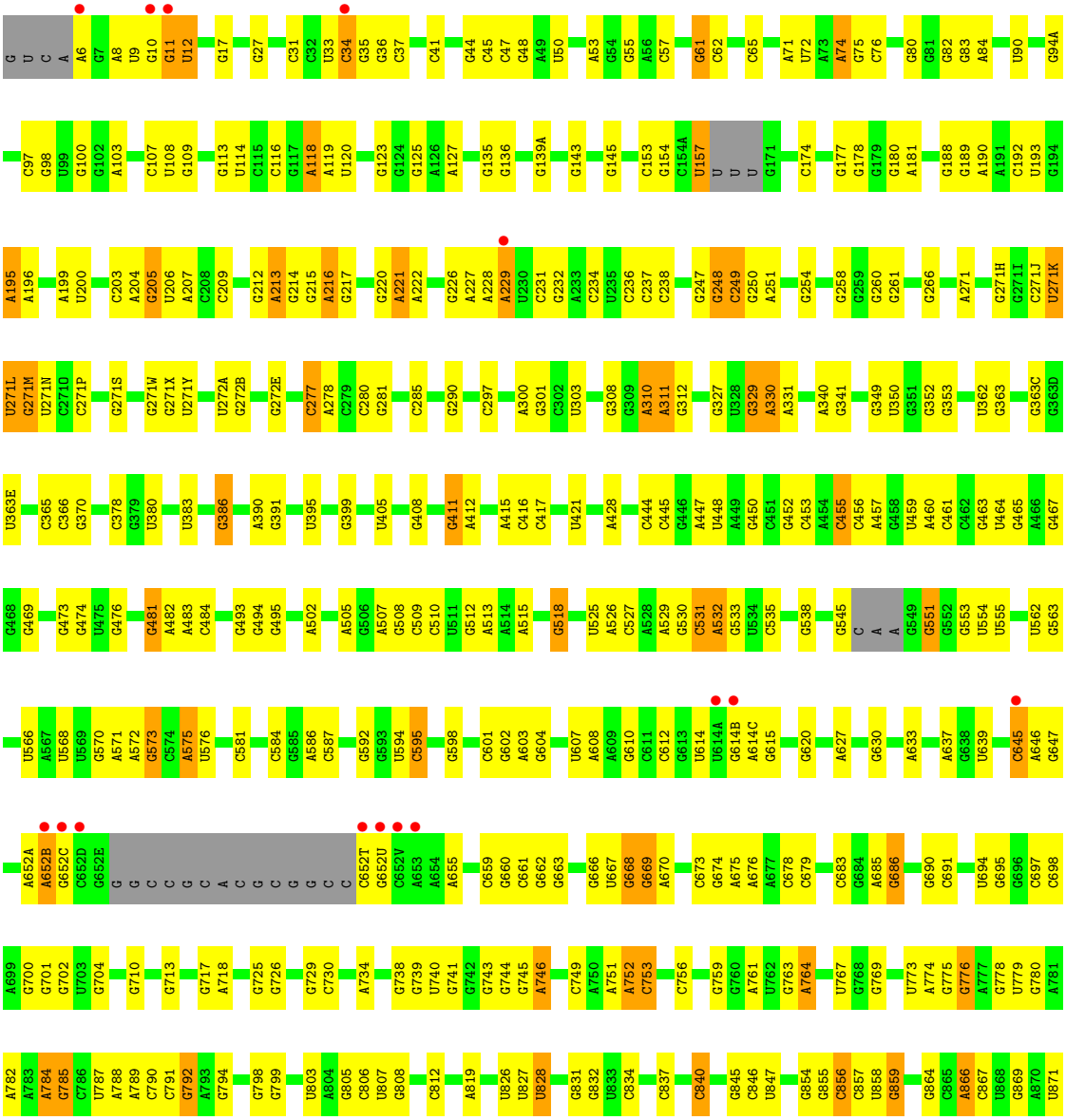


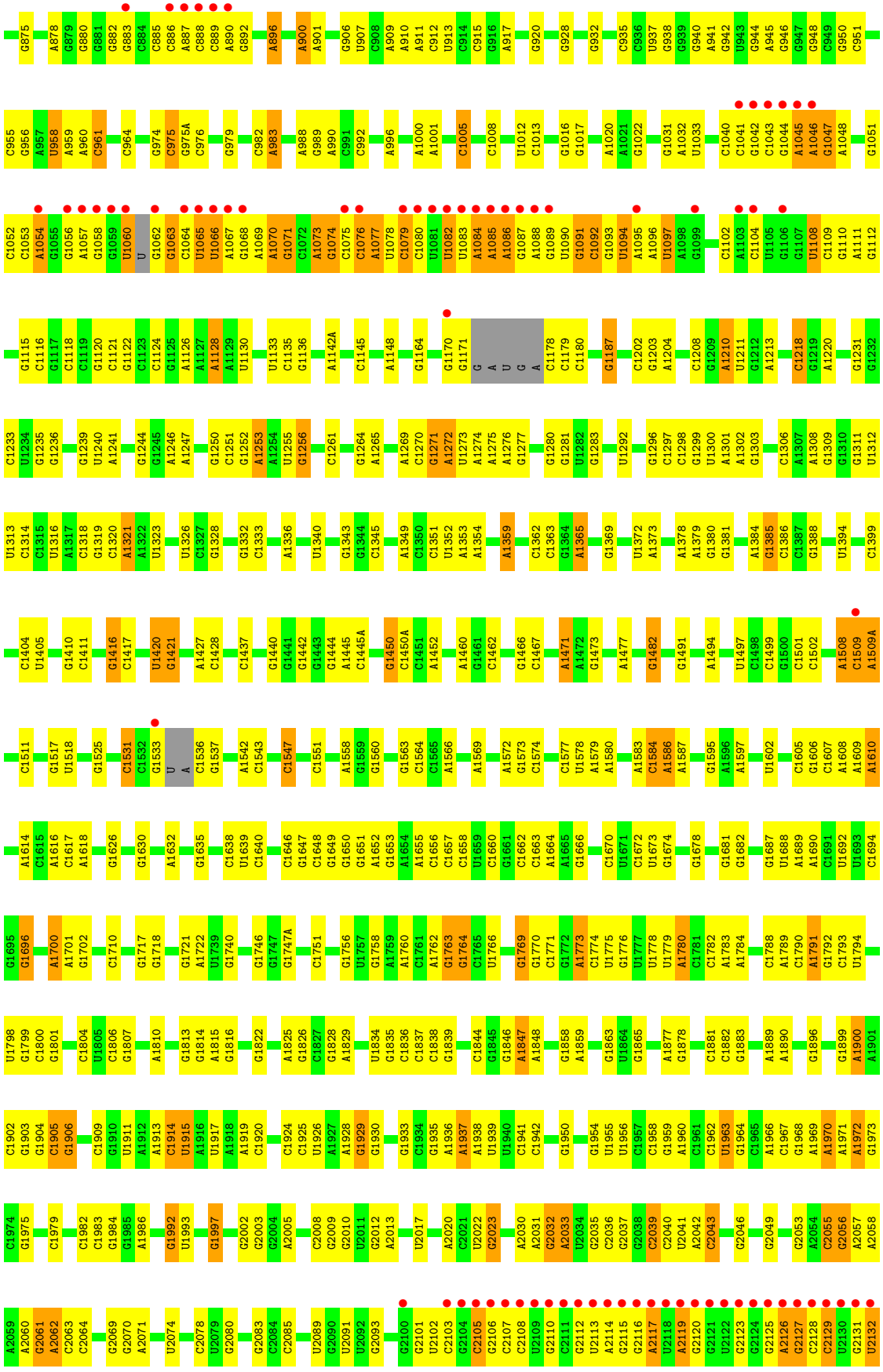


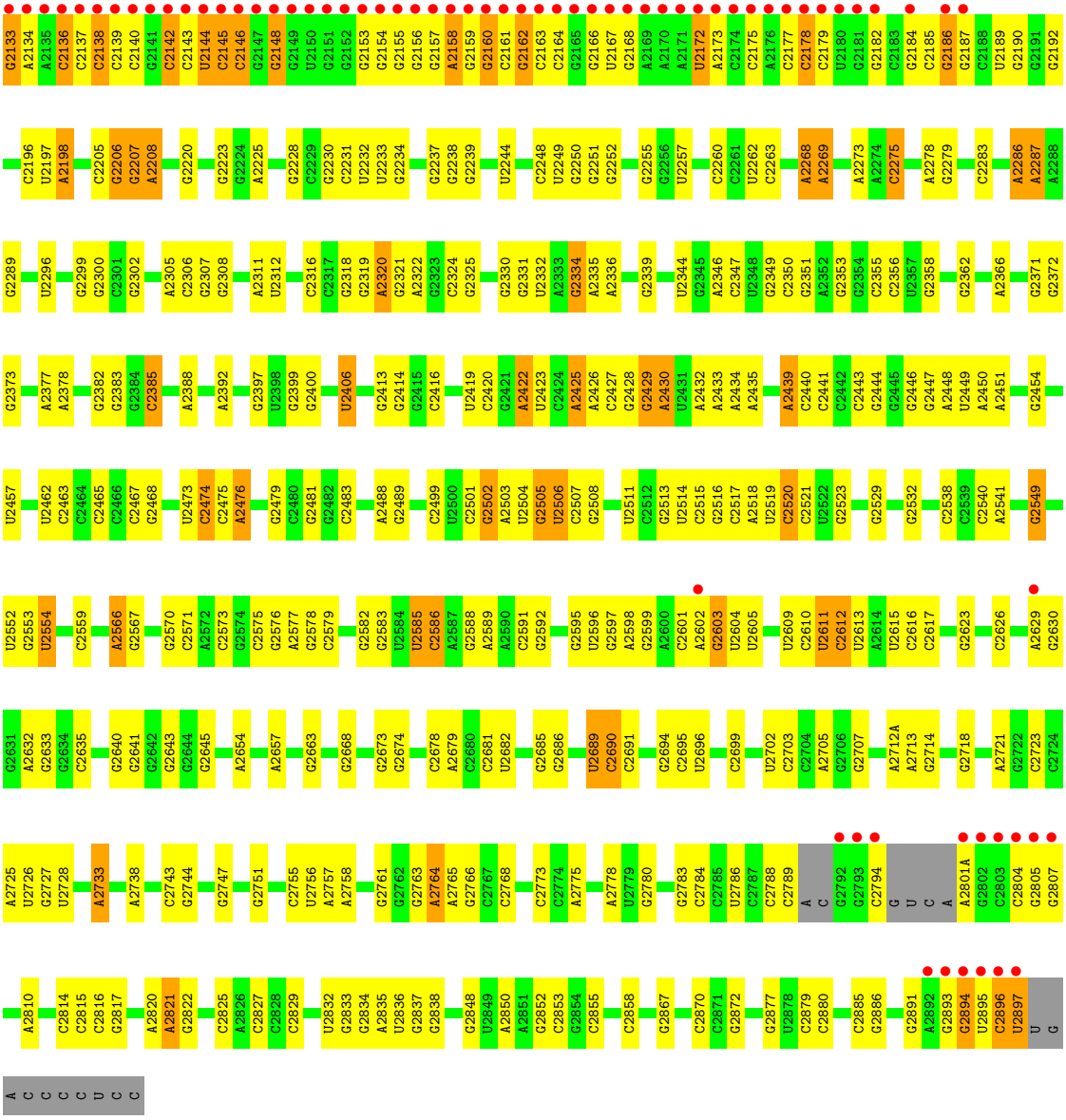


• Molecule 1: 23S ribosomal RNA

Chain 2A:

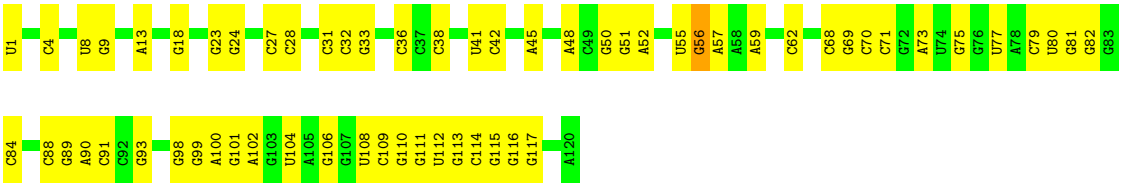






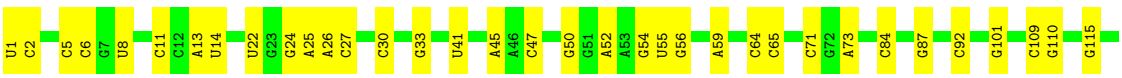
• Molecule 2: 5S ribosomal RNA

Chain 1B:



• Molecule 2: 5S ribosomal RNA

Chain 2B:



• Molecule 3: 50S ribosomal protein L2

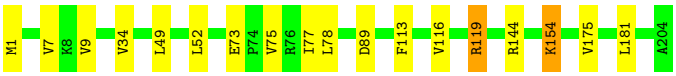
Chain 1D:

• Molecule 3: 50S ribosomal protein L2

Chain 2D:

• Molecule 4: 50S ribosomal protein L3

Chain 1E:

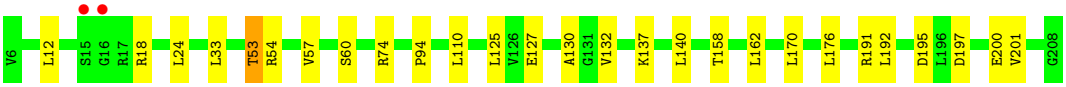


• Molecule 4: 50S ribosomal protein L3

Chain 2E:

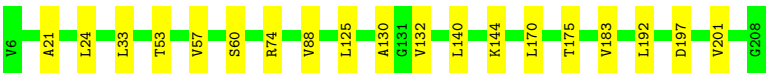
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



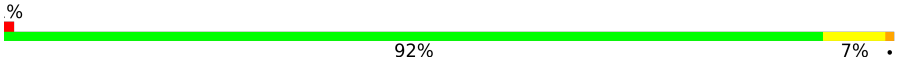
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



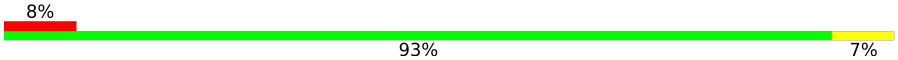
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



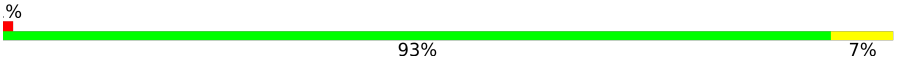
• Molecule 6: 50S ribosomal protein L5

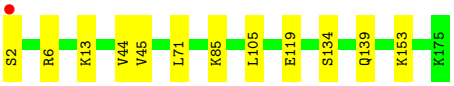
Chain 2G:



• Molecule 7: 50S ribosomal protein L6

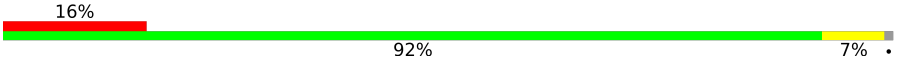
Chain 1H:

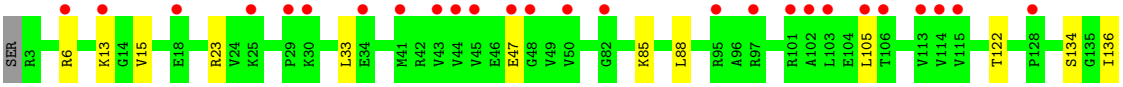




• Molecule 7: 50S ribosomal protein L6

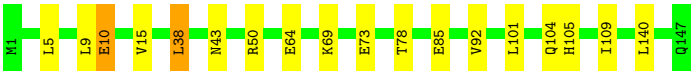
Chain 2H:





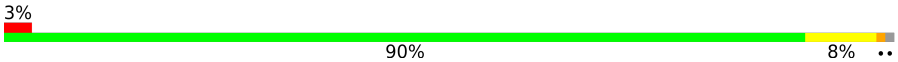
• Molecule 8: 50S ribosomal protein L9

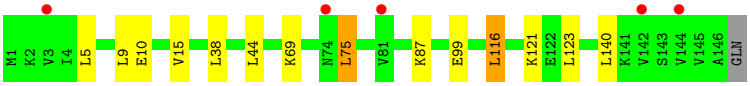
Chain 1I:



• Molecule 8: 50S ribosomal protein L9

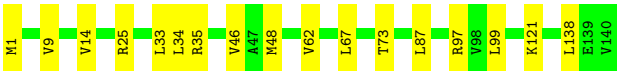
Chain 2I:





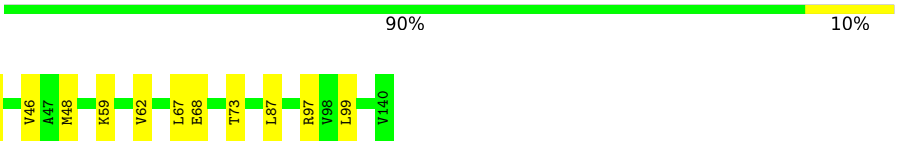
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



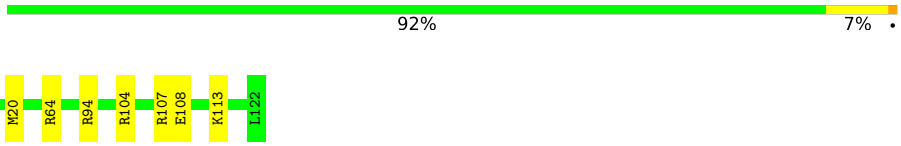
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



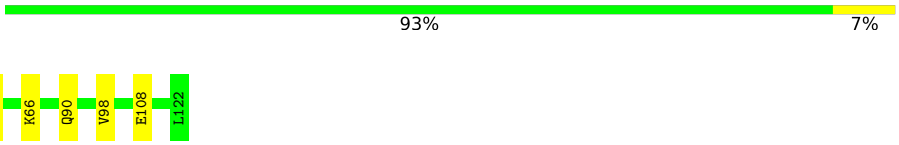
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



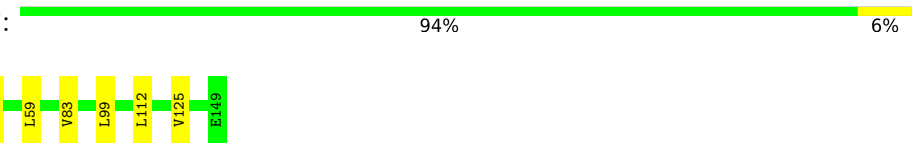
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



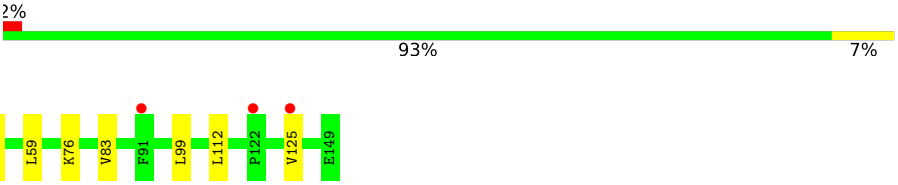
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



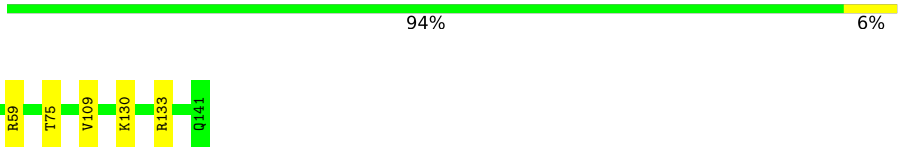
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



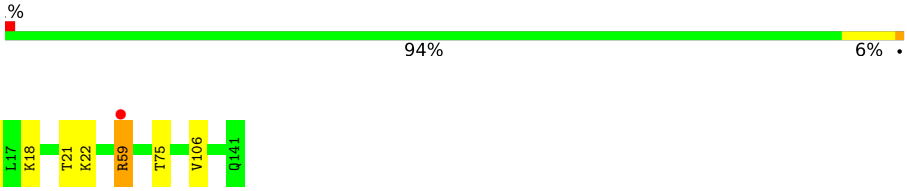
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



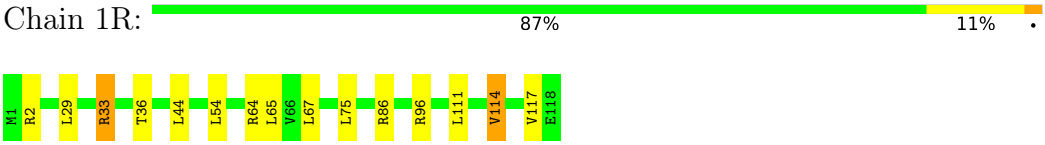
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



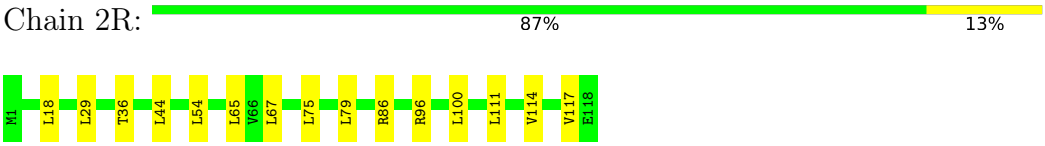
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



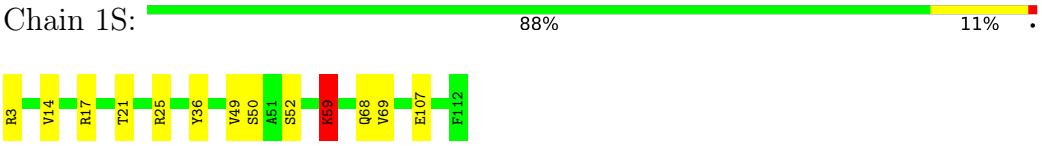
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



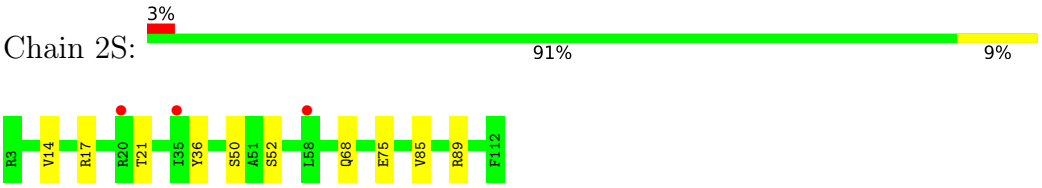
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



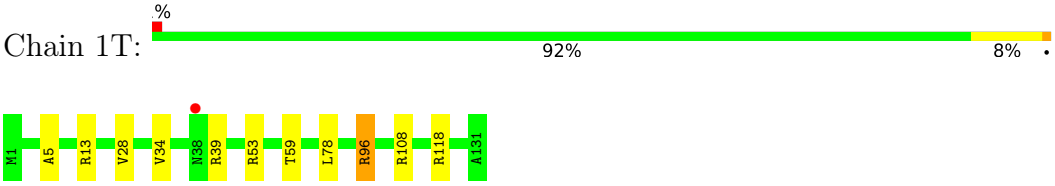
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



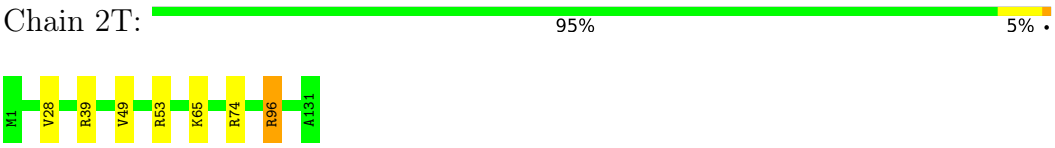
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



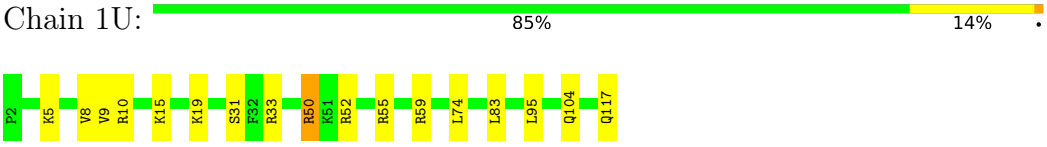
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



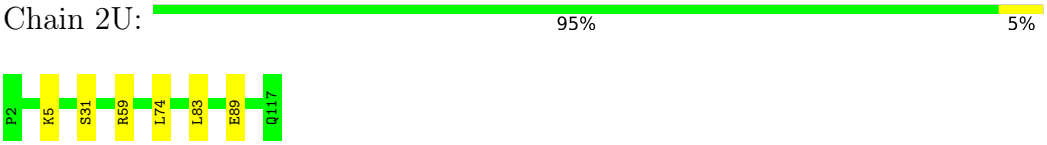
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



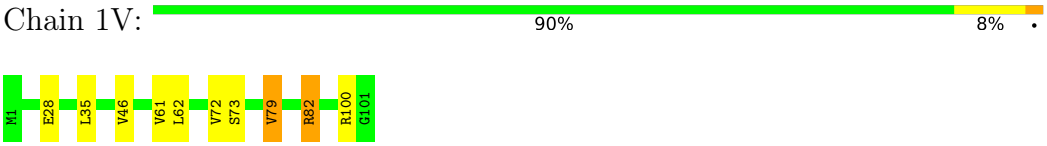
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



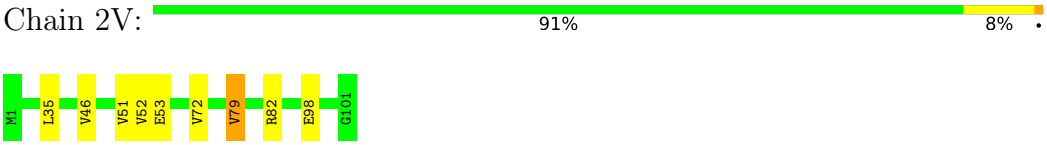
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



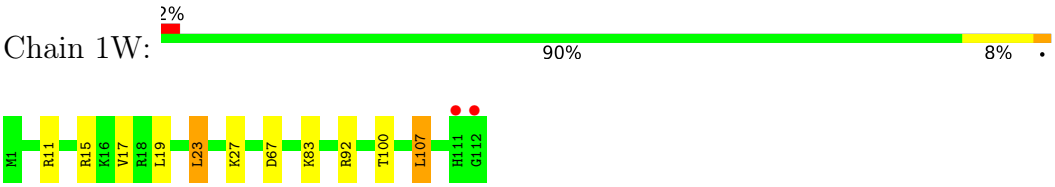
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



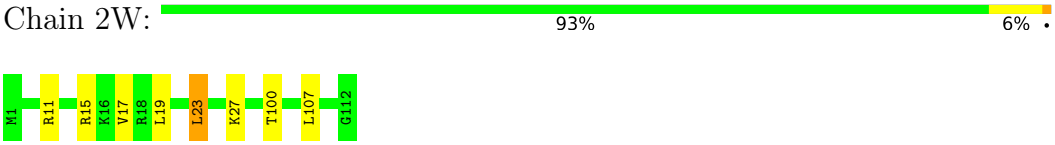
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



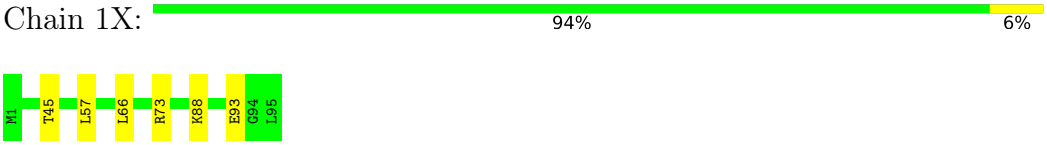
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



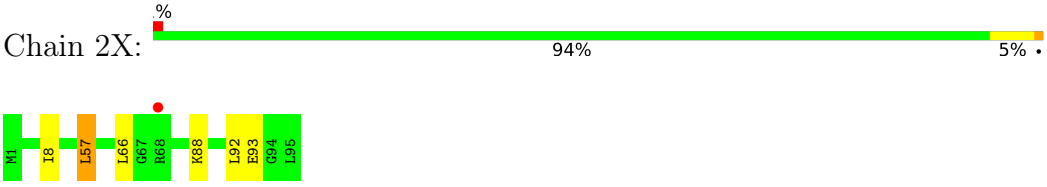
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



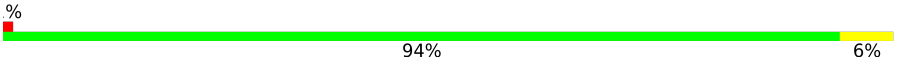
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



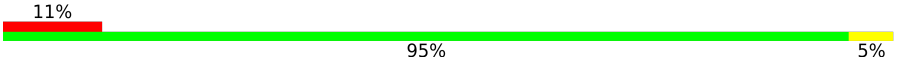
• Molecule 20: 50S ribosomal protein L24

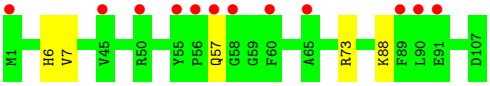
Chain 1Y:



• Molecule 20: 50S ribosomal protein L24

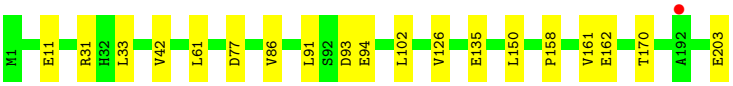
Chain 2Y:





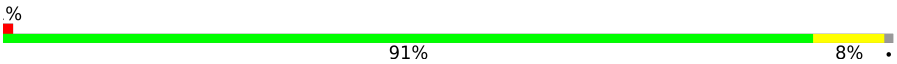
• Molecule 21: 50S ribosomal protein L25

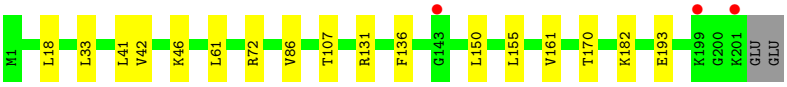
Chain 1Z:



• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



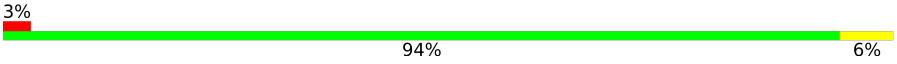


• Molecule 22: 50S ribosomal protein L27

Chain 10:

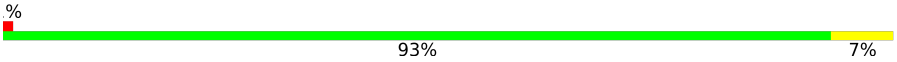
• Molecule 22: 50S ribosomal protein L27

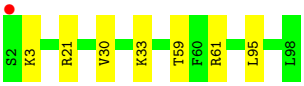
Chain 20:



• Molecule 23: 50S ribosomal protein L28

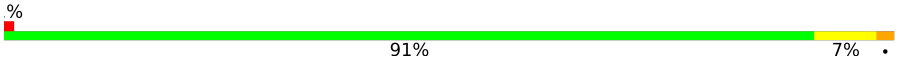
Chain 11:





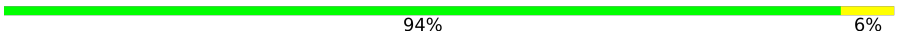
• Molecule 23: 50S ribosomal protein L28

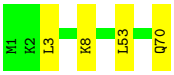
Chain 21:



• Molecule 24: 50S ribosomal protein L29

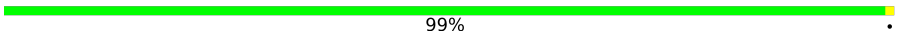
Chain 12:





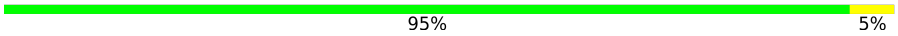
• Molecule 24: 50S ribosomal protein L29

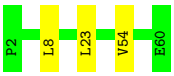
Chain 22:



• Molecule 25: 50S ribosomal protein L30

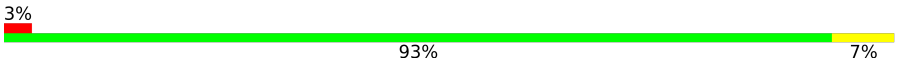
Chain 13:

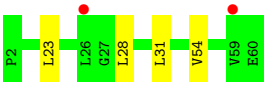




• Molecule 25: 50S ribosomal protein L30

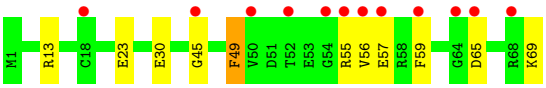
Chain 23:





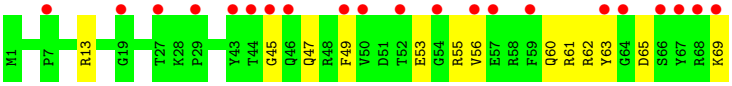
• Molecule 26: 50S ribosomal protein L31

Chain 14:



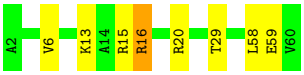
• Molecule 26: 50S ribosomal protein L31

Chain 24:



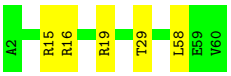
• Molecule 27: 50S ribosomal protein L32

Chain 15:



• Molecule 27: 50S ribosomal protein L32

Chain 25:



• Molecule 28: 50S ribosomal protein L33

Chain 16:

• Molecule 28: 50S ribosomal protein L33

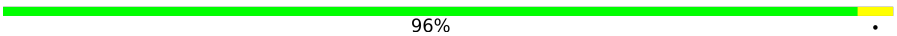
Chain 26:

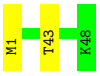
• Molecule 29: 50S ribosomal protein L34

Chain 17:

• Molecule 29: 50S ribosomal protein L34

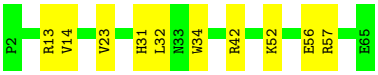
Chain 27:





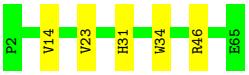
• Molecule 30: 50S ribosomal protein L35

Chain 18:



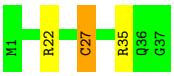
• Molecule 30: 50S ribosomal protein L35

Chain 28:



• Molecule 31: 50S ribosomal protein L36

Chain 19:

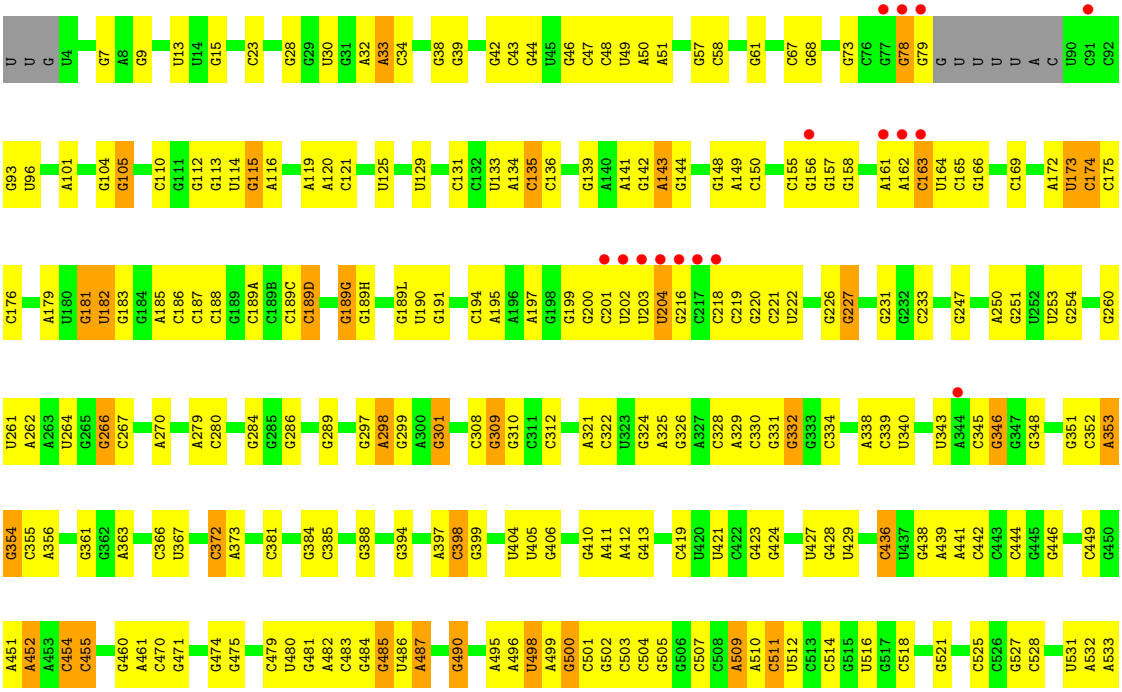


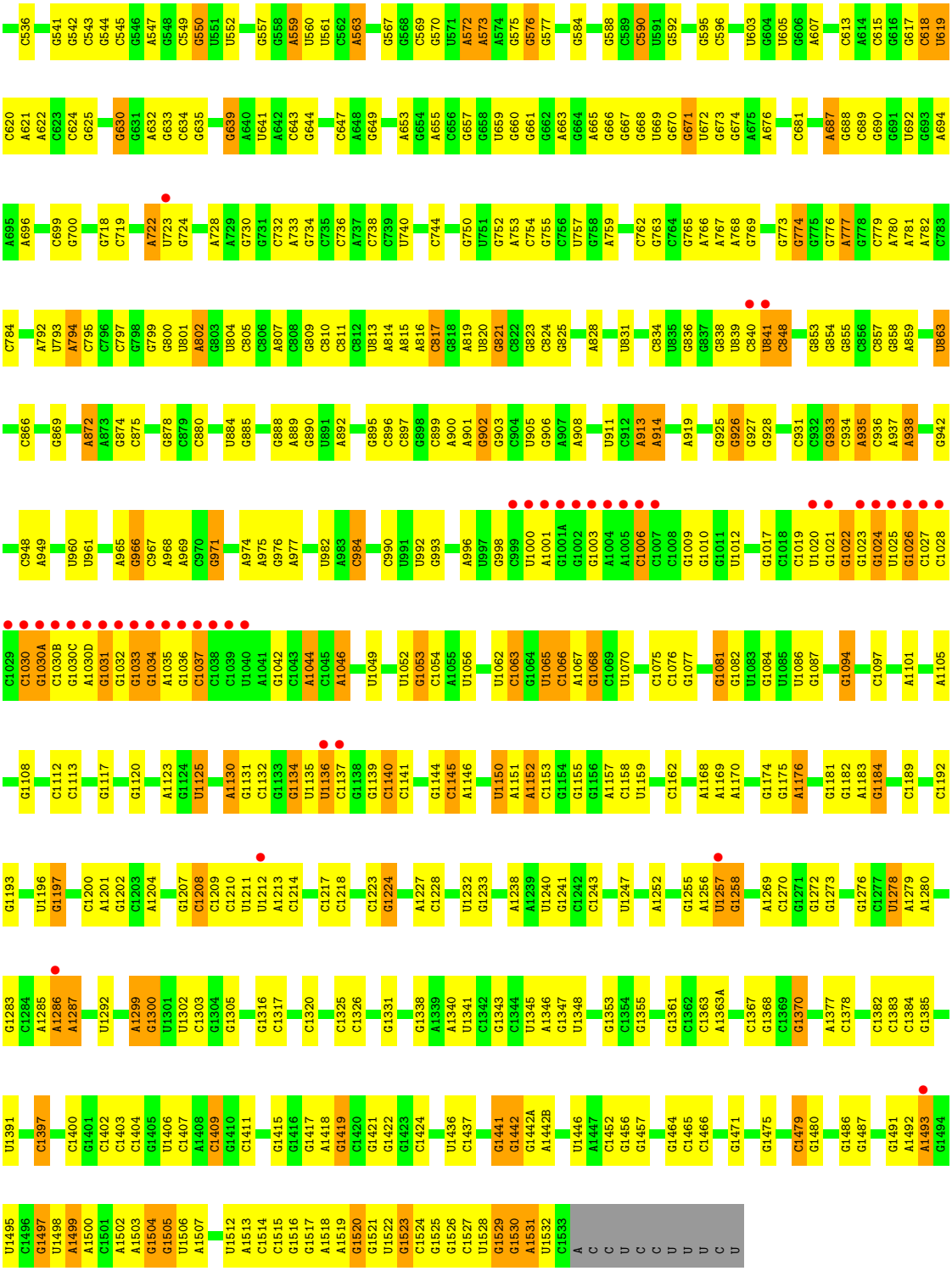
• Molecule 31: 50S ribosomal protein L36

Chain 29:

• Molecule 32: 16S ribosomal RNA

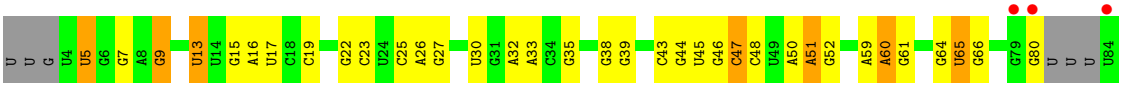
Chain 1a:

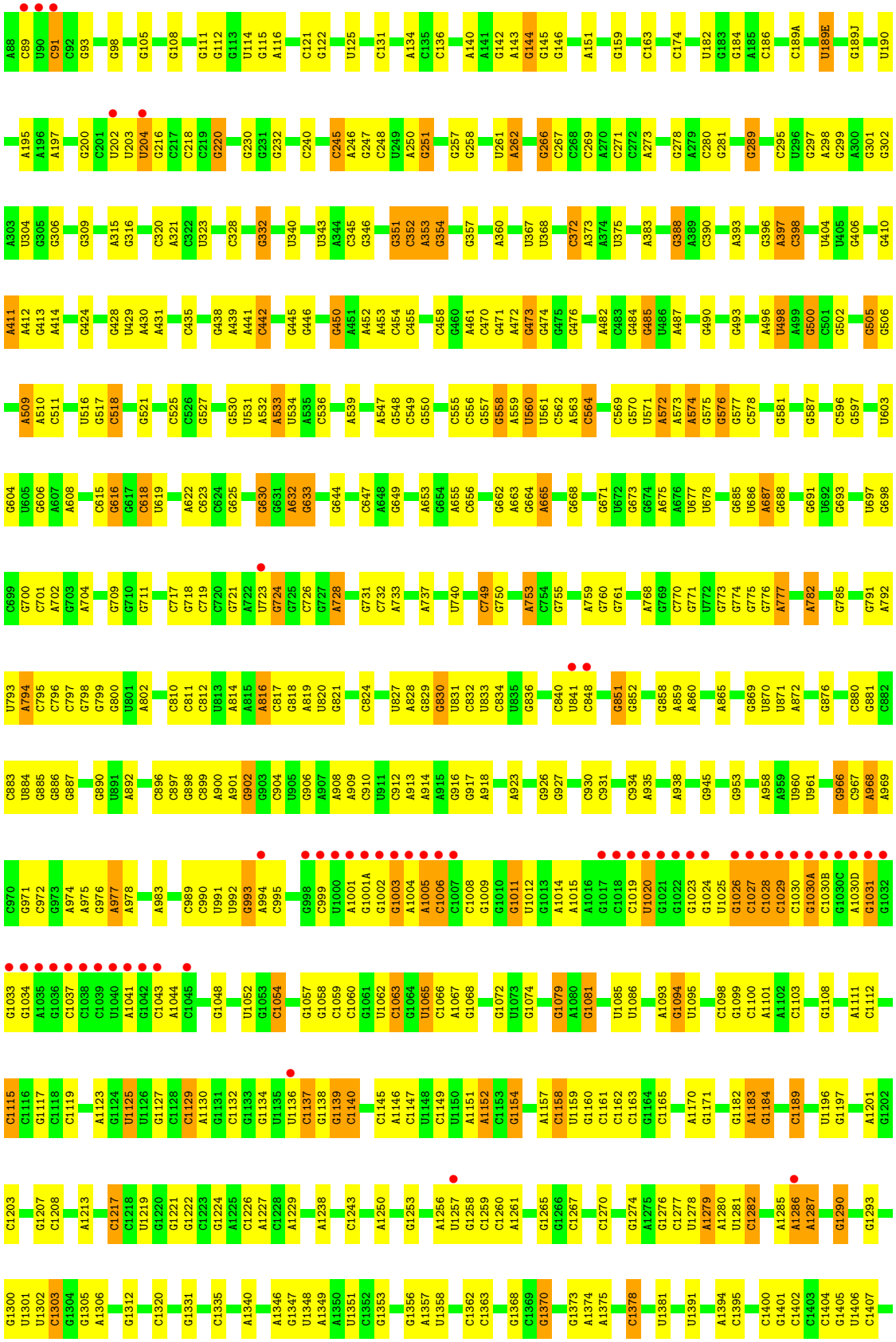




• Molecule 32: 16S ribosomal RNA

Chain 2a:

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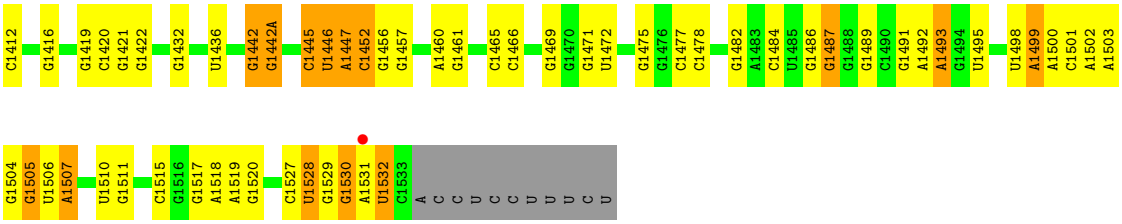
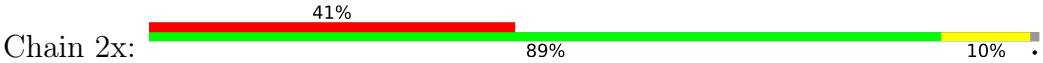
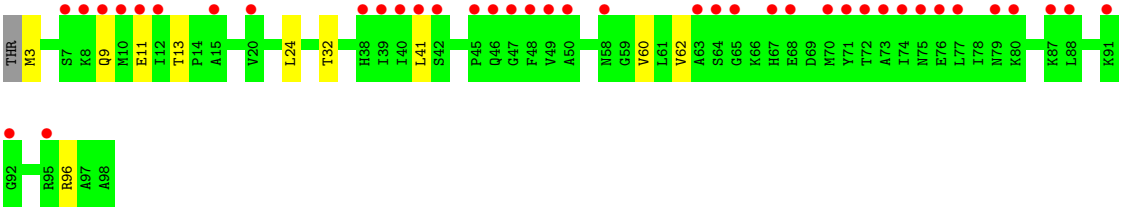
A195 A196 A197 G200 C201 U202 U203 U204 G216 C217 C218 C219 G220 G230 G231 G232 C240 C245 A246 G247 C248 U249 A250 G251 G257 G258 U261 A262 G266 C267 C268 C269 A270 C271 C272 A273 G278 A279 C280 G281 G289 C295 U296 G297 A298 G299 A300 G301 G302
A303 U304 G305 G306 G309 A315 G316 C320 A321 C322 U323 C328 G332 U340 U343 A344 C345 G346 G351 C352 A353 G354 G357 A360 U367 U368 C372 A373 A374 U375 A383 G388 A389 C390 A393 G396 A397 C398 U404 U405 G406 G410
A411 A412 G413 A414 G424 G428 U429 A430 A431 C435 G438 A439 A441 C442 G445 G446 G450 A451 A452 A453 C454 C455 C458 G460 A461 C470 G471 A472 G473 G474 G475 G476 A482 C483 G484 G485 U486 A487 G490 G493 A496 U498 A499 G500 C501 G502 G505 G506
A509 A510 C511 U516 G517 C518 G521 C525 C526 G527 G530 U531 A532 A533 U534 A535 C536 A539 A547 G548 C549 G550 C555 C556 G557 G558 A559 U560 U561 C562 A563 C564 C569 G570 U571 A572 A573 A574 G575 G576 G577 C578 G581 G587 C596 G597 U603
G604 U605 G606 A607 A608 C615 G616 G617 C618 U619 A622 C623 C624 G625 G630 G631 A632 G633 G644 C647 A648 G649 A653 G654 A655 C656 G662 A663 G664 A665 G668 G671 U672 G673 G674 A675 A676 U677 U678 G685 U686 A687 G688 G691 U692 G693 U697 G698
C699 G700 C701 A702 G703 A704 G709 G710 G711 C717 G718 C719 C720 G721 A722 U723 G724 G725 C726 G727 A728 G731 C732 A733 A737 U740 C749 G750 A753 C754 G755 A759 G760 G761 A768 G769 C770 G771 U772 G773 G774 G775 G776 A777 A782 G785 G791 A792
U793 A794 C795 C796 C797 G798 G799 G800 U801 A802 C810 C811 C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 C824 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 C840 U841 C848 G851 G852 G858 A859 A860 A865 G869 U870 U871 A872 G876 C880 G881 C882
C883 U884 G885 G886 G887 G890 U891 A892 C896 C897 G898 C899 A900 A901 G902 G903 C904 U905 G906 A907 A908 A909 C910 U911 C912 A913 A914 A915 G916 G917 A918 A923 G926 G927 C930 C931 C934 A935 A938 G945 G953 G958 A959 U960 U961 G966 C967 A968 A969
C970 G971 C972 G973 A974 A975 G976 A977 A978 A983 C989 C990 U991 U992 G993 A994 C995 G998 C999 U1000 A1001 G1001A U1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 G1011 U1012 G1013 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B G1030C A1030D G1031 G1032
G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 G1048 U1052 G1053 C1054 G1057 G1058 C1059 C1060 G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068 G1072 U1073 G1074 G1079 A1080 G1081 U1085 U1086 A1093 G1094 U1095 C1098 G1099 C1100 A1101 A1102 C1103 G1108 A1111 C1112
C1115 C1116 G1117 C1118 C1119 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 A1157 C1158 U1159 G1160 C1161 C1162 C1163 G1164 C1165 A1170 G1171 G1182 A1183 G1184 C1189 U1196 G1197 A1201 G1202
C1203 G1207 C1208 A1213 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 A1238 C1243 A1250 G1253 A1256 U1257 C1258 C1259 C1260 A1261 G1265 G1266 C1267 C1270 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 A1285 A1286 A1287 G1290 G1293
G1300 U1301 U1302 C1303 G1304 G1305 A1306 G1312 C1320 G1331 C1335 A1340 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 G1356 A1357 U1358 C1362 C1363 G1368 C1369 G1370 G1373 A1374 A1375 C1378 U1381 U1391 A1394 C1395 C1400 G1401 C1402 C1403 C1404 G1405 U1406 C1407

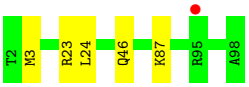


• Molecule 33: Ribosome-associated inhibitor A

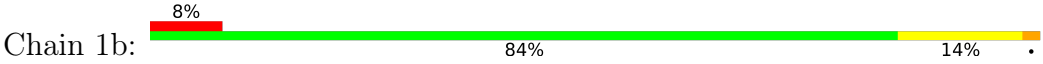


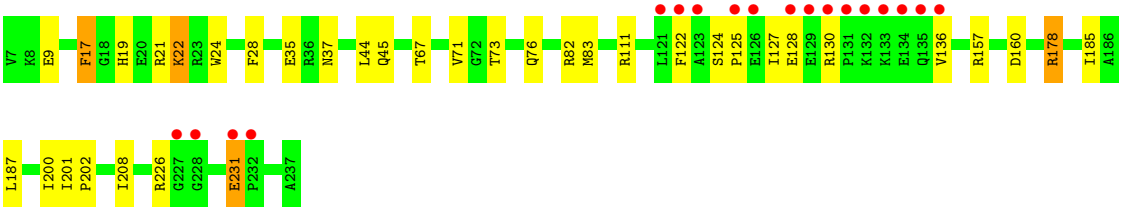


• Molecule 33: Ribosome-associated inhibitor A

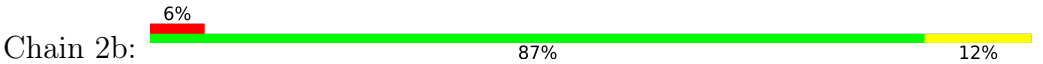


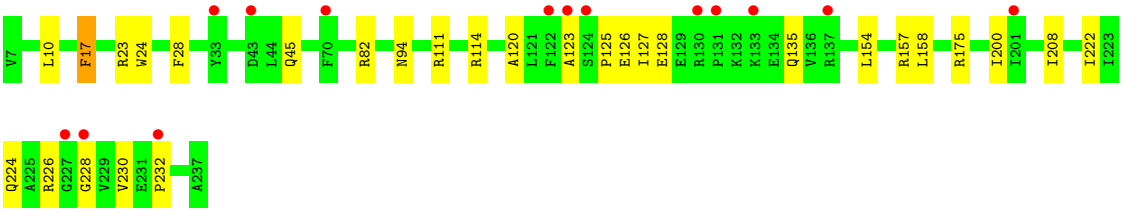
• Molecule 34: 30S ribosomal protein S2



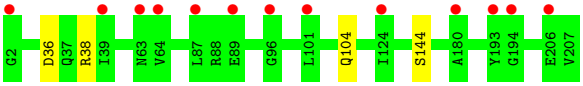


• Molecule 34: 30S ribosomal protein S2



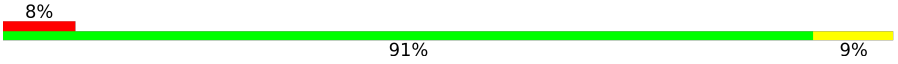


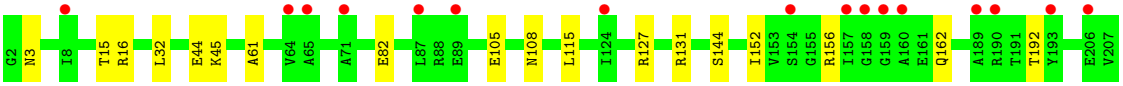
• Molecule 35: 30S ribosomal protein S3



• Molecule 35: 30S ribosomal protein S3

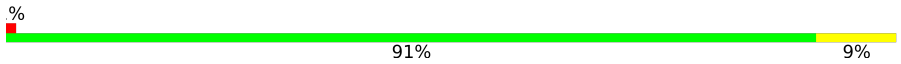
Chain 2c:





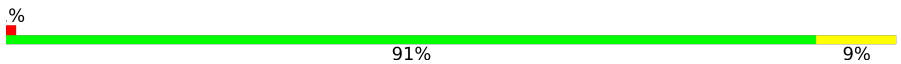
• Molecule 36: 30S ribosomal protein S4

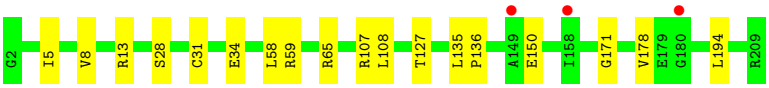
Chain 1d:



• Molecule 36: 30S ribosomal protein S4

Chain 2d:



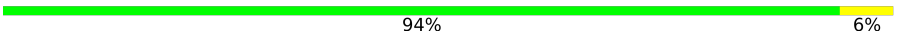


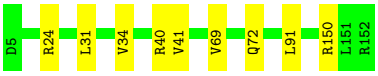
• Molecule 37: 30S ribosomal protein S5

Chain 1e:

• Molecule 37: 30S ribosomal protein S5

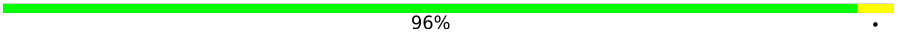
Chain 2e:





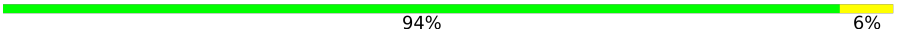
• Molecule 38: 30S ribosomal protein S6

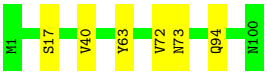
Chain 1f:



• Molecule 38: 30S ribosomal protein S6

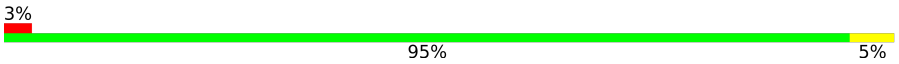
Chain 2f:





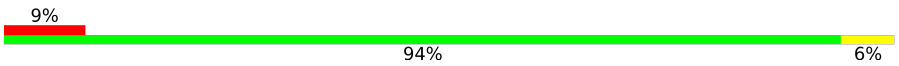
• Molecule 39: 30S ribosomal protein S7

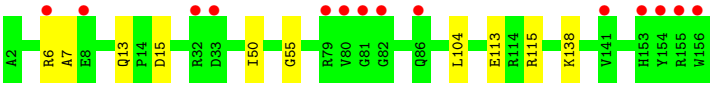
Chain 1g:



• Molecule 39: 30S ribosomal protein S7

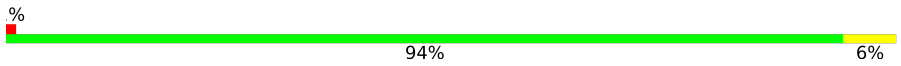
Chain 2g:

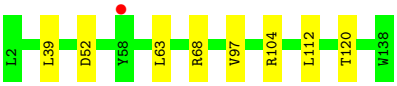




• Molecule 40: 30S ribosomal protein S8

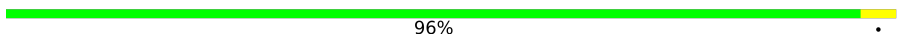
Chain 1h:





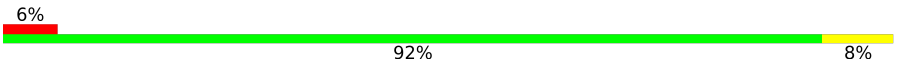
• Molecule 40: 30S ribosomal protein S8

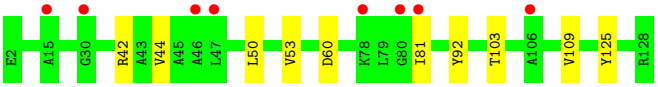
Chain 2h:



• Molecule 41: 30S ribosomal protein S9

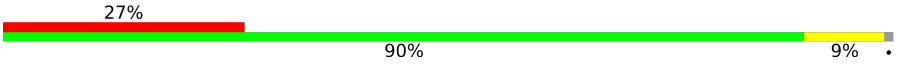
Chain 1i:

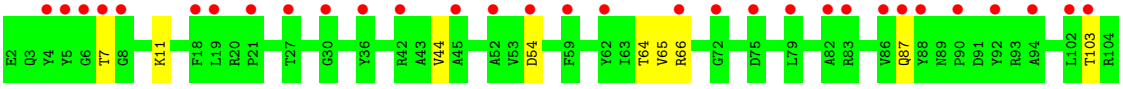


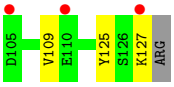


• Molecule 41: 30S ribosomal protein S9

Chain 2i:

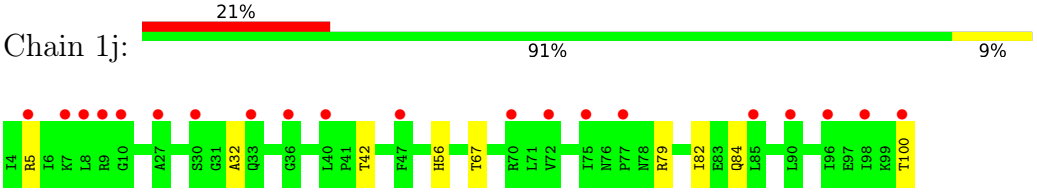






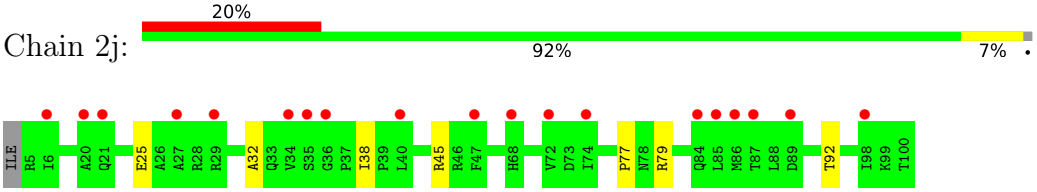
• Molecule 42: 30S ribosomal protein S10

Chain 1j:



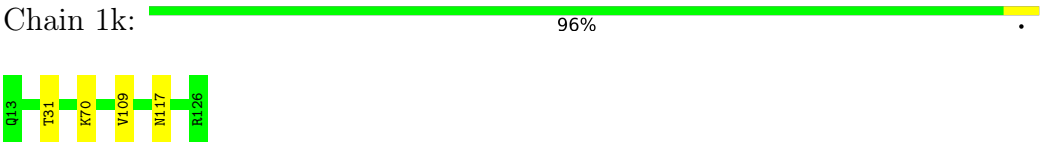
• Molecule 42: 30S ribosomal protein S10

Chain 2j:



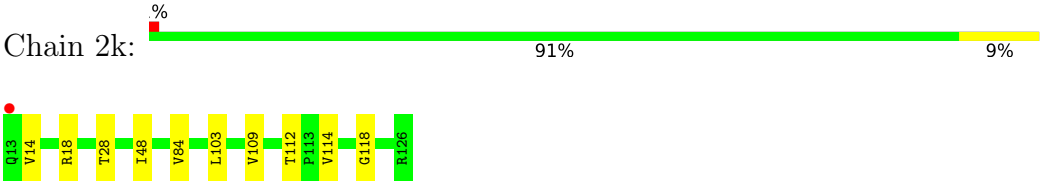
• Molecule 43: 30S ribosomal protein S11

Chain 1k:



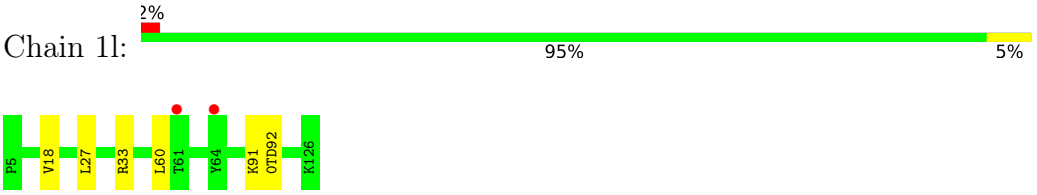
• Molecule 43: 30S ribosomal protein S11

Chain 2k:



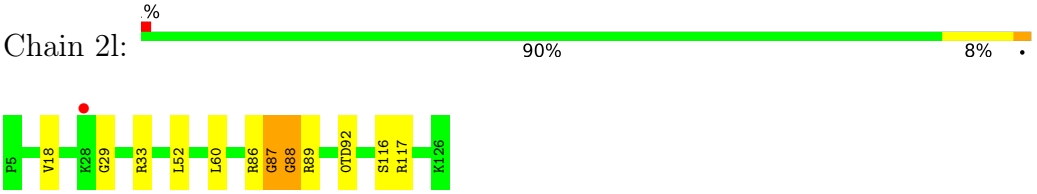
• Molecule 44: 30S ribosomal protein S12

Chain 1l:



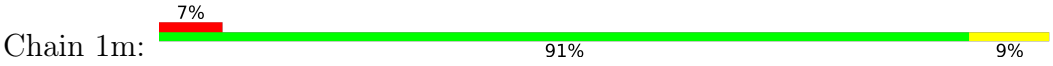
• Molecule 44: 30S ribosomal protein S12

Chain 2l:



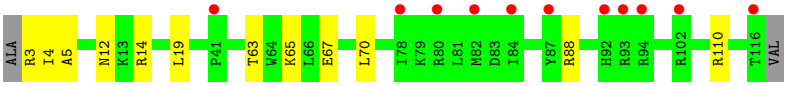
• Molecule 45: 30S ribosomal protein S13

Chain 1m:



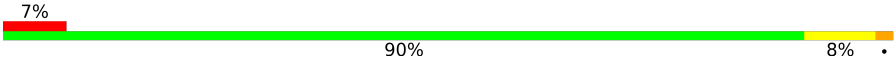
• Molecule 45: 30S ribosomal protein S13

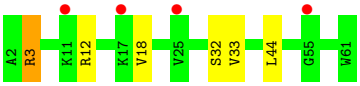
Chain 2m:



• Molecule 46: 30S ribosomal protein S14 type Z

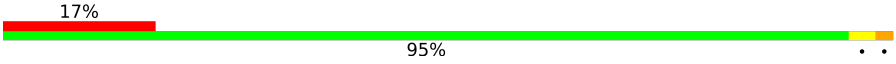
Chain 1n:

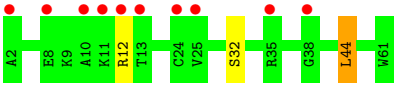




• Molecule 46: 30S ribosomal protein S14 type Z

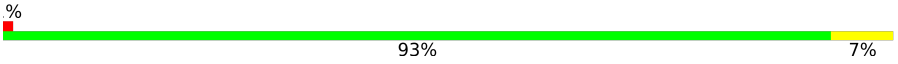
Chain 2n:

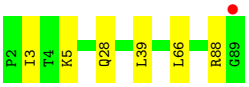




• Molecule 47: 30S ribosomal protein S15

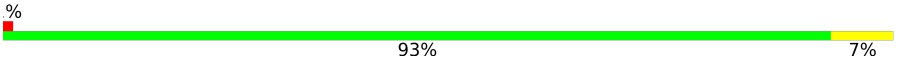
Chain 1o:





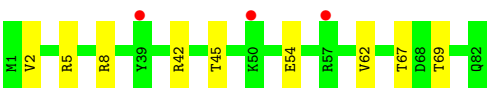
• Molecule 47: 30S ribosomal protein S15

Chain 2o:



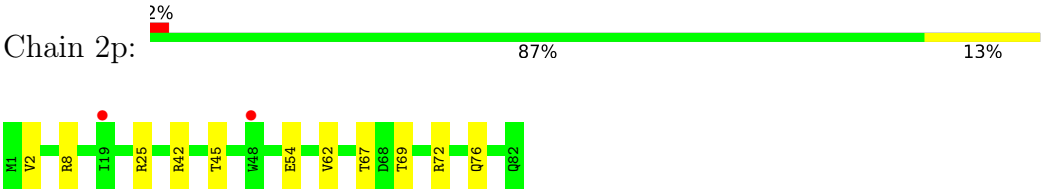
• Molecule 48: 30S ribosomal protein S16

Chain 1p:



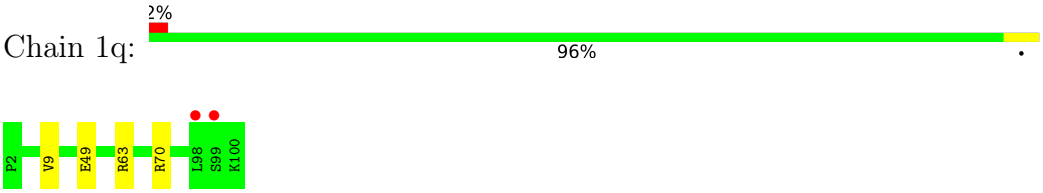
• Molecule 48: 30S ribosomal protein S16

Chain 2p:



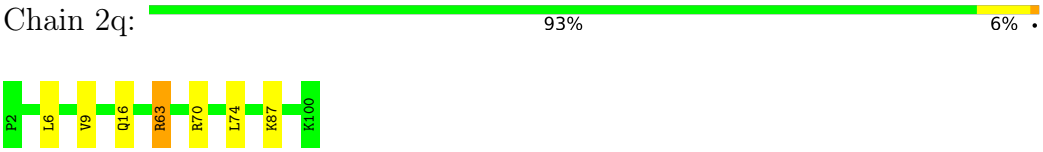
• Molecule 49: 30S ribosomal protein S17

Chain 1q:



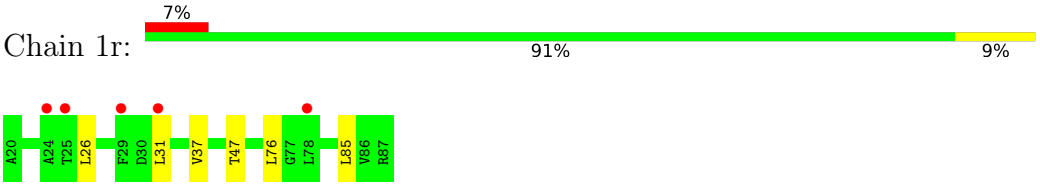
• Molecule 49: 30S ribosomal protein S17

Chain 2q:



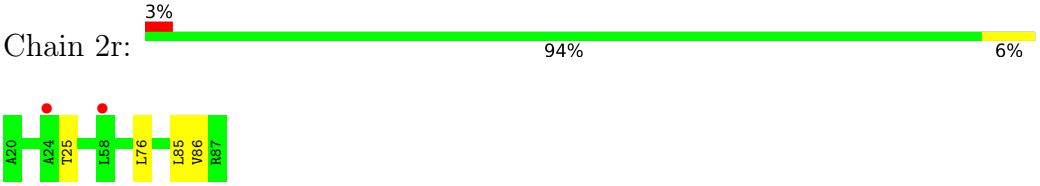
• Molecule 50: 30S ribosomal protein S18

Chain 1r:



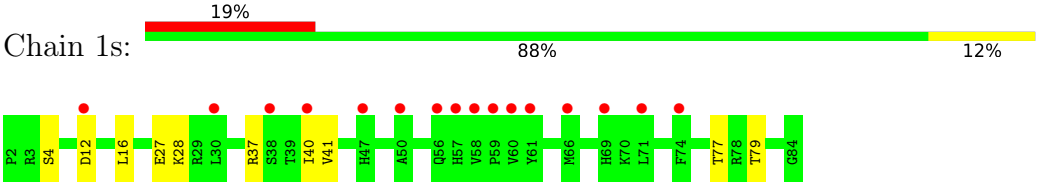
• Molecule 50: 30S ribosomal protein S18

Chain 2r:



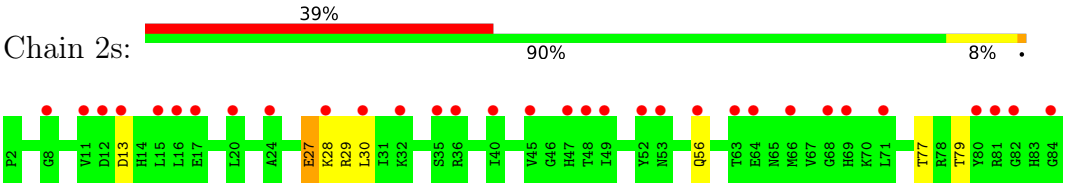
• Molecule 51: 30S ribosomal protein S19

Chain 1s:



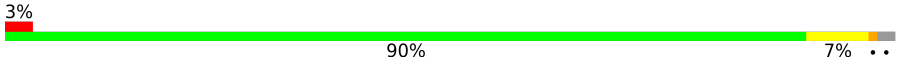
• Molecule 51: 30S ribosomal protein S19

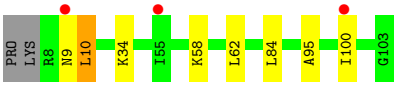
Chain 2s:



• Molecule 52: 30S ribosomal protein S20

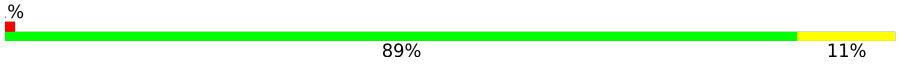
Chain 1t:

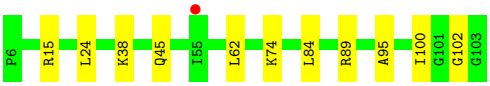




• Molecule 52: 30S ribosomal protein S20

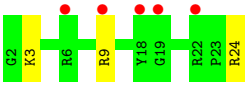
Chain 2t:





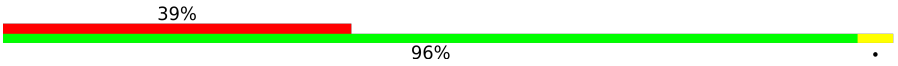
• Molecule 53: 30S ribosomal protein Thx

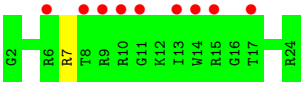
Chain 1u:



• Molecule 53: 30S ribosomal protein Thx

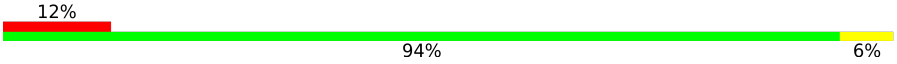
Chain 2u:

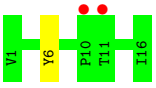




• Molecule 54: Pyrrhocoricin

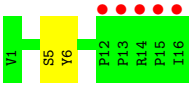
Chain 1y:





• Molecule 54: Pyrrhocoricin

Chain 2y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.94Å 450.10Å 622.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.80 49.81 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.81-2.80) 99.9 (49.81-2.59)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.58Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.189 , 0.240 0.190 , 0.240	Depositor DCC
R_{free} test set	88568 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	293583	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.57	577/69022 (0.8%)	2.06	3825/107739 (3.6%)
1	2A	1.21	119/68893 (0.2%)	1.72	1783/107533 (1.7%)
2	1B	1.15	4/2879 (0.1%)	1.89	110/4490 (2.4%)
2	2B	1.02	1/2874 (0.0%)	1.58	50/4482 (1.1%)
3	1D	0.93	0/2181	1.00	4/2940 (0.1%)
3	2D	0.78	0/2186	0.87	1/2944 (0.0%)
4	1E	0.99	0/1592	1.02	3/2149 (0.1%)
4	2E	0.79	0/1592	0.91	2/2149 (0.1%)
5	1F	0.95	0/1619	0.96	4/2193 (0.2%)
5	2F	0.73	0/1615	0.85	0/2188
6	1G	0.70	0/1451	0.86	0/1961
6	2G	0.78	1/1449 (0.1%)	0.86	0/1957
7	1H	0.80	0/1356	0.89	0/1834
7	2H	0.77	0/1350	0.85	0/1826
8	1I	0.77	2/1109 (0.2%)	0.92	2/1512 (0.1%)
8	2I	0.67	0/1091	0.87	2/1490 (0.1%)
9	1N	0.93	1/1148 (0.1%)	0.97	3/1547 (0.2%)
9	2N	0.64	0/1144	0.83	0/1543
10	1O	1.02	0/943	1.00	2/1269 (0.2%)
10	2O	0.81	0/943	0.86	1/1269 (0.1%)
11	1P	0.89	0/1152	0.96	2/1533 (0.1%)
11	2P	0.68	0/1152	0.83	0/1533
12	1Q	0.94	0/1143	0.94	0/1527
12	2Q	0.68	0/1143	0.83	0/1527
13	1R	0.94	0/982	1.08	7/1312 (0.5%)
13	2R	0.70	0/982	0.90	1/1312 (0.1%)
14	1S	0.79	1/887 (0.1%)	0.98	2/1180 (0.2%)
14	2S	0.68	0/880	0.85	0/1172
15	1T	0.88	1/1105 (0.1%)	1.06	4/1477 (0.3%)
15	2T	0.73	0/1097	0.91	2/1468 (0.1%)
16	1U	1.08	2/977 (0.2%)	1.05	7/1301 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.73	0/977	0.83	0/1301
17	1V	0.94	0/786	0.98	2/1053 (0.2%)
17	2V	0.67	0/782	0.84	0/1049
18	1W	1.04	0/897	1.02	4/1205 (0.3%)
18	2W	0.83	0/897	0.84	1/1205 (0.1%)
19	1X	0.95	0/764	0.96	1/1025 (0.1%)
19	2X	0.76	0/764	0.86	2/1025 (0.2%)
20	1Y	0.86	0/823	0.96	1/1099 (0.1%)
20	2Y	0.79	0/823	0.92	0/1100
21	1Z	0.73	0/1620	0.83	1/2200 (0.0%)
21	2Z	0.70	0/1590	0.84	1/2162 (0.0%)
22	10	0.88	0/616	0.94	0/821
22	20	0.68	0/616	0.86	0/821
23	11	1.01	1/761 (0.1%)	0.96	1/1013 (0.1%)
23	21	0.79	0/766	0.92	2/1018 (0.2%)
24	12	0.87	0/590	0.94	0/781
24	22	0.77	0/594	0.81	0/785
25	13	0.92	0/474	0.94	0/635
25	23	0.62	0/469	0.80	1/630 (0.2%)
26	14	0.89	0/559	0.89	0/754
26	24	1.06	0/549	0.97	0/741
27	15	1.08	3/473 (0.6%)	1.07	6/639 (0.9%)
27	25	0.83	0/469	0.97	2/635 (0.3%)
28	16	0.98	2/460 (0.4%)	1.04	1/613 (0.2%)
28	26	0.68	0/456	0.80	0/608
29	17	1.08	0/426	1.08	1/561 (0.2%)
29	27	0.81	0/426	0.88	0/561
30	18	0.96	1/525 (0.2%)	0.95	2/691 (0.3%)
30	28	0.72	0/525	0.79	0/691
31	19	0.96	1/310 (0.3%)	1.09	2/407 (0.5%)
31	29	0.70	0/310	0.79	0/407
32	1a	1.14	55/35795 (0.2%)	1.70	881/55864 (1.6%)
32	2a	1.10	48/35890 (0.1%)	1.65	737/56012 (1.3%)
33	1x	0.66	0/776	0.79	0/1048
33	2x	0.72	0/761	0.79	0/1030
34	1b	0.77	0/1876	0.93	3/2533 (0.1%)
34	2b	0.78	0/1860	0.89	0/2518
35	1c	0.72	0/1582	0.80	0/2137
35	2c	0.81	0/1566	0.81	0/2119
36	1d	0.71	0/1695	0.84	0/2274
36	2d	0.70	0/1698	0.85	0/2277
37	1e	0.66	0/1149	0.88	0/1548
37	2e	0.68	0/1149	0.87	0/1548

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1f	0.72	0/827	0.81	0/1120
38	2f	0.70	0/829	0.84	0/1123
39	1g	0.71	1/1254 (0.1%)	0.77	0/1683
39	2g	0.73	0/1248	0.76	0/1676
40	1h	0.67	0/1118	0.83	0/1506
40	2h	0.61	0/1108	0.83	0/1494
41	1i	0.77	0/1005	0.82	0/1351
41	2i	0.84	0/985	0.88	0/1329
42	1j	0.79	0/732	0.84	0/993
42	2j	0.81	0/723	0.76	0/984
43	1k	0.73	0/849	0.85	0/1150
43	2k	0.67	0/848	0.86	1/1149 (0.1%)
44	1l	0.69	0/937	0.83	0/1260
44	2l	0.68	0/937	0.95	3/1260 (0.2%)
45	1m	0.68	0/924	0.83	0/1242
45	2m	0.76	0/905	0.82	0/1217
46	1n	0.74	0/501	0.93	2/664 (0.3%)
46	2n	0.75	0/501	0.82	1/664 (0.2%)
47	1o	0.72	0/739	0.86	0/985
47	2o	0.65	0/739	0.79	0/985
48	1p	0.69	0/697	0.85	0/939
48	2p	0.70	0/693	0.90	0/935
49	1q	0.73	0/836	0.86	0/1117
49	2q	0.67	0/836	0.85	1/1117 (0.1%)
50	1r	0.70	0/560	0.87	1/746 (0.1%)
50	2r	0.70	0/560	0.81	0/746
51	1s	0.73	0/663	0.81	0/895
51	2s	0.81	0/660	0.79	1/893 (0.1%)
52	1t	0.68	0/734	0.86	0/969
52	2t	0.64	0/736	0.85	0/976
53	1u	0.69	0/203	0.83	0/266
53	2u	0.73	0/203	0.87	0/266
54	1y	0.83	0/125	0.82	0/173
54	2y	0.69	0/125	0.74	0/173
All	All	1.17	821/310171 (0.3%)	1.62	7479/463547 (1.6%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	2X	0	1
30	18	0	1
44	2l	0	1
All	All	0	4

The worst 5 of 821 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2026	G	N7-C5	-11.28	1.32	1.39
1	1A	2040	G	P-OP2	-11.24	1.29	1.49
1	1A	354	A	N9-C4	-10.67	1.31	1.37
1	1A	1814	A	N3-C4	-10.29	1.28	1.34
1	2A	1046	A	N9-C4	9.81	1.43	1.37

The worst 5 of 7479 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1208	C	O5'-P-OP1	-33.37	70.65	110.70
32	1a	1520	G	O5'-P-OP1	-31.38	73.04	110.70
32	1a	1520	G	O5'-P-OP2	26.23	142.18	110.70
32	1a	1520	G	OP1-P-OP2	-24.67	82.60	119.60
32	2a	1208	C	OP1-P-OP2	-24.65	82.62	119.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	18	13	ARG	Peptide
19	1X	93	GLU	Peptide
19	2X	93	GLU	Peptide
44	2l	86	ARG	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	273/275 (99%)	262 (96%)	11 (4%)	0	100 100
3	2D	273/275 (99%)	258 (94%)	15 (6%)	0	100 100
4	1E	202/204 (99%)	194 (96%)	7 (4%)	1 (0%)	29 61
4	2E	202/204 (99%)	192 (95%)	9 (4%)	1 (0%)	29 61
5	1F	201/203 (99%)	194 (96%)	6 (3%)	1 (0%)	29 61
5	2F	201/203 (99%)	195 (97%)	4 (2%)	2 (1%)	15 44
6	1G	179/181 (99%)	164 (92%)	12 (7%)	3 (2%)	9 29
6	2G	179/181 (99%)	163 (91%)	14 (8%)	2 (1%)	14 41
7	1H	172/174 (99%)	162 (94%)	10 (6%)	0	100 100
7	2H	171/174 (98%)	160 (94%)	11 (6%)	0	100 100
8	1I	145/147 (99%)	128 (88%)	15 (10%)	2 (1%)	11 34
8	2I	144/147 (98%)	125 (87%)	18 (12%)	1 (1%)	22 53
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100 100
9	2N	138/140 (99%)	131 (95%)	7 (5%)	0	100 100
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19 49
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19 49
11	1P	147/149 (99%)	140 (95%)	7 (5%)	0	100 100
11	2P	147/149 (99%)	140 (95%)	6 (4%)	1 (1%)	22 53
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22 53
12	2Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22 53
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100 100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100 100
14	1S	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	17 46
14	2S	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	17 46
15	1T	129/131 (98%)	125 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
16	1U	114/116 (98%)	114 (100%)	0	0	100	100
16	2U	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	44
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	44
18	1W	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
21	1Z	201/203 (99%)	190 (94%)	10 (5%)	1 (0%)	29	61
21	2Z	199/203 (98%)	187 (94%)	12 (6%)	0	100	100
22	10	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
22	20	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
23	11	95/97 (98%)	94 (99%)	0	1 (1%)	14	41
23	21	95/97 (98%)	92 (97%)	2 (2%)	1 (1%)	14	41
24	12	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
24	22	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
25	13	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
25	23	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
26	14	67/69 (97%)	55 (82%)	9 (13%)	3 (4%)	2	8
26	24	67/69 (97%)	54 (81%)	6 (9%)	7 (10%)	0	1
27	15	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
27	25	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
28	16	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
28	26	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
29	17	46/48 (96%)	46 (100%)	0	0	100	100
29	27	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
30	18	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
30	28	62/64 (97%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1x	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
33	2x	94/97 (97%)	92 (98%)	2 (2%)	0	100	100
34	1b	229/231 (99%)	193 (84%)	27 (12%)	9 (4%)	3	10
34	2b	229/231 (99%)	194 (85%)	28 (12%)	7 (3%)	4	14
35	1c	204/206 (99%)	177 (87%)	26 (13%)	1 (0%)	29	61
35	2c	204/206 (99%)	177 (87%)	23 (11%)	4 (2%)	7	24
36	1d	206/208 (99%)	187 (91%)	16 (8%)	3 (2%)	10	33
36	2d	206/208 (99%)	187 (91%)	16 (8%)	3 (2%)	10	33
37	1e	146/148 (99%)	136 (93%)	9 (6%)	1 (1%)	22	53
37	2e	146/148 (99%)	135 (92%)	11 (8%)	0	100	100
38	1f	98/100 (98%)	87 (89%)	11 (11%)	0	100	100
38	2f	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
39	1g	153/155 (99%)	146 (95%)	7 (5%)	0	100	100
39	2g	153/155 (99%)	146 (95%)	4 (3%)	3 (2%)	7	24
40	1h	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
40	2h	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
41	1i	125/127 (98%)	109 (87%)	14 (11%)	2 (2%)	9	31
41	2i	124/127 (98%)	106 (86%)	14 (11%)	4 (3%)	4	13
42	1j	95/97 (98%)	79 (83%)	13 (14%)	3 (3%)	4	13
42	2j	94/97 (97%)	79 (84%)	12 (13%)	3 (3%)	4	13
43	1k	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	17	46
43	2k	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
44	1l	119/122 (98%)	112 (94%)	6 (5%)	1 (1%)	19	49
44	2l	119/122 (98%)	108 (91%)	9 (8%)	2 (2%)	9	29
45	1m	114/116 (98%)	103 (90%)	9 (8%)	2 (2%)	8	28
45	2m	112/116 (97%)	102 (91%)	8 (7%)	2 (2%)	8	28
46	1n	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
46	2n	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
47	1o	86/88 (98%)	83 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	2o	86/88 (98%)	80 (93%)	5 (6%)	1 (1%)	13 39
48	1p	80/82 (98%)	72 (90%)	8 (10%)	0	100 100
48	2p	80/82 (98%)	72 (90%)	8 (10%)	0	100 100
49	1q	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15 44
49	2q	97/99 (98%)	93 (96%)	4 (4%)	0	100 100
50	1r	66/68 (97%)	64 (97%)	2 (3%)	0	100 100
50	2r	66/68 (97%)	64 (97%)	2 (3%)	0	100 100
51	1s	81/83 (98%)	71 (88%)	8 (10%)	2 (2%)	5 19
51	2s	81/83 (98%)	72 (89%)	6 (7%)	3 (4%)	3 11
52	1t	94/98 (96%)	88 (94%)	3 (3%)	3 (3%)	4 13
52	2t	96/98 (98%)	87 (91%)	6 (6%)	3 (3%)	4 14
53	1u	21/23 (91%)	19 (90%)	1 (5%)	1 (5%)	2 7
53	2u	21/23 (91%)	19 (90%)	1 (5%)	1 (5%)	2 7
54	1y	14/16 (88%)	14 (100%)	0	0	100 100
54	2y	14/16 (88%)	14 (100%)	0	0	100 100
All	All	11657/11874 (98%)	10874 (93%)	682 (6%)	101 (1%)	17 46

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	52	LEU
6	1G	49	ASP
6	1G	51	ARG
8	1I	73	GLU
14	1S	59	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	214/217 (99%)	194 (91%)	20 (9%)	9 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	2D	215/217 (99%)	189 (88%)	26 (12%)	5 15
4	1E	164/165 (99%)	148 (90%)	16 (10%)	8 24
4	2E	164/165 (99%)	147 (90%)	17 (10%)	7 21
5	1F	160/161 (99%)	137 (86%)	23 (14%)	3 10
5	2F	159/161 (99%)	142 (89%)	17 (11%)	6 20
6	1G	144/155 (93%)	132 (92%)	12 (8%)	11 32
6	2G	142/155 (92%)	132 (93%)	10 (7%)	15 40
7	1H	144/145 (99%)	132 (92%)	12 (8%)	11 32
7	2H	143/145 (99%)	130 (91%)	13 (9%)	9 27
8	1I	111/123 (90%)	96 (86%)	15 (14%)	4 11
8	2I	108/123 (88%)	95 (88%)	13 (12%)	5 15
9	1N	119/119 (100%)	106 (89%)	13 (11%)	6 19
9	2N	118/119 (99%)	104 (88%)	14 (12%)	5 16
10	1O	100/100 (100%)	92 (92%)	8 (8%)	12 34
10	2O	100/100 (100%)	94 (94%)	6 (6%)	19 48
11	1P	115/116 (99%)	108 (94%)	7 (6%)	18 48
11	2P	115/116 (99%)	105 (91%)	10 (9%)	10 30
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	14 38
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11 33
13	1R	101/101 (100%)	89 (88%)	12 (12%)	5 16
13	2R	101/101 (100%)	87 (86%)	14 (14%)	3 11
14	1S	87/87 (100%)	76 (87%)	11 (13%)	4 14
14	2S	85/87 (98%)	76 (89%)	9 (11%)	6 20
15	1T	115/115 (100%)	107 (93%)	8 (7%)	15 40
15	2T	113/115 (98%)	107 (95%)	6 (5%)	22 54
16	1U	93/93 (100%)	82 (88%)	11 (12%)	5 16
16	2U	93/93 (100%)	87 (94%)	6 (6%)	17 44
17	1V	81/82 (99%)	71 (88%)	10 (12%)	4 15
17	2V	80/82 (98%)	71 (89%)	9 (11%)	6 18
18	1W	90/91 (99%)	81 (90%)	9 (10%)	7 22
18	2W	90/91 (99%)	82 (91%)	8 (9%)	9 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	1X	77/77 (100%)	73 (95%)	4 (5%)	23 55
19	2X	77/77 (100%)	73 (95%)	4 (5%)	23 55
20	1Y	86/88 (98%)	81 (94%)	5 (6%)	20 50
20	2Y	86/88 (98%)	81 (94%)	5 (6%)	20 50
21	1Z	169/176 (96%)	152 (90%)	17 (10%)	7 22
21	2Z	165/176 (94%)	149 (90%)	16 (10%)	8 24
22	10	61/62 (98%)	54 (88%)	7 (12%)	5 17
22	20	61/62 (98%)	56 (92%)	5 (8%)	11 33
23	11	79/82 (96%)	75 (95%)	4 (5%)	24 55
23	21	81/82 (99%)	72 (89%)	9 (11%)	6 19
24	12	65/66 (98%)	61 (94%)	4 (6%)	18 47
24	22	66/66 (100%)	65 (98%)	1 (2%)	65 89
25	13	51/51 (100%)	48 (94%)	3 (6%)	19 49
25	23	50/51 (98%)	47 (94%)	3 (6%)	19 48
26	14	58/62 (94%)	49 (84%)	9 (16%)	2 8
26	24	54/62 (87%)	48 (89%)	6 (11%)	6 19
27	15	51/51 (100%)	49 (96%)	2 (4%)	32 66
27	25	50/51 (98%)	47 (94%)	3 (6%)	19 48
28	16	51/51 (100%)	44 (86%)	7 (14%)	3 11
28	26	50/51 (98%)	46 (92%)	4 (8%)	12 34
29	17	41/41 (100%)	37 (90%)	4 (10%)	8 24
29	27	41/41 (100%)	39 (95%)	2 (5%)	25 57
30	18	54/54 (100%)	48 (89%)	6 (11%)	6 19
30	28	54/54 (100%)	49 (91%)	5 (9%)	9 26
31	19	34/34 (100%)	32 (94%)	2 (6%)	19 49
31	29	34/34 (100%)	34 (100%)	0	100 100
33	1x	82/83 (99%)	77 (94%)	5 (6%)	18 48
33	2x	79/83 (95%)	69 (87%)	10 (13%)	4 14
34	1b	191/199 (96%)	162 (85%)	29 (15%)	3 8
34	2b	187/199 (94%)	164 (88%)	23 (12%)	4 15
35	1c	144/160 (90%)	141 (98%)	3 (2%)	53 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	2c	140/160 (88%)	126 (90%)	14 (10%)	7 22
36	1d	171/180 (95%)	155 (91%)	16 (9%)	8 26
36	2d	172/180 (96%)	157 (91%)	15 (9%)	10 30
37	1e	114/114 (100%)	104 (91%)	10 (9%)	10 29
37	2e	114/114 (100%)	105 (92%)	9 (8%)	12 34
38	1f	85/90 (94%)	81 (95%)	4 (5%)	26 59
38	2f	85/90 (94%)	79 (93%)	6 (7%)	14 39
39	1g	120/126 (95%)	113 (94%)	7 (6%)	20 50
39	2g	119/126 (94%)	112 (94%)	7 (6%)	19 49
40	1h	116/118 (98%)	108 (93%)	8 (7%)	15 41
40	2h	114/118 (97%)	108 (95%)	6 (5%)	22 54
41	1i	91/98 (93%)	83 (91%)	8 (9%)	10 29
41	2i	88/98 (90%)	80 (91%)	8 (9%)	9 27
42	1j	68/87 (78%)	62 (91%)	6 (9%)	10 29
42	2j	68/87 (78%)	64 (94%)	4 (6%)	19 49
43	1k	83/86 (96%)	80 (96%)	3 (4%)	35 69
43	2k	83/86 (96%)	74 (89%)	9 (11%)	6 19
44	1l	96/102 (94%)	92 (96%)	4 (4%)	30 63
44	2l	96/102 (94%)	89 (93%)	7 (7%)	14 38
45	1m	90/94 (96%)	81 (90%)	9 (10%)	7 22
45	2m	87/94 (93%)	77 (88%)	10 (12%)	5 17
46	1n	49/49 (100%)	43 (88%)	6 (12%)	5 15
46	2n	49/49 (100%)	46 (94%)	3 (6%)	18 48
47	1o	78/79 (99%)	72 (92%)	6 (8%)	13 35
47	2o	78/79 (99%)	73 (94%)	5 (6%)	17 45
48	1p	69/71 (97%)	60 (87%)	9 (13%)	4 13
48	2p	68/71 (96%)	57 (84%)	11 (16%)	2 7
49	1q	94/94 (100%)	91 (97%)	3 (3%)	39 73
49	2q	94/94 (100%)	87 (93%)	7 (7%)	13 37
50	1r	59/59 (100%)	54 (92%)	5 (8%)	10 31
50	2r	59/59 (100%)	55 (93%)	4 (7%)	16 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	1s	68/72 (94%)	60 (88%)	8 (12%)	5 16
51	2s	67/72 (93%)	62 (92%)	5 (8%)	13 37
52	1t	71/76 (93%)	65 (92%)	6 (8%)	10 31
52	2t	70/76 (92%)	62 (89%)	8 (11%)	5 18
53	1u	18/18 (100%)	16 (89%)	2 (11%)	6 19
53	2u	18/18 (100%)	18 (100%)	0	100 100
54	1y	14/15 (93%)	13 (93%)	1 (7%)	14 39
54	2y	14/15 (93%)	12 (86%)	2 (14%)	3 10
All	All	9552/9892 (97%)	8702 (91%)	850 (9%)	9 28

5 of 850 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	2E	7	VAL
13	2R	29	LEU
45	2m	19	LEU
4	2E	170	LEU
3	2D	276	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
3	2D	253	GLN
21	2Z	73	GLN
49	2q	26	GLN
5	2F	75	HIS
16	2U	104	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	396 (13%)	51 (1%)
1	2A	2856/2915 (97%)	414 (14%)	49 (1%)
2	1B	119/120 (99%)	5 (4%)	0
2	2B	118/120 (98%)	5 (4%)	0
32	1a	1494/1521 (98%)	319 (21%)	0
32	2a	1498/1521 (98%)	305 (20%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	8950/9112 (98%)	1444 (16%)	100 (1%)

5 of 1444 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	60	G
1	1A	70	A

5 of 100 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	277	C
1	2A	1053	C
1	2A	2756	U
1	2A	573	G
1	2A	827	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	2A	1962	55,1	18,22,23	1.16	4 (22%)	26,32,35	1.49	4 (15%)
32	5MC	2a	1400	32	18,22,23	0.90	0	26,32,35	1.36	5 (19%)
32	MA6	2a	1519	32	19,26,27	1.13	2 (10%)	18,38,41	4.93	3 (16%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	22,30,33	1.71	5 (22%)
1	OMU	1A	2564	55,1	19,22,23	6.38	9 (47%)	26,31,34	2.90	11 (42%)
32	4OC	2a	1402	32	20,23,24	2.61	7 (35%)	26,32,35	1.13	2 (7%)
32	5MC	1a	1404	32	18,22,23	1.23	3 (16%)	26,32,35	1.41	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	G7M	1a	527	55,32	20,26,27	2.89	4 (20%)	17,39,42	0.81	1 (5%)
1	PSU	2A	1911	1	18,21,22	1.42	3 (16%)	22,30,33	1.38	2 (9%)
32	M2G	1a	966	32	20,27,28	2.87	5 (25%)	22,40,43	1.46	6 (27%)
1	OMG	1A	2263	55,1	18,26,27	1.77	6 (33%)	19,38,41	1.51	5 (26%)
1	OMU	2A	2552	55,1	19,22,23	6.64	10 (52%)	26,31,34	2.69	8 (30%)
1	5MC	1A	1964	1	18,22,23	0.99	1 (5%)	26,32,35	1.16	3 (11%)
32	UR3	1a	1498	32	19,22,23	1.89	4 (21%)	26,32,35	1.40	3 (11%)
1	5MC	2A	1942	1	18,22,23	1.02	1 (5%)	26,32,35	1.14	3 (11%)
1	2MA	1A	2515	55,1	17,25,26	1.58	5 (29%)	17,37,40	1.93	3 (17%)
1	PSU	1A	1933	1	18,21,22	1.41	3 (16%)	22,30,33	1.47	3 (13%)
32	5MC	1a	967	32	18,22,23	1.04	2 (11%)	26,32,35	1.33	4 (15%)
32	5MC	2a	1404	32	18,22,23	1.06	2 (11%)	26,32,35	1.44	4 (15%)
1	PSU	1A	2617	1	18,21,22	1.64	4 (22%)	22,30,33	1.78	5 (22%)
32	MA6	1a	1518	32	19,26,27	1.05	1 (5%)	18,38,41	4.70	3 (16%)
32	PSU	1a	516	32	18,21,22	1.43	3 (16%)	22,30,33	2.05	4 (18%)
32	2MG	1a	1207	55,32	18,26,27	1.97	4 (22%)	16,38,41	1.83	5 (31%)
1	5MU	2A	1915	1	19,22,23	1.75	3 (15%)	28,32,35	1.59	5 (17%)
1	OMC	2A	1920	1	19,22,23	2.43	7 (36%)	26,31,34	1.01	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.34	2 (11%)	22,30,33	1.72	5 (22%)
32	G7M	2a	527	32	20,26,27	3.15	6 (30%)	17,39,42	0.97	2 (11%)
32	5MC	2a	1407	32	18,22,23	1.24	1 (5%)	26,32,35	1.42	3 (11%)
1	5MU	1A	1961	55,1	19,22,23	1.00	2 (10%)	28,32,35	1.48	4 (14%)
44	0TD	1l	92	44	7,9,10	2.06	2 (28%)	6,11,13	4.14	4 (66%)
32	4OC	1a	1402	32	20,23,24	2.41	7 (35%)	26,32,35	0.78	0
32	5MC	2a	967	32	18,22,23	0.97	1 (5%)	26,32,35	1.66	4 (15%)
1	OMG	2A	2251	55,1	18,26,27	1.73	3 (16%)	19,38,41	1.64	5 (26%)
32	PSU	2a	516	32	18,21,22	1.84	3 (16%)	22,30,33	2.03	5 (22%)
1	OMC	1A	1942	55,1	19,22,23	2.18	6 (31%)	26,31,34	1.01	3 (11%)
1	PSU	1A	1939	55,1	18,21,22	1.35	2 (11%)	22,30,33	1.75	5 (22%)
32	MA6	2a	1518	32	19,26,27	1.05	1 (5%)	18,38,41	4.81	3 (16%)
32	2MG	2a	1207	32	18,26,27	1.92	4 (22%)	16,38,41	1.12	2 (12%)
1	5MU	2A	1939	55,1	19,22,23	0.91	1 (5%)	28,32,35	1.37	4 (14%)
1	5MC	1A	1984	1	18,22,23	1.11	2 (11%)	26,32,35	1.68	5 (19%)
32	5MC	1a	1400	32	18,22,23	1.03	1 (5%)	26,32,35	1.61	6 (23%)
32	5MC	1a	1407	32	18,22,23	1.37	1 (5%)	26,32,35	1.51	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	MA6	1a	1519	32	19,26,27	1.03	2 (10%)	18,38,41	4.46	3 (16%)
1	5MU	1A	1937	1	19,22,23	1.43	2 (10%)	28,32,35	1.58	6 (21%)
32	M2G	2a	966	32	20,27,28	3.02	7 (35%)	22,40,43	1.37	3 (13%)
44	0TD	2l	92	44	7,9,10	2.21	1 (14%)	6,11,13	2.99	4 (66%)
32	UR3	2a	1498	32	19,22,23	1.89	4 (21%)	26,32,35	1.48	4 (15%)
1	2MA	2A	2503	55,1	17,25,26	1.54	2 (11%)	17,37,40	1.11	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
1	5MC	2A	1962	55,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	2/7/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2564	55,1	-	0/9/27/28	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	55,32	-	1/3/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	OMG	1A	2263	55,1	-	0/5/27/28	0/3/3/3
1	OMU	2A	2552	55,1	-	0/9/27/28	0/2/2/2
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	55,1	-	1/3/25/26	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	PSU	1a	516	32	-	2/7/25/26	0/2/2/2
32	2MG	1a	1207	55,32	-	0/5/27/28	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	1/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	55,1	-	0/7/25/26	0/2/2/2
44	0TD	1l	92	44	-	4/7/12/14	-
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
32	PSU	2a	516	32	-	3/7/25/26	0/2/2/2
1	OMC	1A	1942	55,1	-	3/9/27/28	0/2/2/2
1	PSU	1A	1939	55,1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	5MU	2A	1939	55,1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	1	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	5/7/29/30	0/3/3/3
1	5MU	1A	1937	1	-	4/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
44	0TD	2l	92	44	-	2/7/12/14	-
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	55,1	-	1/3/25/26	0/3/3/3

The worst 5 of 158 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	C4-N3	-15.09	1.11	1.38
1	1A	2564	OMU	C4-N3	-14.97	1.11	1.38
1	2A	2552	OMU	C5-C4	14.92	1.76	1.43
1	1A	2564	OMU	C5-C4	13.65	1.73	1.43
1	1A	2564	OMU	C6-C5	-11.10	1.09	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1519	MA6	N1-C6-N6	-19.44	96.59	117.06
32	2a	1518	MA6	N1-C6-N6	-19.01	97.05	117.06
32	1a	1518	MA6	N1-C6-N6	-18.08	98.03	117.06
32	1a	1519	MA6	N1-C6-N6	-17.64	98.49	117.06
1	2A	2552	OMU	C5-C4-N3	7.23	125.65	114.84

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C1'-N1-C2
1	1A	1937	5MU	O4'-C1'-N1-C6
1	1A	1937	5MU	C3'-C4'-C5'-O5'
1	1A	1937	5MU	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2435 ligands modelled in this entry, 2432 are monoatomic and 1 is modelled with single atom - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	SF4	1d	501	36	0,12,12	-	-	-		
57	SF4	2d	501	36	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	1d	501	36	-	-	0/6/5/5
57	SF4	2d	501	36	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2A	2801(A):A	O3'	2802:G	P	3.56

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, 95^{th} 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%)	0.20	153 (5%) 26 17	18, 37, 90, 99	0
1	2A	2856/2915 (97%)	0.13	161 (5%) 24 16	33, 58, 91, 100	0
2	1B	120/120 (100%)	-0.35	0 100 100	33, 56, 67, 89	0
2	2B	120/120 (100%)	-0.34	0 100 100	63, 76, 81, 86	0
3	1D	275/275 (100%)	-0.29	0 100 100	17, 38, 53, 70	0
3	2D	275/275 (100%)	-0.25	0 100 100	32, 52, 64, 74	0
4	1E	204/204 (100%)	-0.40	0 100 100	19, 41, 61, 70	0
4	2E	204/204 (100%)	-0.23	1 (0%) 91 88	34, 57, 70, 78	0
5	1F	203/203 (100%)	-0.28	2 (0%) 82 77	17, 44, 70, 86	0
5	2F	203/203 (100%)	-0.28	0 100 100	38, 64, 78, 84	0
6	1G	181/181 (100%)	-0.42	2 (1%) 80 75	52, 68, 78, 88	0
6	2G	181/181 (100%)	0.56	15 (8%) 11 6	74, 80, 86, 91	0
7	1H	174/174 (100%)	-0.47	1 (0%) 89 86	39, 55, 66, 70	0
7	2H	173/174 (99%)	0.77	27 (15%) 2 1	65, 79, 85, 87	0
8	1I	147/147 (100%)	-0.26	0 100 100	41, 70, 78, 81	0
8	2I	146/147 (99%)	0.24	5 (3%) 45 35	53, 74, 82, 87	0
9	1N	140/140 (100%)	-0.39	0 100 100	23, 39, 62, 75	0
9	2N	140/140 (100%)	-0.26	0 100 100	48, 63, 73, 82	0
10	1O	122/122 (100%)	-0.33	0 100 100	30, 43, 59, 64	0
10	2O	122/122 (100%)	-0.36	0 100 100	44, 55, 67, 73	0
11	1P	149/149 (100%)	-0.25	0 100 100	19, 46, 65, 78	0
11	2P	149/149 (100%)	0.23	3 (2%) 65 56	42, 66, 79, 82	0
12	1Q	141/141 (100%)	-0.18	0 100 100	28, 43, 56, 69	0
12	2Q	141/141 (100%)	-0.38	2 (1%) 75 70	47, 63, 74, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.16	0 100 100	26, 38, 55, 63	0
13	2R	118/118 (100%)	-0.21	0 100 100	40, 54, 64, 70	0
14	1S	110/110 (100%)	-0.36	0 100 100	44, 55, 67, 71	0
14	2S	110/110 (100%)	0.21	3 (2%) 54 44	64, 72, 78, 82	0
15	1T	131/131 (100%)	-0.34	1 (0%) 86 81	34, 47, 70, 79	0
15	2T	131/131 (100%)	-0.36	0 100 100	50, 60, 75, 83	0
16	1U	116/116 (100%)	-0.25	0 100 100	22, 32, 48, 64	0
16	2U	116/116 (100%)	-0.12	0 100 100	45, 60, 72, 81	0
17	1V	101/101 (100%)	-0.41	0 100 100	22, 41, 60, 71	0
17	2V	101/101 (100%)	-0.24	0 100 100	42, 68, 76, 83	0
18	1W	112/112 (100%)	-0.35	2 (1%) 68 61	22, 32, 54, 85	0
18	2W	112/112 (100%)	-0.30	0 100 100	39, 52, 66, 81	0
19	1X	95/95 (100%)	-0.31	0 100 100	28, 42, 64, 72	0
19	2X	95/95 (100%)	-0.06	1 (1%) 80 75	48, 62, 72, 76	0
20	1Y	107/107 (100%)	-0.35	1 (0%) 84 80	38, 51, 67, 75	0
20	2Y	107/107 (100%)	0.34	12 (11%) 5 3	53, 68, 79, 86	0
21	1Z	203/203 (100%)	-0.40	1 (0%) 91 88	45, 62, 74, 82	0
21	2Z	201/203 (99%)	0.11	3 (1%) 73 68	65, 75, 82, 87	0
22	10	77/77 (100%)	-0.28	0 100 100	29, 41, 58, 63	0
22	20	77/77 (100%)	0.16	2 (2%) 56 46	52, 63, 71, 75	0
23	11	97/97 (100%)	-0.11	1 (1%) 82 77	27, 45, 68, 77	0
23	21	97/97 (100%)	-0.14	1 (1%) 82 77	46, 59, 75, 79	0
24	12	70/70 (100%)	-0.28	0 100 100	40, 51, 63, 77	0
24	22	70/70 (100%)	-0.07	0 100 100	60, 69, 77, 79	0
25	13	59/59 (100%)	-0.32	0 100 100	28, 40, 62, 77	0
25	23	59/59 (100%)	0.32	2 (3%) 45 35	54, 63, 74, 79	0
26	14	69/69 (100%)	0.34	12 (17%) 1 1	64, 79, 87, 91	0
26	24	69/69 (100%)	1.28	21 (30%) 0 0	76, 85, 89, 94	0
27	15	59/59 (100%)	-0.30	0 100 100	18, 38, 57, 66	0
27	25	59/59 (100%)	-0.20	0 100 100	38, 55, 71, 75	0
28	16	53/53 (100%)	-0.43	0 100 100	38, 48, 60, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/53 (100%)	-0.21	0 100 100	56, 64, 71, 77	0
29	17	48/48 (100%)	-0.16	0 100 100	20, 27, 58, 68	0
29	27	48/48 (100%)	-0.10	0 100 100	34, 44, 67, 78	0
30	18	64/64 (100%)	-0.17	0 100 100	28, 35, 46, 59	0
30	28	64/64 (100%)	0.04	0 100 100	46, 58, 65, 70	0
31	19	37/37 (100%)	-0.11	0 100 100	35, 46, 63, 70	0
31	29	37/37 (100%)	0.28	1 (2%) 54 44	63, 69, 75, 75	0
32	1a	1488/1521 (97%)	0.02	59 (3%) 38 28	35, 72, 91, 100	0
32	2a	1492/1521 (98%)	0.01	58 (3%) 39 29	44, 74, 91, 97	0
33	1x	97/97 (100%)	-0.08	1 (1%) 82 77	55, 67, 76, 80	0
33	2x	96/97 (98%)	1.75	40 (41%) 0 0	70, 78, 87, 89	0
34	1b	231/231 (100%)	0.15	18 (7%) 13 7	65, 77, 84, 90	0
34	2b	231/231 (100%)	0.23	14 (6%) 21 13	66, 79, 85, 89	0
35	1c	206/206 (100%)	0.25	13 (6%) 20 12	67, 78, 84, 90	0
35	2c	206/206 (100%)	0.52	16 (7%) 13 7	72, 81, 86, 90	0
36	1d	208/208 (100%)	-0.13	2 (0%) 82 77	59, 73, 80, 87	0
36	2d	208/208 (100%)	-0.16	3 (1%) 75 70	58, 71, 80, 84	0
37	1e	148/148 (100%)	-0.24	0 100 100	45, 68, 75, 89	0
37	2e	148/148 (100%)	-0.27	0 100 100	57, 70, 77, 82	0
38	1f	100/100 (100%)	-0.44	0 100 100	54, 72, 77, 80	0
38	2f	100/100 (100%)	-0.48	0 100 100	59, 68, 78, 80	0
39	1g	155/155 (100%)	-0.03	4 (2%) 56 46	66, 74, 82, 85	0
39	2g	155/155 (100%)	0.35	14 (9%) 9 5	69, 77, 82, 87	0
40	1h	137/137 (100%)	-0.05	1 (0%) 87 84	58, 68, 74, 82	0
40	2h	137/137 (100%)	-0.19	0 100 100	62, 69, 76, 80	0
41	1i	127/127 (100%)	0.58	8 (6%) 20 12	67, 80, 86, 89	0
41	2i	126/127 (99%)	1.16	34 (26%) 0 0	72, 81, 86, 89	0
42	1j	97/97 (100%)	1.13	20 (20%) 1 0	68, 81, 87, 90	0
42	2j	96/97 (98%)	1.06	19 (19%) 1 0	73, 82, 87, 89	0
43	1k	114/114 (100%)	-0.38	0 100 100	44, 64, 75, 81	0
43	2k	114/114 (100%)	-0.29	1 (0%) 84 80	54, 69, 80, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1l	121/122 (99%)	-0.23	2 (1%) 70 63	51, 64, 72, 79	0
44	2l	121/122 (99%)	-0.17	1 (0%) 86 81	56, 66, 74, 77	0
45	1m	116/116 (100%)	0.33	8 (6%) 16 10	69, 77, 82, 83	0
45	2m	114/116 (98%)	0.48	11 (9%) 8 4	75, 81, 85, 88	0
46	1n	60/60 (100%)	0.35	4 (6%) 17 10	69, 77, 81, 83	0
46	2n	60/60 (100%)	0.83	10 (16%) 1 1	73, 81, 84, 88	0
47	1o	88/88 (100%)	-0.01	1 (1%) 80 75	52, 66, 76, 82	0
47	2o	88/88 (100%)	-0.17	1 (1%) 80 75	54, 69, 78, 81	0
48	1p	82/82 (100%)	0.15	3 (3%) 41 31	63, 74, 80, 87	0
48	2p	82/82 (100%)	0.15	2 (2%) 59 49	58, 69, 76, 84	0
49	1q	99/99 (100%)	-0.12	2 (2%) 65 56	54, 68, 77, 79	0
49	2q	99/99 (100%)	-0.26	0 100 100	57, 68, 76, 78	0
50	1r	68/68 (100%)	0.11	5 (7%) 14 8	57, 67, 75, 80	0
50	2r	68/68 (100%)	-0.07	2 (2%) 51 41	62, 69, 77, 79	0
51	1s	83/83 (100%)	0.88	16 (19%) 1 0	73, 79, 84, 85	0
51	2s	83/83 (100%)	1.73	32 (38%) 0 0	77, 83, 88, 90	0
52	1t	96/98 (97%)	0.17	3 (3%) 49 39	63, 72, 81, 83	0
52	2t	98/98 (100%)	0.10	1 (1%) 82 77	59, 69, 78, 80	0
53	1u	23/23 (100%)	1.18	5 (21%) 0 0	72, 75, 78, 81	0
53	2u	23/23 (100%)	1.71	9 (39%) 0 0	76, 79, 82, 84	0
54	1y	16/16 (100%)	0.46	2 (12%) 3 2	36, 50, 60, 61	0
54	2y	16/16 (100%)	1.09	5 (31%) 0 0	53, 59, 69, 72	0
All	All	20798/20986 (99%)	0.04	886 (4%) 35 25	17, 64, 85, 100	0

The worst 5 of 886 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1133	G	17.3
1	1A	1135	G	15.6
1	1A	1137	G	14.1
1	1A	1118	C	12.4
1	1A	1136	U	11.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
1	PSU	1A	1939	20/21	0.91	0.22	60,73,87,88	0
1	5MU	1A	1937	21/22	0.92	0.23	73,79,94,111	0
32	2MG	2a	1207	24/25	0.92	0.21	76,85,87,93	0
32	5MC	2a	967	21/22	0.93	0.15	67,70,79,85	0
32	M2G	2a	966	25/26	0.93	0.14	64,71,79,91	0
32	PSU	2a	516	20/21	0.94	0.16	70,80,85,85	0
32	PSU	1a	516	20/21	0.94	0.15	62,72,77,77	0
1	PSU	2A	1911	20/21	0.94	0.11	68,72,78,81	0
1	PSU	2A	1917	20/21	0.94	0.14	67,76,84,95	0
32	2MG	1a	1207	24/25	0.95	0.12	71,78,82,84	0
32	G7M	2a	527	24/25	0.95	0.17	64,71,75,80	0
32	M2G	1a	966	25/26	0.95	0.14	58,63,73,75	0
1	5MU	2A	1915	21/22	0.95	0.18	76,82,87,102	0
32	5MC	1a	967	21/22	0.95	0.14	62,67,74,77	0
32	5MC	2a	1404	21/22	0.95	0.16	51,55,61,66	0
32	5MC	1a	1407	21/22	0.96	0.17	42,55,59,61	0
32	5MC	2a	1400	21/22	0.96	0.18	61,70,74,75	0
32	4OC	2a	1402	22/23	0.96	0.16	54,61,66,70	0
1	OMC	2A	1920	21/22	0.96	0.15	59,65,69,74	0
44	0TD	2l	92	10/11	0.96	0.12	68,70,74,84	0
1	5MC	2A	1962	21/22	0.97	0.14	38,46,53,61	0
1	2MA	2A	2503	23/24	0.97	0.23	33,38,41,42	0
1	PSU	2A	2605	20/21	0.97	0.18	34,38,44,44	0
32	UR3	1a	1498	21/22	0.97	0.18	48,53,58,64	0
32	MA6	1a	1518	24/25	0.97	0.20	42,51,58,62	0
32	MA6	1a	1519	24/25	0.97	0.18	46,53,58,61	0
44	0TD	1l	92	10/11	0.97	0.13	64,65,70,78	0
1	PSU	1A	1933	20/21	0.97	0.14	62,68,71,72	0
32	G7M	1a	527	24/25	0.97	0.16	50,60,66,69	0
32	4OC	1a	1402	22/23	0.97	0.17	50,53,57,60	0
1	OMC	1A	1942	21/22	0.97	0.14	51,61,63,67	0
32	5MC	2a	1407	21/22	0.97	0.14	51,59,66,69	0
32	UR3	2a	1498	21/22	0.97	0.15	50,60,64,67	0
32	MA6	2a	1518	24/25	0.97	0.17	54,63,68,69	0
32	MA6	2a	1519	24/25	0.97	0.19	51,61,65,68	0
1	5MC	2A	1942	21/22	0.97	0.16	47,52,55,56	0
1	5MU	1A	1961	21/22	0.98	0.17	24,28,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MU	2A	1939	21/22	0.98	0.16	36,39,45,46	0
1	5MC	1A	1964	21/22	0.98	0.13	29,37,42,45	0
1	5MC	1A	1984	21/22	0.98	0.14	31,37,39,44	0
1	OMG	2A	2251	24/25	0.98	0.16	37,44,46,51	0
1	OMG	1A	2263	24/25	0.98	0.18	19,25,27,30	0
1	OMU	1A	2564	21/22	0.98	0.18	23,29,31,33	0
32	5MC	1a	1400	21/22	0.98	0.14	57,61,66,67	0
1	PSU	1A	2617	20/21	0.98	0.21	23,27,33,34	0
32	5MC	1a	1404	21/22	0.98	0.15	45,50,54,55	0
1	2MA	1A	2515	23/24	0.99	0.21	16,20,24,24	0
1	OMU	2A	2552	21/22	0.99	0.16	32,43,45,45	0

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
55	MG	2A	3411	1/1	0.20	0.94	88,88,88,88	0
55	MG	2A	3090	1/1	0.34	0.34	78,78,78,78	0
55	MG	2a	1791	1/1	0.34	0.31	102,102,102,102	0
55	MG	2A	3532	1/1	0.38	0.28	87,87,87,87	0
55	MG	1A	3898	1/1	0.44	0.53	53,53,53,53	0
55	MG	2A	3549	1/1	0.46	0.47	72,72,72,72	0
55	MG	2A	3554	1/1	0.48	0.75	62,62,62,62	0
55	MG	2A	3506	1/1	0.48	0.52	72,72,72,72	0
55	MG	2N	201	1/1	0.49	0.43	90,90,90,90	0
55	MG	2A	3717	1/1	0.50	0.15	89,89,89,89	0
55	MG	1B	206	1/1	0.52	0.17	66,66,66,66	0
55	MG	2A	3454	1/1	0.52	1.21	67,67,67,67	0
55	MG	1A	3758	1/1	0.52	0.60	60,60,60,60	0
55	MG	1A	3496	1/1	0.53	0.08	73,73,73,73	0
55	MG	1A	3185	1/1	0.53	0.18	74,74,74,74	0
55	MG	1A	3359	1/1	0.54	0.12	80,80,80,80	0
55	MG	1a	3078	1/1	0.54	0.71	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2a	1722	1/1	0.54	0.12	77,77,77,77	0
55	MG	2a	1750	1/1	0.54	0.20	103,103,103,103	0
55	MG	1A	3254	1/1	0.54	0.52	59,59,59,59	0
55	MG	2a	1741	1/1	0.55	0.46	91,91,91,91	0
55	MG	2A	3475	1/1	0.55	0.53	66,66,66,66	0
55	MG	1a	3151	1/1	0.55	0.14	81,81,81,81	0
55	MG	2A	3562	1/1	0.56	0.46	81,81,81,81	0
55	MG	1A	3712	1/1	0.56	0.23	96,96,96,96	0
55	MG	2A	3791	1/1	0.56	0.76	73,73,73,73	0
55	MG	2A	3555	1/1	0.56	0.68	70,70,70,70	0
55	MG	1a	3077	1/1	0.57	0.76	68,68,68,68	0
55	MG	1A	3854	1/1	0.57	0.14	74,74,74,74	0
55	MG	2A	3810	1/1	0.58	0.15	68,68,68,68	0
55	MG	1a	3058	1/1	0.58	0.58	81,81,81,81	0
55	MG	1a	3168	1/1	0.58	0.07	75,75,75,75	0
55	MG	2d	504	1/1	0.58	0.25	93,93,93,93	0
55	MG	1A	3213	1/1	0.59	0.52	56,56,56,56	0
55	MG	1A	3886	1/1	0.59	0.22	39,39,39,39	0
55	MG	2A	3113	1/1	0.59	0.23	66,66,66,66	0
55	MG	2B	3013	1/1	0.60	0.06	77,77,77,77	0
55	MG	2a	1719	1/1	0.61	0.23	75,75,75,75	0
55	MG	2A	3103	1/1	0.61	0.25	64,64,64,64	0
55	MG	2A	3773	1/1	0.61	0.10	81,81,81,81	0
55	MG	1A	3609	1/1	0.62	0.40	63,63,63,63	0
55	MG	1D	313	1/1	0.62	0.25	54,54,54,54	0
55	MG	2A	3133	1/1	0.62	0.48	64,64,64,64	0
55	MG	2A	3610	1/1	0.62	0.10	82,82,82,82	0
55	MG	2n	502	1/1	0.62	0.48	77,77,77,77	0
55	MG	2A	3178	1/1	0.63	0.23	73,73,73,73	0
55	MG	1B	220	1/1	0.63	0.22	57,57,57,57	0
55	MG	1A	3721	1/1	0.63	0.24	71,71,71,71	0
55	MG	2A	3635	1/1	0.63	0.23	97,97,97,97	0
55	MG	2A	3695	1/1	0.63	0.10	82,82,82,82	0
55	MG	1H	8001	1/1	0.63	0.23	91,91,91,91	0
55	MG	1A	3608	1/1	0.64	0.18	76,76,76,76	0
55	MG	1A	3839	1/1	0.64	0.18	68,68,68,68	0
55	MG	2A	3574	1/1	0.65	0.31	99,99,99,99	0
55	MG	2A	3727	1/1	0.65	0.61	64,64,64,64	0
55	MG	2A	3128	1/1	0.65	0.59	83,83,83,83	0
55	MG	2a	1731	1/1	0.65	0.13	88,88,88,88	0
55	MG	2A	3627	1/1	0.65	0.19	67,67,67,67	0
55	MG	2A	3049	1/1	0.65	1.70	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3813	1/1	0.65	0.49	59,59,59,59	0
55	MG	1A	3095	1/1	0.65	0.41	58,58,58,58	0
55	MG	2D	302	1/1	0.65	0.35	67,67,67,67	0
55	MG	1B	222	1/1	0.66	0.10	78,78,78,78	0
55	MG	2a	1753	1/1	0.66	0.22	84,84,84,84	0
55	MG	2A	3752	1/1	0.66	0.41	77,77,77,77	0
55	MG	2d	503	1/1	0.66	0.24	72,72,72,72	0
55	MG	2A	3136	1/1	0.66	0.47	59,59,59,59	0
55	MG	2l	201	1/1	0.66	0.80	106,106,106,106	0
55	MG	2P	202	1/1	0.66	0.31	74,74,74,74	0
55	MG	2A	3473	1/1	0.67	0.13	71,71,71,71	0
55	MG	2A	3675	1/1	0.67	0.16	75,75,75,75	0
55	MG	2A	3474	1/1	0.67	0.10	78,78,78,78	0
55	MG	1A	3201	1/1	0.67	0.30	61,61,61,61	0
55	MG	1a	3210	1/1	0.67	0.15	76,76,76,76	0
55	MG	1A	3112	1/1	0.68	0.38	50,50,50,50	0
55	MG	1B	207	1/1	0.68	0.24	60,60,60,60	0
55	MG	2B	3012	1/1	0.68	0.07	80,80,80,80	0
55	MG	1A	3135	1/1	0.69	0.17	71,71,71,71	0
55	MG	2A	3501	1/1	0.69	0.21	57,57,57,57	0
55	MG	1E	303	1/1	0.69	0.29	64,64,64,64	0
55	MG	2A	3376	1/1	0.69	0.15	89,89,89,89	0
55	MG	2A	3672	1/1	0.69	0.32	67,67,67,67	0
55	MG	1F	309	1/1	0.69	0.25	59,59,59,59	0
55	MG	1A	3912	1/1	0.69	0.26	52,52,52,52	0
55	MG	2B	3017	1/1	0.69	0.21	91,91,91,91	0
55	MG	1A	3701	1/1	0.69	0.35	44,44,44,44	0
55	MG	2A	3042	1/1	0.69	0.63	59,59,59,59	0
55	MG	2A	3748	1/1	0.69	0.11	66,66,66,66	0
55	MG	1A	3130	1/1	0.70	0.24	65,65,65,65	0
55	MG	1A	3855	1/1	0.70	0.23	51,51,51,51	0
55	MG	2A	3678	1/1	0.70	0.09	91,91,91,91	0
55	MG	2A	3131	1/1	0.70	0.51	71,71,71,71	0
55	MG	1A	3861	1/1	0.70	0.08	75,75,75,75	0
55	MG	2B	3015	1/1	0.70	0.12	79,79,79,79	0
55	MG	1A	3530	1/1	0.70	0.17	63,63,63,63	0
55	MG	1A	3832	1/1	0.70	0.08	72,72,72,72	0
55	MG	2A	3258	1/1	0.70	0.21	84,84,84,84	0
55	MG	1A	3243	1/1	0.70	0.26	62,62,62,62	0
55	MG	2a	1654	1/1	0.70	0.69	79,79,79,79	0
58	A	2A	3816	1/23	0.70	1.02	85,85,85,85	0
55	MG	1a	3140	1/1	0.71	0.20	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3484	1/1	0.71	0.32	62,62,62,62	0
55	MG	1a	3149	1/1	0.71	0.24	97,97,97,97	0
55	MG	1A	3072	1/1	0.71	0.38	42,42,42,42	0
55	MG	2a	1604	1/1	0.71	0.17	61,61,61,61	0
55	MG	2A	3602	1/1	0.71	0.14	73,73,73,73	0
55	MG	2A	3606	1/1	0.71	0.15	69,69,69,69	0
55	MG	1A	3514	1/1	0.71	0.43	38,38,38,38	0
55	MG	2A	3340	1/1	0.71	0.18	72,72,72,72	0
55	MG	2a	1643	1/1	0.72	0.16	78,78,78,78	0
55	MG	2A	3255	1/1	0.72	0.40	67,67,67,67	0
55	MG	1A	3531	1/1	0.72	0.20	68,68,68,68	0
55	MG	2A	3834	1/1	0.72	0.27	68,68,68,68	0
55	MG	2B	3011	1/1	0.72	0.15	88,88,88,88	0
55	MG	1a	3063	1/1	0.72	0.89	65,65,65,65	0
55	MG	1a	3176	1/1	0.72	0.17	91,91,91,91	0
55	MG	1a	3049	1/1	0.72	0.67	78,78,78,78	0
55	MG	2A	3509	1/1	0.72	0.16	99,99,99,99	0
55	MG	2A	3444	1/1	0.72	0.29	57,57,57,57	0
55	MG	2A	3170	1/1	0.72	0.21	71,71,71,71	0
55	MG	2A	3028	1/1	0.72	0.40	61,61,61,61	0
55	MG	2A	3801	1/1	0.72	0.31	86,86,86,86	0
55	MG	2a	1624	1/1	0.72	0.14	78,78,78,78	0
55	MG	2A	3138	1/1	0.73	0.42	53,53,53,53	0
55	MG	1A	3030	1/1	0.73	0.20	39,39,39,39	0
55	MG	1A	3642	1/1	0.73	0.34	28,28,28,28	0
55	MG	2A	3814	1/1	0.73	0.20	76,76,76,76	0
55	MG	1A	3661	1/1	0.73	0.11	55,55,55,55	0
55	MG	2A	3057	1/1	0.73	0.38	48,48,48,48	0
55	MG	2A	3276	1/1	0.73	0.10	61,61,61,61	0
55	MG	1A	3700	1/1	0.73	0.42	47,47,47,47	0
55	MG	1A	3062	1/1	0.73	0.63	49,49,49,49	0
55	MG	1A	3433	1/1	0.73	0.07	81,81,81,81	0
55	MG	1A	3195	1/1	0.73	0.28	46,46,46,46	0
55	MG	2D	304	1/1	0.73	0.87	58,58,58,58	0
55	MG	1A	3887	1/1	0.73	0.19	58,58,58,58	0
55	MG	1A	3757	1/1	0.73	0.40	59,59,59,59	0
55	MG	1A	3904	1/1	0.73	0.58	53,53,53,53	0
55	MG	1A	3805	1/1	0.74	0.14	72,72,72,72	0
55	MG	2A	3519	1/1	0.74	0.17	68,68,68,68	0
55	MG	1a	3038	1/1	0.74	0.77	78,78,78,78	0
55	MG	2a	1603	1/1	0.74	0.74	65,65,65,65	0
55	MG	2A	3075	1/1	0.74	0.30	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2a	1620	1/1	0.74	0.45	76,76,76,76	0
55	MG	1A	3226	1/1	0.74	0.29	31,31,31,31	0
55	MG	1A	3728	1/1	0.74	0.17	53,53,53,53	0
55	MG	2A	3104	1/1	0.74	0.34	57,57,57,57	0
55	MG	1A	3311	1/1	0.74	0.29	52,52,52,52	0
55	MG	2A	3589	1/1	0.74	0.28	80,80,80,80	0
55	MG	2a	1727	1/1	0.74	0.24	92,92,92,92	0
55	MG	1a	3069	1/1	0.74	0.29	65,65,65,65	0
55	MG	1a	3217	1/1	0.74	0.17	81,81,81,81	0
55	MG	2A	3815	1/1	0.74	0.43	79,79,79,79	0
55	MG	1a	3218	1/1	0.74	0.24	82,82,82,82	0
55	MG	2A	3013	1/1	0.74	0.23	65,65,65,65	0
55	MG	2A	3631	1/1	0.74	0.44	80,80,80,80	0
55	MG	1A	3035	1/1	0.74	0.21	42,42,42,42	0
55	MG	2A	3150	1/1	0.74	0.26	50,50,50,50	0
55	MG	2A	3160	1/1	0.74	0.39	52,52,52,52	0
55	MG	1A	3760	1/1	0.74	0.12	60,60,60,60	0
55	MG	1A	3150	1/1	0.75	0.23	62,62,62,62	0
55	MG	2A	3804	1/1	0.75	0.10	75,75,75,75	0
55	MG	2A	3101	1/1	0.75	0.27	66,66,66,66	0
55	MG	1A	3219	1/1	0.75	0.87	76,76,76,76	0
55	MG	1a	3066	1/1	0.75	0.11	75,75,75,75	0
55	MG	1A	3454	1/1	0.75	0.39	61,61,61,61	0
55	MG	2a	1655	1/1	0.75	0.37	70,70,70,70	0
55	MG	2a	1718	1/1	0.75	0.17	88,88,88,88	0
55	MG	2A	3829	1/1	0.75	0.39	60,60,60,60	0
55	MG	1A	3665	1/1	0.75	0.22	49,49,49,49	0
55	MG	1a	3005	1/1	0.75	0.17	67,67,67,67	0
55	MG	1a	3013	1/1	0.75	0.10	79,79,79,79	0
55	MG	2A	3412	1/1	0.75	0.17	72,72,72,72	0
55	MG	2a	1746	1/1	0.75	0.12	89,89,89,89	0
55	MG	1A	3093	1/1	0.75	0.24	41,41,41,41	0
55	MG	1a	3039	1/1	0.75	0.43	68,68,68,68	0
55	MG	2a	1773	1/1	0.75	0.10	91,91,91,91	0
55	MG	2B	3018	1/1	0.75	0.19	74,74,74,74	0
55	MG	2A	3464	1/1	0.75	0.15	83,83,83,83	0
55	MG	2A	3582	1/1	0.75	0.28	67,67,67,67	0
55	MG	2A	3058	1/1	0.75	0.20	60,60,60,60	0
55	MG	1A	3845	1/1	0.75	0.18	47,47,47,47	0
55	MG	2Q	204	1/1	0.75	0.51	69,69,69,69	0
55	MG	2A	3299	1/1	0.76	0.15	46,46,46,46	0
55	MG	2a	1633	1/1	0.76	0.36	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3302	1/1	0.76	0.14	47,47,47,47	0
55	MG	1a	3150	1/1	0.76	0.23	94,94,94,94	0
55	MG	2A	3141	1/1	0.76	0.48	51,51,51,51	0
55	MG	2A	3533	1/1	0.76	1.28	79,79,79,79	0
55	MG	2A	3694	1/1	0.76	0.10	61,61,61,61	0
55	MG	2A	3148	1/1	0.76	0.27	72,72,72,72	0
55	MG	1A	3171	1/1	0.76	0.29	48,48,48,48	0
55	MG	2A	3151	1/1	0.76	0.92	50,50,50,50	0
55	MG	2a	1732	1/1	0.76	0.13	83,83,83,83	0
55	MG	1A	3319	1/1	0.76	0.21	64,64,64,64	0
55	MG	2A	3457	1/1	0.76	0.16	77,77,77,77	0
55	MG	1A	3877	1/1	0.76	0.14	69,69,69,69	0
55	MG	1a	3136	1/1	0.76	0.57	82,82,82,82	0
55	MG	1A	3880	1/1	0.76	0.09	73,73,73,73	0
55	MG	1A	3724	1/1	0.76	0.41	40,40,40,40	0
55	MG	2X	102	1/1	0.76	0.44	82,82,82,82	0
55	MG	28	101	1/1	0.76	0.60	67,67,67,67	0
55	MG	2A	3808	1/1	0.76	0.31	73,73,73,73	0
55	MG	2A	3260	1/1	0.76	0.31	74,74,74,74	0
55	MG	1d	505	1/1	0.76	0.10	76,76,76,76	0
55	MG	2A	3594	1/1	0.77	0.12	55,55,55,55	0
55	MG	1A	3766	1/1	0.77	0.08	58,58,58,58	0
55	MG	2A	3337	1/1	0.77	0.04	74,74,74,74	0
55	MG	1a	3175	1/1	0.77	0.17	87,87,87,87	0
55	MG	10	101	1/1	0.77	0.38	51,51,51,51	0
55	MG	2a	1729	1/1	0.77	0.19	68,68,68,68	0
55	MG	1a	3074	1/1	0.77	0.48	70,70,70,70	0
55	MG	1A	3139	1/1	0.77	0.30	38,38,38,38	0
55	MG	2a	1733	1/1	0.77	0.53	66,66,66,66	0
55	MG	2A	3424	1/1	0.77	0.21	76,76,76,76	0
55	MG	1B	216	1/1	0.77	0.17	74,74,74,74	0
55	MG	2a	1601	1/1	0.77	0.31	59,59,59,59	0
55	MG	1a	3117	1/1	0.77	0.32	71,71,71,71	0
55	MG	2a	1771	1/1	0.77	0.37	83,83,83,83	0
55	MG	1A	3890	1/1	0.77	0.20	45,45,45,45	0
55	MG	1A	3396	1/1	0.77	0.32	40,40,40,40	0
55	MG	2A	3706	1/1	0.77	0.07	93,93,93,93	0
55	MG	1A	3899	1/1	0.77	0.10	52,52,52,52	0
55	MG	2a	1641	1/1	0.77	0.96	65,65,65,65	0
55	MG	1A	3685	1/1	0.77	0.13	31,31,31,31	0
55	MG	1A	3567	1/1	0.77	0.18	51,51,51,51	0
55	MG	2A	3183	1/1	0.78	0.58	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3188	1/1	0.78	0.43	57,57,57,57	0
55	MG	1a	3114	1/1	0.78	0.10	79,79,79,79	0
55	MG	1a	3048	1/1	0.78	0.13	75,75,75,75	0
55	MG	1a	3129	1/1	0.78	0.11	83,83,83,83	0
55	MG	2a	1659	1/1	0.78	0.13	76,76,76,76	0
55	MG	2A	3008	1/1	0.78	0.37	68,68,68,68	0
55	MG	2A	3292	1/1	0.78	0.08	55,55,55,55	0
55	MG	1F	301	1/1	0.78	0.20	51,51,51,51	0
55	MG	1A	3131	1/1	0.78	0.21	44,44,44,44	0
55	MG	1A	3816	1/1	0.78	0.27	72,72,72,72	0
55	MG	1A	3179	1/1	0.78	0.35	44,44,44,44	0
55	MG	2A	3538	1/1	0.78	0.07	73,73,73,73	0
55	MG	1A	3725	1/1	0.78	0.25	33,33,33,33	0
55	MG	2G	3003	1/1	0.78	0.10	83,83,83,83	0
55	MG	1a	3152	1/1	0.78	0.14	90,90,90,90	0
55	MG	1a	3073	1/1	0.78	0.17	75,75,75,75	0
55	MG	2A	3754	1/1	0.78	0.18	85,85,85,85	0
55	MG	2A	3416	1/1	0.78	0.53	50,50,50,50	0
55	MG	27	102	1/1	0.78	0.17	72,72,72,72	0
55	MG	2A	3787	1/1	0.78	0.18	84,84,84,84	0
55	MG	2A	3422	1/1	0.78	0.12	71,71,71,71	0
55	MG	1A	3123	1/1	0.78	0.18	61,61,61,61	0
55	MG	2A	3161	1/1	0.78	0.28	83,83,83,83	0
55	MG	1A	3848	1/1	0.78	0.27	60,60,60,60	0
55	MG	1A	3920	1/1	0.78	0.40	45,45,45,45	0
55	MG	2A	3132	1/1	0.79	0.72	68,68,68,68	0
55	MG	2A	3263	1/1	0.79	0.17	65,65,65,65	0
55	MG	2A	3811	1/1	0.79	0.48	57,57,57,57	0
55	MG	1A	3647	1/1	0.79	0.05	85,85,85,85	0
55	MG	2a	1636	1/1	0.79	0.30	67,67,67,67	0
55	MG	1A	3655	1/1	0.79	0.18	72,72,72,72	0
55	MG	1B	224	1/1	0.79	0.18	55,55,55,55	0
55	MG	1A	3169	1/1	0.79	0.36	37,37,37,37	0
55	MG	2A	3303	1/1	0.79	0.09	73,73,73,73	0
55	MG	1A	3174	1/1	0.79	0.71	60,60,60,60	0
55	MG	2a	1714	1/1	0.79	0.36	73,73,73,73	0
55	MG	2A	3682	1/1	0.79	0.21	68,68,68,68	0
55	MG	1A	3501	1/1	0.79	0.19	58,58,58,58	0
55	MG	1a	3194	1/1	0.79	0.11	80,80,80,80	0
55	MG	2a	1725	1/1	0.79	0.12	89,89,89,89	0
55	MG	1A	3729	1/1	0.79	0.17	68,68,68,68	0
55	MG	1A	3622	1/1	0.79	0.27	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3561	1/1	0.79	0.17	55,55,55,55	0
55	MG	1a	3144	1/1	0.79	0.39	74,74,74,74	0
55	MG	2F	305	1/1	0.79	0.19	51,51,51,51	0
55	MG	2A	3105	1/1	0.79	0.14	83,83,83,83	0
55	MG	2A	3439	1/1	0.79	0.15	73,73,73,73	0
55	MG	2A	3765	1/1	0.79	0.42	60,60,60,60	0
55	MG	2A	3766	1/1	0.79	0.13	78,78,78,78	0
55	MG	2R	8001	1/1	0.79	0.35	77,77,77,77	0
55	MG	2V	202	1/1	0.79	0.17	70,70,70,70	0
55	MG	2A	3002	1/1	0.79	0.23	68,68,68,68	0
55	MG	20	103	1/1	0.79	0.20	77,77,77,77	0
55	MG	2A	3228	1/1	0.79	0.33	84,84,84,84	0
55	MG	10	103	1/1	0.79	0.11	51,51,51,51	0
55	MG	2A	3011	1/1	0.79	0.41	57,57,57,57	0
55	MG	2A	3605	1/1	0.79	0.38	68,68,68,68	0
55	MG	1A	3723	1/1	0.80	0.10	77,77,77,77	0
55	MG	1A	3482	1/1	0.80	0.27	64,64,64,64	0
55	MG	2A	3795	1/1	0.80	0.59	61,61,61,61	0
55	MG	2A	3798	1/1	0.80	0.14	81,81,81,81	0
55	MG	1a	3022	1/1	0.80	0.68	66,66,66,66	0
55	MG	2A	3250	1/1	0.80	0.15	68,68,68,68	0
55	MG	2A	3109	1/1	0.80	0.50	63,63,63,63	0
55	MG	2A	3461	1/1	0.80	0.25	72,72,72,72	0
55	MG	1A	3806	1/1	0.80	0.18	59,59,59,59	0
55	MG	1A	3143	1/1	0.80	0.48	69,69,69,69	0
55	MG	2a	1644	1/1	0.80	0.29	71,71,71,71	0
55	MG	1A	3824	1/1	0.80	0.15	57,57,57,57	0
55	MG	1D	303	1/1	0.80	0.62	48,48,48,48	0
55	MG	2A	3819	1/1	0.80	0.86	51,51,51,51	0
55	MG	2A	3671	1/1	0.80	0.14	76,76,76,76	0
55	MG	1a	3057	1/1	0.80	0.48	89,89,89,89	0
55	MG	2B	3005	1/1	0.80	0.14	71,71,71,71	0
55	MG	1A	3536	1/1	0.80	0.17	56,56,56,56	0
55	MG	2A	3041	1/1	0.80	0.83	62,62,62,62	0
55	MG	2A	3681	1/1	0.80	0.06	65,65,65,65	0
55	MG	1A	3628	1/1	0.80	0.20	66,66,66,66	0
55	MG	2A	3513	1/1	0.80	0.85	62,62,62,62	0
55	MG	2A	3327	1/1	0.80	0.20	88,88,88,88	0
55	MG	1A	3752	1/1	0.80	0.14	65,65,65,65	0
55	MG	1a	3157	1/1	0.80	0.11	75,75,75,75	0
55	MG	2F	303	1/1	0.80	0.31	57,57,57,57	0
55	MG	2a	1747	1/1	0.80	0.15	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3725	1/1	0.80	0.09	58,58,58,58	0
55	MG	2A	3343	1/1	0.80	0.29	79,79,79,79	0
55	MG	1A	3547	1/1	0.80	0.23	29,29,29,29	0
55	MG	1A	3021	1/1	0.80	0.12	50,50,50,50	0
55	MG	2A	3076	1/1	0.80	0.34	50,50,50,50	0
55	MG	2A	3558	1/1	0.80	0.19	67,67,67,67	0
55	MG	1A	3258	1/1	0.80	0.14	53,53,53,53	0
55	MG	1A	3856	1/1	0.80	0.26	53,53,53,53	0
55	MG	2A	3777	1/1	0.80	0.21	83,83,83,83	0
55	MG	2A	3785	1/1	0.80	0.08	53,53,53,53	0
55	MG	2A	3803	1/1	0.81	0.20	47,47,47,47	0
55	MG	1A	3528	1/1	0.81	0.20	61,61,61,61	0
55	MG	2A	3129	1/1	0.81	0.17	64,64,64,64	0
55	MG	2A	3130	1/1	0.81	0.41	66,66,66,66	0
55	MG	2A	3668	1/1	0.81	0.14	72,72,72,72	0
55	MG	2A	3481	1/1	0.81	0.56	57,57,57,57	0
55	MG	1A	3849	1/1	0.81	0.23	86,86,86,86	0
55	MG	1A	3026	1/1	0.81	0.21	59,59,59,59	0
55	MG	1a	3146	1/1	0.81	0.12	71,71,71,71	0
55	MG	2a	1645	1/1	0.81	0.21	64,64,64,64	0
55	MG	2A	3035	1/1	0.81	0.16	53,53,53,53	0
55	MG	2A	3305	1/1	0.81	0.09	52,52,52,52	0
55	MG	2A	3686	1/1	0.81	0.10	93,93,93,93	0
55	MG	2a	1682	1/1	0.81	0.16	78,78,78,78	0
55	MG	2a	1708	1/1	0.81	0.10	89,89,89,89	0
55	MG	1A	3170	1/1	0.81	0.31	40,40,40,40	0
55	MG	1A	3374	1/1	0.81	0.08	74,74,74,74	0
55	MG	1A	3240	1/1	0.81	0.31	42,42,42,42	0
55	MG	2A	3712	1/1	0.81	0.14	69,69,69,69	0
55	MG	2A	3050	1/1	0.81	0.20	63,63,63,63	0
55	MG	1A	3862	1/1	0.81	0.36	55,55,55,55	0
55	MG	1A	3550	1/1	0.81	0.37	47,47,47,47	0
55	MG	1A	3878	1/1	0.81	0.13	36,36,36,36	0
55	MG	1A	3697	1/1	0.81	0.31	64,64,64,64	0
55	MG	1A	3147	1/1	0.81	0.21	62,62,62,62	0
55	MG	2G	3002	1/1	0.81	0.18	79,79,79,79	0
55	MG	2A	3564	1/1	0.81	0.13	58,58,58,58	0
55	MG	1A	3246	1/1	0.81	0.12	87,87,87,87	0
55	MG	2P	201	1/1	0.81	0.33	67,67,67,67	0
55	MG	2A	3771	1/1	0.81	0.15	65,65,65,65	0
55	MG	2A	3427	1/1	0.81	0.43	81,81,81,81	0
55	MG	1A	3252	1/1	0.81	0.80	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3200	1/1	0.81	0.53	65,65,65,65	0
55	MG	1A	3101	1/1	0.81	0.52	55,55,55,55	0
55	MG	1A	3209	1/1	0.81	0.43	49,49,49,49	0
55	MG	1A	3623	1/1	0.81	0.34	43,43,43,43	0
55	MG	1A	3177	1/1	0.81	0.54	54,54,54,54	0
56	ZN	14	501	1/1	0.81	0.05	149,149,149,149	0
55	MG	2A	3621	1/1	0.81	0.73	64,64,64,64	0
55	MG	1a	3197	1/1	0.82	0.12	78,78,78,78	0
55	MG	2A	3380	1/1	0.82	0.10	83,83,83,83	0
55	MG	2A	3690	1/1	0.82	0.22	82,82,82,82	0
55	MG	2A	3821	1/1	0.82	0.30	54,54,54,54	0
55	MG	2A	3545	1/1	0.82	0.07	84,84,84,84	0
55	MG	2A	3173	1/1	0.82	0.97	72,72,72,72	0
55	MG	2B	3002	1/1	0.82	0.12	67,67,67,67	0
55	MG	2a	1652	1/1	0.82	0.11	65,65,65,65	0
55	MG	1A	3267	1/1	0.82	0.12	77,77,77,77	0
55	MG	1A	3166	1/1	0.82	0.18	54,54,54,54	0
55	MG	2a	1657	1/1	0.82	0.34	64,64,64,64	0
55	MG	1A	3167	1/1	0.82	0.11	54,54,54,54	0
55	MG	2A	3194	1/1	0.82	0.08	83,83,83,83	0
55	MG	2a	1696	1/1	0.82	0.07	78,78,78,78	0
55	MG	2a	1697	1/1	0.82	0.07	79,79,79,79	0
55	MG	1A	3207	1/1	0.82	0.29	35,35,35,35	0
55	MG	2a	1710	1/1	0.82	0.16	84,84,84,84	0
55	MG	1A	3236	1/1	0.82	0.27	53,53,53,53	0
55	MG	1A	3382	1/1	0.82	0.54	58,58,58,58	0
55	MG	2A	3009	1/1	0.82	0.69	64,64,64,64	0
55	MG	1A	3632	1/1	0.82	0.29	53,53,53,53	0
55	MG	2F	301	1/1	0.82	0.30	52,52,52,52	0
55	MG	1A	3257	1/1	0.82	0.54	44,44,44,44	0
55	MG	2A	3019	1/1	0.82	0.20	43,43,43,43	0
55	MG	1A	3118	1/1	0.82	0.31	39,39,39,39	0
55	MG	2A	3774	1/1	0.82	0.22	81,81,81,81	0
55	MG	1A	3444	1/1	0.82	0.22	57,57,57,57	0
55	MG	1A	3260	1/1	0.82	0.18	75,75,75,75	0
55	MG	2A	3479	1/1	0.82	0.11	73,73,73,73	0
55	MG	1A	3907	1/1	0.82	0.44	58,58,58,58	0
55	MG	1A	3477	1/1	0.82	0.17	40,40,40,40	0
55	MG	2A	3647	1/1	0.82	0.19	77,77,77,77	0
55	MG	2a	1755	1/1	0.82	0.13	66,66,66,66	0
55	MG	2A	3650	1/1	0.82	0.35	57,57,57,57	0
55	MG	2A	3802	1/1	0.82	0.68	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	21	102	1/1	0.82	0.19	66,66,66,66	0
55	MG	1A	3670	1/1	0.82	0.27	51,51,51,51	0
55	MG	1a	3184	1/1	0.82	0.15	82,82,82,82	0
55	MG	2A	3329	1/1	0.82	0.44	72,72,72,72	0
55	MG	1a	3186	1/1	0.82	0.08	69,69,69,69	0
55	MG	1A	3683	1/1	0.82	0.16	50,50,50,50	0
55	MG	1a	3196	1/1	0.82	0.13	82,82,82,82	0
55	MG	20	102	1/1	0.83	0.31	63,63,63,63	0
55	MG	1g	3001	1/1	0.83	0.25	79,79,79,79	0
55	MG	1h	3001	1/1	0.83	0.56	52,52,52,52	0
55	MG	2A	3768	1/1	0.83	0.44	94,94,94,94	0
55	MG	2A	3326	1/1	0.83	0.13	69,69,69,69	0
55	MG	1A	3039	1/1	0.83	0.34	55,55,55,55	0
55	MG	1a	3131	1/1	0.83	0.17	70,70,70,70	0
55	MG	2A	3336	1/1	0.83	0.80	76,76,76,76	0
55	MG	1A	3558	1/1	0.83	0.19	72,72,72,72	0
55	MG	2A	3010	1/1	0.83	0.20	62,62,62,62	0
55	MG	1A	3431	1/1	0.83	0.58	53,53,53,53	0
55	MG	2A	3585	1/1	0.83	0.19	75,75,75,75	0
55	MG	2a	1638	1/1	0.83	0.86	70,70,70,70	0
55	MG	1A	3142	1/1	0.83	0.47	43,43,43,43	0
55	MG	1a	3019	1/1	0.83	0.15	67,67,67,67	0
55	MG	2A	3385	1/1	0.83	0.23	86,86,86,86	0
55	MG	2A	3027	1/1	0.83	0.35	66,66,66,66	0
55	MG	2a	1646	1/1	0.83	0.41	62,62,62,62	0
55	MG	1A	3919	1/1	0.83	0.45	33,33,33,33	0
55	MG	1A	3786	1/1	0.83	0.30	58,58,58,58	0
55	MG	2A	3162	1/1	0.83	0.76	79,79,79,79	0
55	MG	1A	3803	1/1	0.83	0.10	78,78,78,78	0
55	MG	2A	3172	1/1	0.83	0.39	64,64,64,64	0
55	MG	2A	3431	1/1	0.83	0.15	74,74,74,74	0
55	MG	2A	3638	1/1	0.83	0.19	85,85,85,85	0
55	MG	2A	3641	1/1	0.83	0.16	72,72,72,72	0
55	MG	2A	3643	1/1	0.83	0.51	56,56,56,56	0
55	MG	1A	3857	1/1	0.83	0.16	67,67,67,67	0
55	MG	1A	3804	1/1	0.83	0.10	71,71,71,71	0
55	MG	2A	3655	1/1	0.83	0.24	60,60,60,60	0
55	MG	2A	3179	1/1	0.83	0.72	63,63,63,63	0
55	MG	2B	3007	1/1	0.83	0.14	79,79,79,79	0
55	MG	1B	217	1/1	0.83	0.08	57,57,57,57	0
55	MG	1A	3603	1/1	0.83	0.48	46,46,46,46	0
55	MG	2A	3674	1/1	0.83	0.12	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2B	3014	1/1	0.83	0.09	73,73,73,73	0
55	MG	1A	3188	1/1	0.83	0.35	44,44,44,44	0
55	MG	1A	3034	1/1	0.83	0.19	60,60,60,60	0
55	MG	2a	1737	1/1	0.83	0.84	87,87,87,87	0
55	MG	2A	3203	1/1	0.83	1.25	58,58,58,58	0
55	MG	2A	3209	1/1	0.83	0.07	89,89,89,89	0
55	MG	1A	3468	1/1	0.83	0.17	30,30,30,30	0
55	MG	2A	3243	1/1	0.83	0.46	55,55,55,55	0
55	MG	2a	1752	1/1	0.83	0.49	69,69,69,69	0
55	MG	1A	3882	1/1	0.83	0.19	67,67,67,67	0
55	MG	2A	3486	1/1	0.83	0.15	57,57,57,57	0
55	MG	1A	3215	1/1	0.83	0.21	51,51,51,51	0
55	MG	2A	3707	1/1	0.83	0.15	73,73,73,73	0
55	MG	1A	3245	1/1	0.83	0.10	74,74,74,74	0
55	MG	1A	3840	1/1	0.83	0.26	64,64,64,64	0
55	MG	1a	3216	1/1	0.83	0.11	96,96,96,96	0
55	MG	1a	3079	1/1	0.83	0.14	54,54,54,54	0
55	MG	1A	3843	1/1	0.83	0.22	47,47,47,47	0
55	MG	1a	3226	1/1	0.83	0.41	74,74,74,74	0
55	MG	1P	202	1/1	0.83	0.19	85,85,85,85	0
55	MG	1A	3903	1/1	0.84	0.10	34,34,34,34	0
55	MG	2A	3612	1/1	0.84	0.18	41,41,41,41	0
55	MG	2a	1607	1/1	0.84	0.88	73,73,73,73	0
55	MG	2A	3229	1/1	0.84	0.46	64,64,64,64	0
55	MG	1A	3552	1/1	0.84	0.20	64,64,64,64	0
55	MG	2A	3030	1/1	0.84	0.25	66,66,66,66	0
55	MG	1a	3208	1/1	0.84	0.29	70,70,70,70	0
55	MG	2A	3462	1/1	0.84	0.19	62,62,62,62	0
55	MG	1A	3164	1/1	0.84	0.29	78,78,78,78	0
55	MG	1A	3182	1/1	0.84	0.41	38,38,38,38	0
55	MG	1A	3259	1/1	0.84	0.24	36,36,36,36	0
55	MG	2A	3147	1/1	0.84	0.17	81,81,81,81	0
55	MG	2A	3277	1/1	0.84	0.17	54,54,54,54	0
55	MG	1F	302	1/1	0.84	0.43	37,37,37,37	0
55	MG	2A	3297	1/1	0.84	0.13	68,68,68,68	0
55	MG	2A	3053	1/1	0.84	0.96	60,60,60,60	0
55	MG	2A	3835	1/1	0.84	1.05	65,65,65,65	0
55	MG	2A	3838	1/1	0.84	0.38	54,54,54,54	0
55	MG	1a	3222	1/1	0.84	0.35	72,72,72,72	0
55	MG	2A	3154	1/1	0.84	0.73	53,53,53,53	0
55	MG	1A	3572	1/1	0.84	0.23	67,67,67,67	0
55	MG	1A	3932	1/1	0.84	0.33	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1B	204	1/1	0.84	0.27	72,72,72,72	0
55	MG	2A	3169	1/1	0.84	0.29	73,73,73,73	0
55	MG	2A	3085	1/1	0.84	0.17	67,67,67,67	0
55	MG	2A	3534	1/1	0.84	0.16	82,82,82,82	0
55	MG	1a	3071	1/1	0.84	0.28	56,56,56,56	0
55	MG	2A	3542	1/1	0.84	0.23	75,75,75,75	0
55	MG	1y	101	1/1	0.84	0.35	50,50,50,50	0
55	MG	2A	3177	1/1	0.84	0.98	50,50,50,50	0
55	MG	2a	1730	1/1	0.84	0.13	84,84,84,84	0
55	MG	2A	3716	1/1	0.84	0.10	85,85,85,85	0
55	MG	2A	3553	1/1	0.84	0.13	66,66,66,66	0
55	MG	2A	3347	1/1	0.84	0.05	72,72,72,72	0
55	MG	2F	309	1/1	0.84	0.14	72,72,72,72	0
55	MG	2A	3374	1/1	0.84	0.59	60,60,60,60	0
55	MG	1A	3218	1/1	0.84	0.22	53,53,53,53	0
55	MG	2A	3378	1/1	0.84	0.07	58,58,58,58	0
55	MG	1A	3253	1/1	0.84	0.42	63,63,63,63	0
55	MG	1A	3541	1/1	0.84	0.30	55,55,55,55	0
55	MG	1A	3671	1/1	0.84	0.17	46,46,46,46	0
55	MG	2A	3192	1/1	0.84	0.66	64,64,64,64	0
55	MG	2a	1769	1/1	0.84	0.23	83,83,83,83	0
55	MG	1A	3211	1/1	0.84	0.40	41,41,41,41	0
55	MG	2A	3197	1/1	0.84	0.28	53,53,53,53	0
55	MG	2a	1785	1/1	0.84	0.17	83,83,83,83	0
55	MG	2A	3115	1/1	0.84	0.29	65,65,65,65	0
55	MG	2A	3603	1/1	0.84	0.12	70,70,70,70	0
55	MG	2A	3604	1/1	0.84	0.30	77,77,77,77	0
55	MG	2g	3001	1/1	0.84	0.18	75,75,75,75	0
55	MG	27	101	1/1	0.84	0.33	57,57,57,57	0
55	MG	1A	3315	1/1	0.84	0.07	74,74,74,74	0
55	MG	1a	3036	1/1	0.84	0.20	50,50,50,50	0
55	MG	2A	3608	1/1	0.84	0.15	63,63,63,63	0
55	MG	1A	3566	1/1	0.85	0.18	70,70,70,70	0
55	MG	2A	3644	1/1	0.85	0.44	66,66,66,66	0
55	MG	2A	3499	1/1	0.85	0.38	51,51,51,51	0
55	MG	2A	3159	1/1	0.85	0.43	53,53,53,53	0
55	MG	1A	3876	1/1	0.85	0.07	61,61,61,61	0
55	MG	2A	3658	1/1	0.85	0.26	76,76,76,76	0
55	MG	2A	3054	1/1	0.85	0.34	54,54,54,54	0
55	MG	18	3302	1/1	0.85	0.60	43,43,43,43	0
55	MG	2A	3166	1/1	0.85	0.28	54,54,54,54	0
55	MG	1A	3287	1/1	0.85	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3162	1/1	0.85	0.24	62,62,62,62	0
55	MG	2A	3338	1/1	0.85	0.22	55,55,55,55	0
55	MG	1a	3018	1/1	0.85	0.11	66,66,66,66	0
55	MG	2A	3077	1/1	0.85	0.34	58,58,58,58	0
55	MG	1A	3472	1/1	0.85	0.15	64,64,64,64	0
55	MG	1d	502	1/1	0.85	0.28	71,71,71,71	0
55	MG	1d	504	1/1	0.85	0.21	77,77,77,77	0
55	MG	1A	3837	1/1	0.85	0.13	78,78,78,78	0
55	MG	2A	3184	1/1	0.85	0.64	57,57,57,57	0
55	MG	1a	3033	1/1	0.85	0.12	56,56,56,56	0
55	MG	1A	3392	1/1	0.85	0.37	57,57,57,57	0
55	MG	1A	3148	1/1	0.85	0.47	48,48,48,48	0
55	MG	2a	1721	1/1	0.85	0.14	86,86,86,86	0
55	MG	2A	3110	1/1	0.85	0.61	58,58,58,58	0
55	MG	2A	3579	1/1	0.85	0.17	61,61,61,61	0
55	MG	2a	1726	1/1	0.85	0.15	73,73,73,73	0
55	MG	2A	3581	1/1	0.85	0.09	73,73,73,73	0
55	MG	2A	3737	1/1	0.85	0.12	79,79,79,79	0
55	MG	1A	3104	1/1	0.85	0.21	42,42,42,42	0
55	MG	2A	3749	1/1	0.85	0.06	81,81,81,81	0
55	MG	1a	3041	1/1	0.85	0.11	76,76,76,76	0
55	MG	2A	3587	1/1	0.85	0.06	63,63,63,63	0
55	MG	1D	301	1/1	0.85	0.45	54,54,54,54	0
55	MG	1A	3499	1/1	0.85	0.13	62,62,62,62	0
55	MG	1D	312	1/1	0.85	0.26	65,65,65,65	0
55	MG	2A	3240	1/1	0.85	0.15	50,50,50,50	0
55	MG	1A	3551	1/1	0.85	0.27	36,36,36,36	0
55	MG	1A	3357	1/1	0.85	0.06	75,75,75,75	0
55	MG	20	101	1/1	0.85	0.27	84,84,84,84	0
55	MG	2A	3458	1/1	0.85	0.12	74,74,74,74	0
55	MG	2a	1759	1/1	0.85	0.04	86,86,86,86	0
55	MG	1A	3706	1/1	0.85	0.40	70,70,70,70	0
55	MG	1a	3180	1/1	0.85	0.20	97,97,97,97	0
55	MG	1A	3793	1/1	0.85	0.33	60,60,60,60	0
55	MG	2a	1780	1/1	0.85	0.27	73,73,73,73	0
55	MG	1a	3070	1/1	0.85	0.35	60,60,60,60	0
55	MG	1A	3505	1/1	0.85	0.38	50,50,50,50	0
55	MG	1A	3720	1/1	0.85	0.36	64,64,64,64	0
55	MG	2A	3634	1/1	0.85	0.20	81,81,81,81	0
55	MG	2e	202	1/1	0.85	0.31	73,73,73,73	0
55	MG	2A	3045	1/1	0.85	0.11	75,75,75,75	0
55	MG	2h	3002	1/1	0.85	0.24	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3280	1/1	0.85	0.16	33,33,33,33	0
55	MG	2a	1608	1/1	0.85	0.30	57,57,57,57	0
55	MG	2a	1610	1/1	0.85	0.96	70,70,70,70	0
55	MG	2A	3152	1/1	0.85	0.24	66,66,66,66	0
55	MG	25	104	1/1	0.86	0.16	83,83,83,83	0
55	MG	1A	3002	1/1	0.86	0.23	55,55,55,55	0
55	MG	2A	3731	1/1	0.86	0.07	65,65,65,65	0
55	MG	1A	3834	1/1	0.86	0.17	73,73,73,73	0
55	MG	2A	3266	1/1	0.86	0.20	66,66,66,66	0
55	MG	1a	3020	1/1	0.86	0.34	71,71,71,71	0
55	MG	1A	3036	1/1	0.86	0.25	40,40,40,40	0
55	MG	1A	3152	1/1	0.86	0.17	46,46,46,46	0
55	MG	1A	3518	1/1	0.86	0.21	71,71,71,71	0
55	MG	1A	3073	1/1	0.86	0.19	44,44,44,44	0
55	MG	2a	1612	1/1	0.86	0.19	54,54,54,54	0
55	MG	2a	1615	1/1	0.86	1.49	78,78,78,78	0
55	MG	1a	3201	1/1	0.86	0.10	80,80,80,80	0
55	MG	1A	3180	1/1	0.86	0.15	64,64,64,64	0
55	MG	1A	3629	1/1	0.86	0.16	63,63,63,63	0
55	MG	1a	3046	1/1	0.86	0.30	50,50,50,50	0
55	MG	1A	3138	1/1	0.86	0.29	57,57,57,57	0
55	MG	1A	3636	1/1	0.86	0.41	27,27,27,27	0
55	MG	1a	3050	1/1	0.86	0.25	54,54,54,54	0
55	MG	1a	3223	1/1	0.86	0.22	65,65,65,65	0
55	MG	1a	3056	1/1	0.86	0.09	74,74,74,74	0
55	MG	1A	3733	1/1	0.86	0.26	42,42,42,42	0
55	MG	2a	1648	1/1	0.86	0.08	82,82,82,82	0
55	MG	2A	3142	1/1	0.86	0.77	57,57,57,57	0
55	MG	2A	3599	1/1	0.86	0.10	78,78,78,78	0
55	MG	1A	3734	1/1	0.86	0.25	29,29,29,29	0
55	MG	1A	3113	1/1	0.86	0.25	26,26,26,26	0
55	MG	1A	3013	1/1	0.86	0.16	62,62,62,62	0
55	MG	2a	1667	1/1	0.86	0.25	75,75,75,75	0
55	MG	1a	3068	1/1	0.86	0.23	71,71,71,71	0
55	MG	1B	225	1/1	0.86	0.34	68,68,68,68	0
55	MG	1A	3436	1/1	0.86	0.16	58,58,58,58	0
55	MG	1A	3869	1/1	0.86	0.19	40,40,40,40	0
55	MG	1A	3270	1/1	0.86	0.33	60,60,60,60	0
55	MG	1A	3190	1/1	0.86	0.17	72,72,72,72	0
55	MG	1A	3669	1/1	0.86	0.30	62,62,62,62	0
55	MG	2A	3825	1/1	0.86	1.51	60,60,60,60	0
55	MG	2A	3165	1/1	0.86	0.35	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3191	1/1	0.86	0.28	39,39,39,39	0
55	MG	1A	3881	1/1	0.86	0.20	51,51,51,51	0
55	MG	1F	308	1/1	0.86	0.56	62,62,62,62	0
55	MG	1A	3058	1/1	0.86	0.08	50,50,50,50	0
55	MG	2B	3003	1/1	0.86	0.16	71,71,71,71	0
55	MG	1A	3199	1/1	0.86	0.63	41,41,41,41	0
55	MG	2A	3032	1/1	0.86	0.35	63,63,63,63	0
55	MG	1A	3316	1/1	0.86	0.40	69,69,69,69	0
55	MG	1A	3127	1/1	0.86	0.14	36,36,36,36	0
55	MG	1A	3895	1/1	0.86	0.37	45,45,45,45	0
55	MG	2A	3463	1/1	0.86	0.18	77,77,77,77	0
55	MG	2A	3664	1/1	0.86	0.13	81,81,81,81	0
55	MG	1a	3143	1/1	0.86	0.10	82,82,82,82	0
55	MG	11	102	1/1	0.86	0.22	56,56,56,56	0
55	MG	11	103	1/1	0.86	0.20	50,50,50,50	0
55	MG	17	101	1/1	0.86	0.28	64,64,64,64	0
55	MG	1A	3809	1/1	0.86	0.14	35,35,35,35	0
55	MG	18	3303	1/1	0.86	0.04	63,63,63,63	0
55	MG	1a	3004	1/1	0.86	0.19	67,67,67,67	0
55	MG	2A	3065	1/1	0.86	0.08	70,70,70,70	0
55	MG	2A	3488	1/1	0.86	0.17	75,75,75,75	0
55	MG	2a	1775	1/1	0.86	0.10	74,74,74,74	0
55	MG	2A	3223	1/1	0.86	0.16	68,68,68,68	0
55	MG	2A	3691	1/1	0.86	0.08	75,75,75,75	0
55	MG	2a	1786	1/1	0.86	0.12	72,72,72,72	0
55	MG	2A	3693	1/1	0.86	0.06	78,78,78,78	0
55	MG	1a	3153	1/1	0.86	0.12	66,66,66,66	0
55	MG	1A	3322	1/1	0.86	0.17	49,49,49,49	0
55	MG	1a	3164	1/1	0.86	0.20	68,68,68,68	0
55	MG	2A	3512	1/1	0.86	0.59	59,59,59,59	0
55	MG	2A	3078	1/1	0.86	0.23	50,50,50,50	0
55	MG	1a	3007	1/1	0.86	0.28	71,71,71,71	0
55	MG	1A	3602	1/1	0.86	0.18	56,56,56,56	0
55	MG	2A	3721	1/1	0.86	0.23	50,50,50,50	0
55	MG	2A	3098	1/1	0.86	0.23	60,60,60,60	0
55	MG	1A	3217	1/1	0.87	0.45	35,35,35,35	0
55	MG	28	102	1/1	0.87	0.07	73,73,73,73	0
55	MG	2A	3139	1/1	0.87	0.20	51,51,51,51	0
55	MG	2A	3140	1/1	0.87	0.34	56,56,56,56	0
55	MG	1A	3859	1/1	0.87	0.19	81,81,81,81	0
55	MG	2A	3756	1/1	0.87	0.64	86,86,86,86	0
55	MG	2A	3563	1/1	0.87	0.28	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1a	3139	1/1	0.87	0.28	67,67,67,67	0
55	MG	1A	3607	1/1	0.87	0.19	67,67,67,67	0
55	MG	1A	3049	1/1	0.87	0.57	36,36,36,36	0
55	MG	2a	1618	1/1	0.87	0.59	66,66,66,66	0
55	MG	1A	3866	1/1	0.87	0.25	62,62,62,62	0
55	MG	1A	3532	1/1	0.87	0.13	56,56,56,56	0
55	MG	2A	3583	1/1	0.87	0.11	72,72,72,72	0
55	MG	2A	3782	1/1	0.87	0.19	79,79,79,79	0
55	MG	2A	3783	1/1	0.87	0.31	93,93,93,93	0
55	MG	1a	3028	1/1	0.87	0.30	63,63,63,63	0
55	MG	2a	1642	1/1	0.87	0.16	82,82,82,82	0
55	MG	1A	3870	1/1	0.87	0.36	54,54,54,54	0
55	MG	1A	3063	1/1	0.87	0.52	45,45,45,45	0
55	MG	2A	3033	1/1	0.87	0.62	66,66,66,66	0
55	MG	1A	3255	1/1	0.87	0.23	41,41,41,41	0
55	MG	2A	3037	1/1	0.87	0.43	48,48,48,48	0
55	MG	1A	3546	1/1	0.87	0.24	40,40,40,40	0
55	MG	1a	3040	1/1	0.87	0.25	73,73,73,73	0
55	MG	2A	3043	1/1	0.87	0.18	68,68,68,68	0
55	MG	1a	3163	1/1	0.87	0.16	79,79,79,79	0
55	MG	1A	3052	1/1	0.87	0.54	24,24,24,24	0
55	MG	1D	306	1/1	0.87	0.22	45,45,45,45	0
55	MG	2a	1676	1/1	0.87	0.14	65,65,65,65	0
55	MG	1D	310	1/1	0.87	0.13	68,68,68,68	0
55	MG	1A	3235	1/1	0.87	0.42	72,72,72,72	0
55	MG	1A	3054	1/1	0.87	0.22	41,41,41,41	0
55	MG	2a	1707	1/1	0.87	0.10	82,82,82,82	0
55	MG	2A	3445	1/1	0.87	0.41	61,61,61,61	0
55	MG	2A	3448	1/1	0.87	0.15	80,80,80,80	0
55	MG	1a	3054	1/1	0.87	0.19	79,79,79,79	0
55	MG	2a	1717	1/1	0.87	0.06	71,71,71,71	0
55	MG	2A	3063	1/1	0.87	0.22	65,65,65,65	0
55	MG	1A	3638	1/1	0.87	0.25	35,35,35,35	0
55	MG	1A	3836	1/1	0.87	0.14	54,54,54,54	0
55	MG	1A	3889	1/1	0.87	0.09	55,55,55,55	0
55	MG	1A	3239	1/1	0.87	0.45	50,50,50,50	0
55	MG	1a	3199	1/1	0.87	0.14	71,71,71,71	0
55	MG	1A	3089	1/1	0.87	0.19	48,48,48,48	0
55	MG	1A	3090	1/1	0.87	0.22	41,41,41,41	0
55	MG	2A	3661	1/1	0.87	0.11	88,88,88,88	0
55	MG	2A	3094	1/1	0.87	1.35	58,58,58,58	0
55	MG	1A	3044	1/1	0.87	0.23	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1R	203	1/1	0.87	0.26	48,48,48,48	0
55	MG	2a	1734	1/1	0.87	0.06	73,73,73,73	0
55	MG	1A	3406	1/1	0.87	0.21	37,37,37,37	0
55	MG	2A	3673	1/1	0.87	0.22	70,70,70,70	0
55	MG	1A	3568	1/1	0.87	0.29	53,53,53,53	0
55	MG	2A	3244	1/1	0.87	0.06	87,87,87,87	0
55	MG	1A	3193	1/1	0.87	0.36	29,29,29,29	0
55	MG	2A	3254	1/1	0.87	0.12	87,87,87,87	0
55	MG	1A	3853	1/1	0.87	0.09	22,22,22,22	0
55	MG	2A	3256	1/1	0.87	0.14	61,61,61,61	0
55	MG	1a	3225	1/1	0.87	0.10	74,74,74,74	0
55	MG	2G	3001	1/1	0.87	0.19	82,82,82,82	0
55	MG	1A	3579	1/1	0.87	0.52	41,41,41,41	0
55	MG	2A	3114	1/1	0.87	0.40	62,62,62,62	0
55	MG	2A	3528	1/1	0.87	0.09	67,67,67,67	0
55	MG	1A	3764	1/1	0.87	0.09	41,41,41,41	0
55	MG	2A	3705	1/1	0.87	0.21	65,65,65,65	0
55	MG	1a	3096	1/1	0.87	0.17	81,81,81,81	0
55	MG	1a	3097	1/1	0.87	0.10	58,58,58,58	0
55	MG	2a	1792	1/1	0.87	0.20	74,74,74,74	0
55	MG	2A	3536	1/1	0.87	0.15	62,62,62,62	0
55	MG	2A	3537	1/1	0.87	0.73	65,65,65,65	0
55	MG	1A	3929	1/1	0.87	0.64	40,40,40,40	0
55	MG	2A	3540	1/1	0.87	0.07	70,70,70,70	0
55	MG	1A	3299	1/1	0.87	0.21	37,37,37,37	0
55	MG	1a	3124	1/1	0.87	0.30	88,88,88,88	0
55	MG	1B	203	1/1	0.87	0.25	66,66,66,66	0
55	MG	2q	201	1/1	0.87	0.39	63,63,63,63	0
55	MG	2A	3736	1/1	0.87	0.14	88,88,88,88	0
55	MG	2A	3004	1/1	0.87	0.23	52,52,52,52	0
55	MG	2A	3134	1/1	0.88	0.89	70,70,70,70	0
55	MG	1a	3133	1/1	0.88	0.42	77,77,77,77	0
55	MG	1A	3594	1/1	0.88	0.18	59,59,59,59	0
55	MG	1A	3922	1/1	0.88	0.21	39,39,39,39	0
55	MG	1A	3159	1/1	0.88	0.87	40,40,40,40	0
55	MG	2A	3732	1/1	0.88	0.56	60,60,60,60	0
55	MG	2A	3544	1/1	0.88	0.14	89,89,89,89	0
55	MG	1A	3176	1/1	0.88	0.29	45,45,45,45	0
55	MG	2A	3547	1/1	0.88	0.06	67,67,67,67	0
55	MG	2A	3318	1/1	0.88	0.06	77,77,77,77	0
55	MG	1A	3940	1/1	0.88	0.23	40,40,40,40	0
55	MG	2A	3753	1/1	0.88	0.09	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2a	1616	1/1	0.88	0.12	55,55,55,55	0
55	MG	2A	3144	1/1	0.88	0.15	78,78,78,78	0
55	MG	1A	3606	1/1	0.88	0.23	62,62,62,62	0
55	MG	2a	1621	1/1	0.88	0.11	80,80,80,80	0
55	MG	2A	3757	1/1	0.88	0.25	64,64,64,64	0
55	MG	2A	3762	1/1	0.88	0.63	57,57,57,57	0
55	MG	1A	3220	1/1	0.88	0.22	61,61,61,61	0
55	MG	2a	1637	1/1	0.88	0.48	87,87,87,87	0
55	MG	1A	3515	1/1	0.88	0.28	63,63,63,63	0
55	MG	1A	3517	1/1	0.88	0.20	51,51,51,51	0
55	MG	1a	3035	1/1	0.88	1.05	69,69,69,69	0
55	MG	2A	3568	1/1	0.88	0.31	46,46,46,46	0
55	MG	1A	3198	1/1	0.88	0.26	30,30,30,30	0
55	MG	2A	3576	1/1	0.88	0.52	57,57,57,57	0
55	MG	2A	3157	1/1	0.88	0.26	63,63,63,63	0
55	MG	2a	1647	1/1	0.88	0.23	60,60,60,60	0
55	MG	1a	3154	1/1	0.88	0.12	90,90,90,90	0
55	MG	2a	1649	1/1	0.88	0.11	71,71,71,71	0
55	MG	1A	3521	1/1	0.88	0.30	66,66,66,66	0
55	MG	1A	3384	1/1	0.88	0.11	70,70,70,70	0
55	MG	1A	3234	1/1	0.88	0.26	43,43,43,43	0
55	MG	2A	3794	1/1	0.88	0.10	70,70,70,70	0
55	MG	1A	3737	1/1	0.88	0.39	38,38,38,38	0
55	MG	2A	3400	1/1	0.88	0.28	77,77,77,77	0
55	MG	1A	3749	1/1	0.88	0.10	50,50,50,50	0
55	MG	2A	3596	1/1	0.88	0.16	63,63,63,63	0
55	MG	1A	3160	1/1	0.88	0.26	52,52,52,52	0
55	MG	1a	3179	1/1	0.88	0.04	73,73,73,73	0
55	MG	2A	3420	1/1	0.88	0.15	58,58,58,58	0
55	MG	1A	3032	1/1	0.88	0.39	53,53,53,53	0
55	MG	1A	3203	1/1	0.88	0.36	38,38,38,38	0
55	MG	2A	3174	1/1	0.88	0.39	47,47,47,47	0
55	MG	1D	308	1/1	0.88	0.13	46,46,46,46	0
55	MG	2A	3437	1/1	0.88	0.06	75,75,75,75	0
55	MG	1A	3285	1/1	0.88	0.22	49,49,49,49	0
55	MG	1A	3644	1/1	0.88	0.43	51,51,51,51	0
55	MG	1A	3206	1/1	0.88	0.28	42,42,42,42	0
55	MG	2A	3446	1/1	0.88	0.13	78,78,78,78	0
55	MG	1A	3774	1/1	0.88	0.22	79,79,79,79	0
55	MG	2A	3185	1/1	0.88	0.44	65,65,65,65	0
55	MG	2A	3637	1/1	0.88	0.05	63,63,63,63	0
55	MG	2A	3455	1/1	0.88	0.25	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1a	3200	1/1	0.88	0.08	87,87,87,87	0
55	MG	2A	3642	1/1	0.88	0.07	80,80,80,80	0
55	MG	2A	3080	1/1	0.88	0.26	66,66,66,66	0
55	MG	1A	3442	1/1	0.88	0.13	80,80,80,80	0
55	MG	1A	3792	1/1	0.88	0.08	63,63,63,63	0
55	MG	1A	3443	1/1	0.88	0.27	59,59,59,59	0
55	MG	2A	3653	1/1	0.88	0.23	70,70,70,70	0
55	MG	1A	3078	1/1	0.88	0.29	50,50,50,50	0
55	MG	2B	3016	1/1	0.88	0.29	81,81,81,81	0
55	MG	2a	1751	1/1	0.88	0.12	77,77,77,77	0
55	MG	1A	3667	1/1	0.88	0.09	74,74,74,74	0
55	MG	2A	3102	1/1	0.88	0.39	55,55,55,55	0
55	MG	1a	3072	1/1	0.88	0.09	59,59,59,59	0
55	MG	2a	1756	1/1	0.88	0.17	76,76,76,76	0
55	MG	1A	3079	1/1	0.88	0.78	45,45,45,45	0
55	MG	2A	3234	1/1	0.88	0.10	71,71,71,71	0
55	MG	1R	201	1/1	0.88	0.22	59,59,59,59	0
55	MG	1A	3312	1/1	0.88	0.17	61,61,61,61	0
55	MG	1W	3001	1/1	0.88	0.31	44,44,44,44	0
55	MG	2A	3498	1/1	0.88	0.11	68,68,68,68	0
55	MG	1A	3080	1/1	0.88	0.32	45,45,45,45	0
55	MG	1A	3682	1/1	0.88	0.44	61,61,61,61	0
55	MG	2a	1788	1/1	0.88	0.10	83,83,83,83	0
55	MG	1A	3823	1/1	0.88	0.16	32,32,32,32	0
55	MG	2A	3127	1/1	0.88	0.18	76,76,76,76	0
55	MG	1a	3106	1/1	0.88	0.06	56,56,56,56	0
55	MG	1A	3476	1/1	0.88	0.10	33,33,33,33	0
55	MG	1A	3011	1/1	0.88	0.49	48,48,48,48	0
55	MG	2A	3520	1/1	0.88	0.15	70,70,70,70	0
55	MG	2A	3523	1/1	0.88	0.07	65,65,65,65	0
55	MG	2A	3524	1/1	0.88	0.10	47,47,47,47	0
55	MG	1A	3038	1/1	0.88	0.23	50,50,50,50	0
55	MG	1A	3116	1/1	0.88	0.14	49,49,49,49	0
55	MG	1A	3348	1/1	0.88	0.09	42,42,42,42	0
55	MG	2A	3291	1/1	0.88	0.17	40,40,40,40	0
55	MG	2A	3005	1/1	0.89	0.20	47,47,47,47	0
55	MG	1A	3328	1/1	0.89	0.10	40,40,40,40	0
55	MG	1a	3084	1/1	0.89	0.30	58,58,58,58	0
55	MG	2A	3646	1/1	0.89	0.36	57,57,57,57	0
55	MG	1A	3790	1/1	0.89	0.07	38,38,38,38	0
55	MG	1A	3333	1/1	0.89	0.19	29,29,29,29	0
55	MG	2U	201	1/1	0.89	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3225	1/1	0.89	0.20	32,32,32,32	0
55	MG	1A	3074	1/1	0.89	0.68	39,39,39,39	0
55	MG	2A	3026	1/1	0.89	0.14	37,37,37,37	0
55	MG	1A	3204	1/1	0.89	0.30	43,43,43,43	0
55	MG	1a	3120	1/1	0.89	0.08	65,65,65,65	0
55	MG	20	105	1/1	0.89	0.21	80,80,80,80	0
55	MG	1A	3571	1/1	0.89	0.45	33,33,33,33	0
55	MG	25	101	1/1	0.89	0.31	58,58,58,58	0
55	MG	2A	3456	1/1	0.89	0.25	91,91,91,91	0
55	MG	1A	3263	1/1	0.89	0.15	48,48,48,48	0
55	MG	15	202	1/1	0.89	0.25	39,39,39,39	0
55	MG	1a	3132	1/1	0.89	0.11	71,71,71,71	0
55	MG	1A	3902	1/1	0.89	0.32	25,25,25,25	0
55	MG	1A	3576	1/1	0.89	0.16	77,77,77,77	0
55	MG	2a	1602	1/1	0.89	0.40	76,76,76,76	0
55	MG	1A	3577	1/1	0.89	0.18	68,68,68,68	0
55	MG	2A	3469	1/1	0.89	0.09	62,62,62,62	0
55	MG	1a	3001	1/1	0.89	0.07	73,73,73,73	0
55	MG	2A	3689	1/1	0.89	0.18	66,66,66,66	0
55	MG	1A	3906	1/1	0.89	0.36	40,40,40,40	0
55	MG	2A	3046	1/1	0.89	0.10	72,72,72,72	0
55	MG	1A	3504	1/1	0.89	0.12	66,66,66,66	0
55	MG	2A	3480	1/1	0.89	0.16	65,65,65,65	0
55	MG	1A	3586	1/1	0.89	0.19	60,60,60,60	0
55	MG	2A	3189	1/1	0.89	0.33	53,53,53,53	0
55	MG	2A	3051	1/1	0.89	0.42	53,53,53,53	0
55	MG	1A	3830	1/1	0.89	0.07	51,51,51,51	0
55	MG	2a	1630	1/1	0.89	0.16	83,83,83,83	0
55	MG	2A	3195	1/1	0.89	0.18	60,60,60,60	0
55	MG	1A	3588	1/1	0.89	0.06	41,41,41,41	0
55	MG	2A	3055	1/1	0.89	0.30	56,56,56,56	0
55	MG	2A	3502	1/1	0.89	0.52	69,69,69,69	0
55	MG	2A	3505	1/1	0.89	0.25	44,44,44,44	0
55	MG	2A	3201	1/1	0.89	0.27	50,50,50,50	0
55	MG	1A	3704	1/1	0.89	0.34	57,57,57,57	0
55	MG	2A	3207	1/1	0.89	0.15	65,65,65,65	0
55	MG	1A	3205	1/1	0.89	0.19	34,34,34,34	0
55	MG	1A	3598	1/1	0.89	0.13	76,76,76,76	0
55	MG	2A	3740	1/1	0.89	0.26	78,78,78,78	0
55	MG	2A	3742	1/1	0.89	0.59	61,61,61,61	0
55	MG	1A	3838	1/1	0.89	0.22	46,46,46,46	0
55	MG	2a	1651	1/1	0.89	0.77	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3521	1/1	0.89	0.13	74,74,74,74	0
55	MG	2A	3522	1/1	0.89	0.15	67,67,67,67	0
55	MG	2A	3066	1/1	0.89	0.29	64,64,64,64	0
55	MG	1a	3029	1/1	0.89	0.14	55,55,55,55	0
55	MG	2A	3525	1/1	0.89	0.18	77,77,77,77	0
55	MG	2A	3236	1/1	0.89	0.09	65,65,65,65	0
55	MG	1a	3030	1/1	0.89	1.08	75,75,75,75	0
55	MG	2A	3242	1/1	0.89	0.07	75,75,75,75	0
55	MG	1a	3032	1/1	0.89	0.16	39,39,39,39	0
55	MG	1a	3166	1/1	0.89	0.13	70,70,70,70	0
55	MG	1A	3944	1/1	0.89	0.77	47,47,47,47	0
55	MG	2A	3083	1/1	0.89	0.29	60,60,60,60	0
55	MG	1a	3170	1/1	0.89	0.22	80,80,80,80	0
55	MG	1a	3173	1/1	0.89	0.23	68,68,68,68	0
55	MG	2A	3091	1/1	0.89	0.23	52,52,52,52	0
55	MG	1A	3717	1/1	0.89	0.16	69,69,69,69	0
55	MG	2A	3095	1/1	0.89	0.23	58,58,58,58	0
55	MG	1A	3719	1/1	0.89	0.10	70,70,70,70	0
55	MG	2A	3552	1/1	0.89	0.55	57,57,57,57	0
55	MG	2A	3271	1/1	0.89	0.10	58,58,58,58	0
55	MG	1A	3507	1/1	0.89	0.32	32,32,32,32	0
55	MG	1A	3055	1/1	0.89	0.21	48,48,48,48	0
55	MG	1B	213	1/1	0.89	0.09	54,54,54,54	0
55	MG	1A	3273	1/1	0.89	0.11	35,35,35,35	0
55	MG	1A	3004	1/1	0.89	0.16	50,50,50,50	0
55	MG	2A	3107	1/1	0.89	0.12	58,58,58,58	0
55	MG	2A	3567	1/1	0.89	0.22	72,72,72,72	0
55	MG	1A	3404	1/1	0.89	0.15	62,62,62,62	0
55	MG	2a	1735	1/1	0.89	0.17	74,74,74,74	0
55	MG	2A	3569	1/1	0.89	0.17	56,56,56,56	0
55	MG	1A	3050	1/1	0.89	0.25	37,37,37,37	0
55	MG	2A	3112	1/1	0.89	1.04	68,68,68,68	0
55	MG	2A	3315	1/1	0.89	0.12	68,68,68,68	0
55	MG	1A	3084	1/1	0.89	0.56	43,43,43,43	0
55	MG	2A	3322	1/1	0.89	0.21	69,69,69,69	0
55	MG	1a	3052	1/1	0.89	0.30	59,59,59,59	0
55	MG	1A	3732	1/1	0.89	0.70	34,34,34,34	0
55	MG	1a	3055	1/1	0.89	0.32	44,44,44,44	0
55	MG	2A	3588	1/1	0.89	0.17	66,66,66,66	0
55	MG	2A	3332	1/1	0.89	0.18	63,63,63,63	0
55	MG	2A	3593	1/1	0.89	0.23	72,72,72,72	0
55	MG	1A	3172	1/1	0.89	0.53	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3308	1/1	0.89	0.31	38,38,38,38	0
55	MG	1A	3441	1/1	0.89	0.17	21,21,21,21	0
55	MG	2a	1776	1/1	0.89	0.09	74,74,74,74	0
55	MG	1A	3214	1/1	0.89	0.23	33,33,33,33	0
55	MG	1a	3064	1/1	0.89	0.34	82,82,82,82	0
55	MG	1a	3065	1/1	0.89	0.53	67,67,67,67	0
55	MG	2A	3359	1/1	0.89	0.08	64,64,64,64	0
55	MG	1A	3865	1/1	0.89	0.11	82,82,82,82	0
55	MG	1A	3173	1/1	0.89	0.22	45,45,45,45	0
55	MG	1A	3051	1/1	0.89	0.17	35,35,35,35	0
55	MG	1A	3031	1/1	0.89	0.21	27,27,27,27	0
55	MG	1E	304	1/1	0.89	0.25	35,35,35,35	0
55	MG	2A	3393	1/1	0.89	0.14	67,67,67,67	0
55	MG	1A	3465	1/1	0.89	0.18	28,28,28,28	0
55	MG	1A	3163	1/1	0.89	0.27	69,69,69,69	0
55	MG	1o	3001	1/1	0.89	0.46	62,62,62,62	0
55	MG	1A	3029	1/1	0.89	0.17	39,39,39,39	0
55	MG	1A	3773	1/1	0.89	0.15	53,53,53,53	0
55	MG	1A	3659	1/1	0.89	0.33	61,61,61,61	0
55	MG	1A	3457	1/1	0.90	0.48	70,70,70,70	0
55	MG	2A	3320	1/1	0.90	0.17	71,71,71,71	0
55	MG	1A	3244	1/1	0.90	0.28	49,49,49,49	0
55	MG	2A	3021	1/1	0.90	0.27	50,50,50,50	0
55	MG	2A	3719	1/1	0.90	0.07	67,67,67,67	0
55	MG	1A	3937	1/1	0.90	1.57	52,52,52,52	0
55	MG	1A	3161	1/1	0.90	0.66	38,38,38,38	0
55	MG	1A	3584	1/1	0.90	0.08	48,48,48,48	0
55	MG	2A	3729	1/1	0.90	0.42	72,72,72,72	0
55	MG	1A	3755	1/1	0.90	0.18	44,44,44,44	0
55	MG	1a	3148	1/1	0.90	0.23	88,88,88,88	0
55	MG	1A	3756	1/1	0.90	0.16	38,38,38,38	0
55	MG	2a	1614	1/1	0.90	0.42	61,61,61,61	0
55	MG	1A	3402	1/1	0.90	0.07	62,62,62,62	0
55	MG	1a	3031	1/1	0.90	0.12	71,71,71,71	0
55	MG	2A	3550	1/1	0.90	0.11	75,75,75,75	0
55	MG	2a	1619	1/1	0.90	0.57	76,76,76,76	0
55	MG	2A	3744	1/1	0.90	0.26	72,72,72,72	0
55	MG	2A	3344	1/1	0.90	0.12	78,78,78,78	0
55	MG	1A	3474	1/1	0.90	0.20	50,50,50,50	0
55	MG	1A	3759	1/1	0.90	0.19	61,61,61,61	0
55	MG	1A	3077	1/1	0.90	0.29	48,48,48,48	0
55	MG	2a	1634	1/1	0.90	0.34	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2a	1635	1/1	0.90	0.60	81,81,81,81	0
55	MG	2A	3556	1/1	0.90	0.15	63,63,63,63	0
55	MG	1A	3674	1/1	0.90	0.39	51,51,51,51	0
55	MG	1a	3161	1/1	0.90	0.60	67,67,67,67	0
55	MG	1A	3067	1/1	0.90	0.74	47,47,47,47	0
55	MG	1A	3600	1/1	0.90	0.46	81,81,81,81	0
55	MG	1A	3534	1/1	0.90	0.09	40,40,40,40	0
55	MG	2A	3395	1/1	0.90	0.12	76,76,76,76	0
55	MG	2A	3398	1/1	0.90	0.10	45,45,45,45	0
55	MG	1A	3782	1/1	0.90	0.14	59,59,59,59	0
55	MG	2A	3403	1/1	0.90	0.05	67,67,67,67	0
55	MG	2A	3404	1/1	0.90	0.11	47,47,47,47	0
55	MG	1B	226	1/1	0.90	0.11	72,72,72,72	0
55	MG	2a	1650	1/1	0.90	0.08	84,84,84,84	0
55	MG	1A	3689	1/1	0.90	0.16	62,62,62,62	0
55	MG	1a	3174	1/1	0.90	0.11	70,70,70,70	0
55	MG	2A	3417	1/1	0.90	0.12	52,52,52,52	0
55	MG	1A	3874	1/1	0.90	0.17	67,67,67,67	0
55	MG	2A	3059	1/1	0.90	1.20	55,55,55,55	0
55	MG	2A	3180	1/1	0.90	0.43	72,72,72,72	0
55	MG	2A	3590	1/1	0.90	0.38	63,63,63,63	0
55	MG	2a	1671	1/1	0.90	0.16	80,80,80,80	0
55	MG	1A	3478	1/1	0.90	0.12	33,33,33,33	0
55	MG	1A	3791	1/1	0.90	0.16	58,58,58,58	0
55	MG	2a	1686	1/1	0.90	0.20	61,61,61,61	0
55	MG	1A	3409	1/1	0.90	0.17	48,48,48,48	0
55	MG	2A	3072	1/1	0.90	0.64	64,64,64,64	0
55	MG	2A	3074	1/1	0.90	0.39	51,51,51,51	0
55	MG	1a	3183	1/1	0.90	0.15	82,82,82,82	0
55	MG	2a	1709	1/1	0.90	0.16	87,87,87,87	0
55	MG	1A	3493	1/1	0.90	0.14	46,46,46,46	0
55	MG	2a	1712	1/1	0.90	0.40	68,68,68,68	0
55	MG	1A	3237	1/1	0.90	0.28	42,42,42,42	0
55	MG	2A	3452	1/1	0.90	0.11	63,63,63,63	0
55	MG	1A	3498	1/1	0.90	0.41	67,67,67,67	0
55	MG	1A	3621	1/1	0.90	0.14	58,58,58,58	0
55	MG	2A	3611	1/1	0.90	0.30	79,79,79,79	0
55	MG	2A	3822	1/1	0.90	0.78	65,65,65,65	0
55	MG	2a	1723	1/1	0.90	0.21	98,98,98,98	0
55	MG	1A	3087	1/1	0.90	0.46	34,34,34,34	0
55	MG	1A	3888	1/1	0.90	0.28	54,54,54,54	0
55	MG	2A	3832	1/1	0.90	0.90	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3500	1/1	0.90	0.14	67,67,67,67	0
55	MG	1A	3553	1/1	0.90	0.06	47,47,47,47	0
55	MG	2A	3211	1/1	0.90	0.15	64,64,64,64	0
55	MG	1F	311	1/1	0.90	0.22	67,67,67,67	0
55	MG	1A	3369	1/1	0.90	0.16	70,70,70,70	0
55	MG	2A	3097	1/1	0.90	0.23	39,39,39,39	0
55	MG	2A	3470	1/1	0.90	0.17	75,75,75,75	0
55	MG	1a	3213	1/1	0.90	0.16	67,67,67,67	0
55	MG	2a	1740	1/1	0.90	0.06	73,73,73,73	0
55	MG	1A	3722	1/1	0.90	0.08	50,50,50,50	0
55	MG	1A	3371	1/1	0.90	0.12	62,62,62,62	0
55	MG	1A	3900	1/1	0.90	0.45	57,57,57,57	0
55	MG	1U	203	1/1	0.90	0.19	51,51,51,51	0
55	MG	2A	3649	1/1	0.90	0.38	52,52,52,52	0
55	MG	1A	3831	1/1	0.90	0.20	43,43,43,43	0
55	MG	1A	3098	1/1	0.90	0.21	37,37,37,37	0
55	MG	1A	3833	1/1	0.90	0.13	70,70,70,70	0
55	MG	10	107	1/1	0.90	0.43	46,46,46,46	0
55	MG	1A	3276	1/1	0.90	0.23	35,35,35,35	0
55	MG	2a	1765	1/1	0.90	0.07	88,88,88,88	0
55	MG	2a	1767	1/1	0.90	0.09	74,74,74,74	0
55	MG	1A	3508	1/1	0.90	0.12	72,72,72,72	0
55	MG	2A	3666	1/1	0.90	0.07	63,63,63,63	0
55	MG	2A	3500	1/1	0.90	0.11	78,78,78,78	0
55	MG	1A	3909	1/1	0.90	0.28	38,38,38,38	0
55	MG	1A	3383	1/1	0.90	0.14	53,53,53,53	0
55	MG	2a	1777	1/1	0.90	0.05	85,85,85,85	0
55	MG	2A	3118	1/1	0.90	0.39	54,54,54,54	0
55	MG	2A	3267	1/1	0.90	0.13	50,50,50,50	0
55	MG	2A	3508	1/1	0.90	0.97	52,52,52,52	0
55	MG	1l	201	1/1	0.90	0.14	71,71,71,71	0
55	MG	2a	1789	1/1	0.90	0.53	82,82,82,82	0
55	MG	2A	3511	1/1	0.90	0.17	54,54,54,54	0
55	MG	18	3301	1/1	0.90	0.62	64,64,64,64	0
55	MG	1A	3914	1/1	0.90	0.33	68,68,68,68	0
55	MG	2A	3001	1/1	0.90	0.18	50,50,50,50	0
55	MG	1A	3730	1/1	0.90	0.10	75,75,75,75	0
55	MG	1A	3061	1/1	0.90	0.14	36,36,36,36	0
55	MG	2h	3001	1/1	0.90	0.56	64,64,64,64	0
55	MG	1A	3921	1/1	0.90	0.44	40,40,40,40	0
55	MG	1a	3130	1/1	0.90	0.34	75,75,75,75	0
55	MG	2l	202	1/1	0.90	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3575	1/1	0.90	0.56	45,45,45,45	0
55	MG	2A	3700	1/1	0.90	0.15	79,79,79,79	0
55	MG	1A	3926	1/1	0.90	0.64	44,44,44,44	0
55	MG	1a	3009	1/1	0.90	0.89	62,62,62,62	0
55	MG	1A	3549	1/1	0.91	0.24	52,52,52,52	0
55	MG	1A	3489	1/1	0.91	0.19	46,46,46,46	0
55	MG	2A	3146	1/1	0.91	0.66	57,57,57,57	0
55	MG	1A	3913	1/1	0.91	0.42	64,64,64,64	0
55	MG	2A	3720	1/1	0.91	0.36	58,58,58,58	0
55	MG	2A	3541	1/1	0.91	0.14	85,85,85,85	0
55	MG	1A	3146	1/1	0.91	0.19	39,39,39,39	0
55	MG	2a	1609	1/1	0.91	0.20	46,46,46,46	0
55	MG	1A	3047	1/1	0.91	0.37	45,45,45,45	0
55	MG	1a	3135	1/1	0.91	0.26	77,77,77,77	0
55	MG	1A	3064	1/1	0.91	0.39	59,59,59,59	0
55	MG	1A	3426	1/1	0.91	0.12	72,72,72,72	0
55	MG	1A	3183	1/1	0.91	0.21	44,44,44,44	0
55	MG	2A	3358	1/1	0.91	0.15	59,59,59,59	0
55	MG	2A	3158	1/1	0.91	0.74	56,56,56,56	0
55	MG	1A	3924	1/1	0.91	0.93	43,43,43,43	0
55	MG	2A	3743	1/1	0.91	0.22	48,48,48,48	0
55	MG	1A	3565	1/1	0.91	0.17	26,26,26,26	0
55	MG	2A	3747	1/1	0.91	0.09	78,78,78,78	0
55	MG	1A	3168	1/1	0.91	0.27	56,56,56,56	0
55	MG	1A	3931	1/1	0.91	0.32	35,35,35,35	0
55	MG	2A	3559	1/1	0.91	0.10	51,51,51,51	0
55	MG	1a	3017	1/1	0.91	0.40	75,75,75,75	0
55	MG	1A	3132	1/1	0.91	0.60	34,34,34,34	0
55	MG	2A	3167	1/1	0.91	0.60	56,56,56,56	0
55	MG	1A	3934	1/1	0.91	0.30	30,30,30,30	0
55	MG	1A	3744	1/1	0.91	0.05	55,55,55,55	0
55	MG	1A	3747	1/1	0.91	0.14	66,66,66,66	0
55	MG	2A	3572	1/1	0.91	0.16	51,51,51,51	0
55	MG	1a	3026	1/1	0.91	0.30	64,64,64,64	0
55	MG	2A	3769	1/1	0.91	0.13	66,66,66,66	0
55	MG	2A	3405	1/1	0.91	0.23	60,60,60,60	0
55	MG	1A	3657	1/1	0.91	0.32	45,45,45,45	0
55	MG	1A	3151	1/1	0.91	0.27	48,48,48,48	0
55	MG	1A	3133	1/1	0.91	0.13	62,62,62,62	0
55	MG	1A	3275	1/1	0.91	0.20	38,38,38,38	0
55	MG	1a	3165	1/1	0.91	0.78	74,74,74,74	0
55	MG	2a	1653	1/1	0.91	0.44	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3115	1/1	0.91	0.14	69,69,69,69	0
55	MG	2A	3062	1/1	0.91	0.29	56,56,56,56	0
55	MG	1A	3668	1/1	0.91	0.55	63,63,63,63	0
55	MG	1A	3453	1/1	0.91	0.08	51,51,51,51	0
55	MG	2a	1661	1/1	0.91	0.17	74,74,74,74	0
55	MG	1A	3277	1/1	0.91	0.20	56,56,56,56	0
55	MG	1A	3863	1/1	0.91	0.28	68,68,68,68	0
55	MG	2A	3799	1/1	0.91	0.25	97,97,97,97	0
55	MG	2A	3440	1/1	0.91	0.11	78,78,78,78	0
55	MG	2a	1683	1/1	0.91	0.21	79,79,79,79	0
55	MG	2A	3193	1/1	0.91	0.09	80,80,80,80	0
55	MG	2A	3073	1/1	0.91	0.35	52,52,52,52	0
55	MG	1A	3455	1/1	0.91	0.15	21,21,21,21	0
55	MG	1A	3216	1/1	0.91	0.46	50,50,50,50	0
55	MG	1A	3526	1/1	0.91	0.08	52,52,52,52	0
55	MG	1A	3527	1/1	0.91	0.22	56,56,56,56	0
55	MG	2A	3812	1/1	0.91	0.53	68,68,68,68	0
55	MG	2A	3202	1/1	0.91	0.25	59,59,59,59	0
55	MG	1A	3593	1/1	0.91	0.05	63,63,63,63	0
55	MG	1A	3372	1/1	0.91	0.11	68,68,68,68	0
55	MG	1A	3789	1/1	0.91	0.12	89,89,89,89	0
55	MG	2A	3615	1/1	0.91	0.23	59,59,59,59	0
55	MG	1a	3188	1/1	0.91	0.24	65,65,65,65	0
55	MG	2A	3824	1/1	0.91	0.38	55,55,55,55	0
55	MG	2A	3624	1/1	0.91	0.34	55,55,55,55	0
55	MG	2A	3221	1/1	0.91	0.49	68,68,68,68	0
55	MG	2A	3831	1/1	0.91	1.10	52,52,52,52	0
55	MG	1D	307	1/1	0.91	0.38	22,22,22,22	0
55	MG	1a	3053	1/1	0.91	0.23	76,76,76,76	0
55	MG	1A	3529	1/1	0.91	0.07	45,45,45,45	0
55	MG	2A	3636	1/1	0.91	0.06	67,67,67,67	0
55	MG	1A	3281	1/1	0.91	0.14	31,31,31,31	0
55	MG	2A	3472	1/1	0.91	0.11	55,55,55,55	0
55	MG	1A	3014	1/1	0.91	0.40	41,41,41,41	0
55	MG	1A	3068	1/1	0.91	0.51	41,41,41,41	0
55	MG	1A	3883	1/1	0.91	0.06	58,58,58,58	0
55	MG	1A	3885	1/1	0.91	0.21	33,33,33,33	0
55	MG	1A	3802	1/1	0.91	0.09	41,41,41,41	0
55	MG	1A	3705	1/1	0.91	0.12	53,53,53,53	0
55	MG	2A	3648	1/1	0.91	0.08	39,39,39,39	0
55	MG	1A	3289	1/1	0.91	0.19	33,33,33,33	0
55	MG	1A	3711	1/1	0.91	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3651	1/1	0.91	0.23	56,56,56,56	0
55	MG	2A	3487	1/1	0.91	0.23	75,75,75,75	0
55	MG	1F	310	1/1	0.91	0.40	43,43,43,43	0
55	MG	2D	310	1/1	0.91	0.27	61,61,61,61	0
55	MG	2E	301	1/1	0.91	0.15	47,47,47,47	0
55	MG	2a	1764	1/1	0.91	0.50	70,70,70,70	0
55	MG	1A	3110	1/1	0.91	0.29	41,41,41,41	0
55	MG	2A	3660	1/1	0.91	0.15	80,80,80,80	0
55	MG	1A	3893	1/1	0.91	0.23	66,66,66,66	0
55	MG	1A	3111	1/1	0.91	0.22	55,55,55,55	0
55	MG	1A	3812	1/1	0.91	0.09	32,32,32,32	0
55	MG	1A	3718	1/1	0.91	0.11	46,46,46,46	0
55	MG	2A	3268	1/1	0.91	0.18	54,54,54,54	0
55	MG	2H	201	1/1	0.91	0.72	95,95,95,95	0
55	MG	2a	1779	1/1	0.91	0.20	85,85,85,85	0
55	MG	1U	202	1/1	0.91	0.32	34,34,34,34	0
55	MG	2A	3124	1/1	0.91	0.95	53,53,53,53	0
55	MG	1A	3545	1/1	0.91	0.21	30,30,30,30	0
55	MG	2A	3288	1/1	0.91	0.32	67,67,67,67	0
55	MG	1A	3615	1/1	0.91	0.04	50,50,50,50	0
55	MG	2a	1790	1/1	0.91	0.23	72,72,72,72	0
55	MG	1W	3002	1/1	0.91	0.27	51,51,51,51	0
55	MG	2A	3296	1/1	0.91	0.16	60,60,60,60	0
55	MG	2b	3001	1/1	0.91	0.18	79,79,79,79	0
55	MG	1a	3092	1/1	0.91	0.09	86,86,86,86	0
55	MG	2X	103	1/1	0.91	0.13	58,58,58,58	0
55	MG	1A	3825	1/1	0.91	0.08	67,67,67,67	0
55	MG	10	102	1/1	0.91	0.26	69,69,69,69	0
55	MG	1A	3826	1/1	0.91	0.07	65,65,65,65	0
55	MG	1a	3113	1/1	0.91	0.26	65,65,65,65	0
55	MG	10	105	1/1	0.91	0.14	63,63,63,63	0
55	MG	2A	3526	1/1	0.91	0.19	64,64,64,64	0
55	MG	10	106	1/1	0.91	0.06	73,73,73,73	0
55	MG	1A	3178	1/1	0.91	0.53	37,37,37,37	0
55	MG	1A	3488	1/1	0.91	0.22	64,64,64,64	0
56	ZN	24	501	1/1	0.91	0.14	132,132,132,132	0
55	MG	1a	3127	1/1	0.91	0.16	52,52,52,52	0
55	MG	2W	3001	1/1	0.92	0.25	57,57,57,57	0
55	MG	2A	3485	1/1	0.92	0.81	57,57,57,57	0
55	MG	1A	3037	1/1	0.92	0.11	51,51,51,51	0
55	MG	2A	3092	1/1	0.92	0.52	49,49,49,49	0
55	MG	1a	3185	1/1	0.92	0.21	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3493	1/1	0.92	0.09	75,75,75,75	0
55	MG	1A	3688	1/1	0.92	0.17	76,76,76,76	0
55	MG	1a	3051	1/1	0.92	0.39	59,59,59,59	0
55	MG	1A	3192	1/1	0.92	0.32	51,51,51,51	0
55	MG	1A	3690	1/1	0.92	0.14	21,21,21,21	0
55	MG	1A	3692	1/1	0.92	0.09	40,40,40,40	0
55	MG	1A	3800	1/1	0.92	0.06	65,65,65,65	0
55	MG	1A	3695	1/1	0.92	0.09	33,33,33,33	0
55	MG	1F	305	1/1	0.92	0.11	35,35,35,35	0
55	MG	1A	3241	1/1	0.92	0.28	32,32,32,32	0
55	MG	1a	3060	1/1	0.92	0.41	74,74,74,74	0
55	MG	1A	3596	1/1	0.92	0.17	83,83,83,83	0
55	MG	2A	3702	1/1	0.92	0.17	38,38,38,38	0
55	MG	1a	3215	1/1	0.92	0.23	74,74,74,74	0
55	MG	1A	3048	1/1	0.92	0.16	29,29,29,29	0
55	MG	1A	3894	1/1	0.92	0.04	87,87,87,87	0
55	MG	1A	3467	1/1	0.92	0.23	59,59,59,59	0
55	MG	1a	3067	1/1	0.92	0.06	66,66,66,66	0
55	MG	2A	3119	1/1	0.92	0.22	47,47,47,47	0
55	MG	1H	8002	1/1	0.92	0.19	58,58,58,58	0
55	MG	1N	8001	1/1	0.92	0.26	49,49,49,49	0
55	MG	1A	3144	1/1	0.92	0.26	33,33,33,33	0
55	MG	2A	3724	1/1	0.92	0.14	46,46,46,46	0
55	MG	1A	3145	1/1	0.92	0.15	60,60,60,60	0
55	MG	2A	3529	1/1	0.92	0.37	48,48,48,48	0
55	MG	1d	503	1/1	0.92	0.27	72,72,72,72	0
55	MG	1R	202	1/1	0.92	0.32	51,51,51,51	0
55	MG	2a	1631	1/1	0.92	0.42	52,52,52,52	0
55	MG	2A	3316	1/1	0.92	0.27	69,69,69,69	0
55	MG	1A	3814	1/1	0.92	0.25	46,46,46,46	0
55	MG	1A	3041	1/1	0.92	0.25	63,63,63,63	0
55	MG	1a	3076	1/1	0.92	0.20	69,69,69,69	0
55	MG	2A	3539	1/1	0.92	0.13	64,64,64,64	0
55	MG	1A	3820	1/1	0.92	0.24	45,45,45,45	0
55	MG	1A	3250	1/1	0.92	0.42	43,43,43,43	0
55	MG	1A	3714	1/1	0.92	0.04	80,80,80,80	0
55	MG	1A	3537	1/1	0.92	0.25	63,63,63,63	0
55	MG	1a	3087	1/1	0.92	0.11	63,63,63,63	0
55	MG	1A	3388	1/1	0.92	0.17	26,26,26,26	0
55	MG	2A	3548	1/1	0.92	0.05	72,72,72,72	0
55	MG	1A	3105	1/1	0.92	0.29	35,35,35,35	0
55	MG	1A	3480	1/1	0.92	0.28	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3342	1/1	0.92	0.19	49,49,49,49	0
55	MG	1a	3101	1/1	0.92	0.13	46,46,46,46	0
55	MG	2A	3764	1/1	0.92	0.13	80,80,80,80	0
55	MG	1A	3394	1/1	0.92	0.66	75,75,75,75	0
55	MG	2A	3149	1/1	0.92	0.23	58,58,58,58	0
55	MG	2A	3348	1/1	0.92	0.16	59,59,59,59	0
55	MG	2A	3355	1/1	0.92	0.14	58,58,58,58	0
55	MG	1A	3548	1/1	0.92	0.19	47,47,47,47	0
55	MG	2A	3772	1/1	0.92	0.10	68,68,68,68	0
55	MG	1A	3307	1/1	0.92	0.19	37,37,37,37	0
55	MG	2a	1662	1/1	0.92	0.30	61,61,61,61	0
55	MG	2A	3360	1/1	0.92	0.20	58,58,58,58	0
55	MG	2A	3015	1/1	0.92	0.36	46,46,46,46	0
55	MG	1A	3399	1/1	0.92	0.05	65,65,65,65	0
55	MG	2A	3155	1/1	0.92	0.64	42,42,42,42	0
55	MG	1A	3022	1/1	0.92	0.24	28,28,28,28	0
55	MG	2A	3786	1/1	0.92	0.14	66,66,66,66	0
55	MG	2a	1694	1/1	0.92	0.26	77,77,77,77	0
55	MG	2A	3025	1/1	0.92	0.23	53,53,53,53	0
55	MG	15	203	1/1	0.92	0.32	45,45,45,45	0
55	MG	2a	1699	1/1	0.92	0.14	67,67,67,67	0
55	MG	1A	3633	1/1	0.92	0.22	48,48,48,48	0
55	MG	2A	3396	1/1	0.92	0.04	64,64,64,64	0
55	MG	2A	3397	1/1	0.92	0.16	83,83,83,83	0
55	MG	1A	3221	1/1	0.92	0.60	32,32,32,32	0
55	MG	2A	3029	1/1	0.92	0.53	72,72,72,72	0
55	MG	2A	3584	1/1	0.92	0.18	65,65,65,65	0
55	MG	1A	3928	1/1	0.92	0.22	32,32,32,32	0
55	MG	1A	3405	1/1	0.92	0.08	59,59,59,59	0
55	MG	2A	3805	1/1	0.92	0.22	68,68,68,68	0
55	MG	19	103	1/1	0.92	0.21	63,63,63,63	0
55	MG	2A	3809	1/1	0.92	0.28	45,45,45,45	0
55	MG	2A	3034	1/1	0.92	0.17	58,58,58,58	0
55	MG	2a	1724	1/1	0.92	0.23	92,92,92,92	0
55	MG	1A	3639	1/1	0.92	0.28	30,30,30,30	0
55	MG	2A	3415	1/1	0.92	0.19	69,69,69,69	0
55	MG	1A	3554	1/1	0.92	0.18	15,15,15,15	0
55	MG	1A	3119	1/1	0.92	0.39	35,35,35,35	0
55	MG	2A	3419	1/1	0.92	0.18	58,58,58,58	0
55	MG	2A	3818	1/1	0.92	0.49	69,69,69,69	0
55	MG	1A	3136	1/1	0.92	0.62	42,42,42,42	0
55	MG	1A	3938	1/1	0.92	0.24	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3741	1/1	0.92	0.41	56,56,56,56	0
55	MG	2A	3823	1/1	0.92	0.79	53,53,53,53	0
55	MG	2A	3425	1/1	0.92	0.27	67,67,67,67	0
55	MG	1A	3942	1/1	0.92	0.32	32,32,32,32	0
55	MG	2A	3827	1/1	0.92	0.67	58,58,58,58	0
55	MG	2a	1744	1/1	0.92	0.36	69,69,69,69	0
55	MG	1A	3648	1/1	0.92	0.19	33,33,33,33	0
55	MG	2A	3830	1/1	0.92	0.70	65,65,65,65	0
55	MG	2a	1748	1/1	0.92	0.10	85,85,85,85	0
55	MG	2A	3432	1/1	0.92	0.15	58,58,58,58	0
55	MG	2A	3434	1/1	0.92	0.14	78,78,78,78	0
55	MG	2A	3181	1/1	0.92	0.58	67,67,67,67	0
55	MG	1A	3945	1/1	0.92	0.22	56,56,56,56	0
55	MG	2A	3616	1/1	0.92	0.06	57,57,57,57	0
55	MG	1A	3425	1/1	0.92	0.10	46,46,46,46	0
55	MG	2A	3441	1/1	0.92	0.29	88,88,88,88	0
55	MG	2A	3626	1/1	0.92	0.21	68,68,68,68	0
55	MG	1A	3228	1/1	0.92	0.20	76,76,76,76	0
55	MG	1a	3024	1/1	0.92	0.31	61,61,61,61	0
55	MG	2A	3632	1/1	0.92	0.37	94,94,94,94	0
55	MG	1A	3232	1/1	0.92	0.34	68,68,68,68	0
55	MG	2a	1772	1/1	0.92	0.10	81,81,81,81	0
55	MG	1a	3027	1/1	0.92	0.89	75,75,75,75	0
55	MG	2a	1774	1/1	0.92	0.07	65,65,65,65	0
55	MG	1A	3120	1/1	0.92	0.24	54,54,54,54	0
55	MG	1A	3860	1/1	0.92	0.22	56,56,56,56	0
55	MG	2A	3060	1/1	0.92	0.35	48,48,48,48	0
55	MG	2A	3640	1/1	0.92	0.17	76,76,76,76	0
55	MG	2A	3196	1/1	0.92	0.12	75,75,75,75	0
55	MG	2D	303	1/1	0.92	0.26	54,54,54,54	0
55	MG	1A	3186	1/1	0.92	0.10	58,58,58,58	0
55	MG	1A	3156	1/1	0.92	0.10	53,53,53,53	0
55	MG	1A	3344	1/1	0.92	0.20	54,54,54,54	0
55	MG	1A	3057	1/1	0.92	0.18	26,26,26,26	0
55	MG	1A	3353	1/1	0.92	0.25	62,62,62,62	0
55	MG	1A	3519	1/1	0.92	0.23	52,52,52,52	0
55	MG	2F	307	1/1	0.92	0.83	58,58,58,58	0
55	MG	1a	3169	1/1	0.92	0.25	90,90,90,90	0
55	MG	1A	3583	1/1	0.92	0.09	59,59,59,59	0
55	MG	1A	3772	1/1	0.92	0.11	48,48,48,48	0
55	MG	1A	3678	1/1	0.92	0.23	40,40,40,40	0
55	MG	1A	3679	1/1	0.92	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1a	3043	1/1	0.92	0.61	66,66,66,66	0
55	MG	2A	3476	1/1	0.92	0.17	67,67,67,67	0
55	MG	2A	3231	1/1	0.92	0.17	74,74,74,74	0
55	MG	1a	3044	1/1	0.92	0.17	62,62,62,62	0
55	MG	2A	3665	1/1	0.92	0.09	54,54,54,54	0
55	MG	1A	3238	1/1	0.92	0.15	37,37,37,37	0
55	MG	2U	202	1/1	0.92	0.54	60,60,60,60	0
55	MG	1A	3522	1/1	0.92	0.30	57,57,57,57	0
55	MG	2Q	202	1/1	0.93	0.13	65,65,65,65	0
55	MG	2A	3662	1/1	0.93	0.07	65,65,65,65	0
55	MG	1A	3395	1/1	0.93	0.05	68,68,68,68	0
55	MG	2A	3086	1/1	0.93	0.42	60,60,60,60	0
55	MG	2A	3483	1/1	0.93	0.26	44,44,44,44	0
55	MG	2A	3253	1/1	0.93	0.09	66,66,66,66	0
55	MG	2A	3089	1/1	0.93	0.15	58,58,58,58	0
55	MG	1F	307	1/1	0.93	0.69	34,34,34,34	0
55	MG	1A	3817	1/1	0.93	0.08	21,21,21,21	0
55	MG	1A	3247	1/1	0.93	0.26	47,47,47,47	0
55	MG	2A	3489	1/1	0.93	0.26	38,38,38,38	0
55	MG	2A	3492	1/1	0.93	0.28	46,46,46,46	0
55	MG	2A	3680	1/1	0.93	0.12	63,63,63,63	0
55	MG	1a	3189	1/1	0.93	0.17	81,81,81,81	0
55	MG	1a	3193	1/1	0.93	0.41	75,75,75,75	0
55	MG	25	102	1/1	0.93	0.31	63,63,63,63	0
55	MG	2A	3684	1/1	0.93	0.13	61,61,61,61	0
55	MG	1A	3821	1/1	0.93	0.13	64,64,64,64	0
55	MG	1A	3470	1/1	0.93	0.26	52,52,52,52	0
55	MG	1A	3006	1/1	0.93	0.20	26,26,26,26	0
55	MG	1A	3329	1/1	0.93	0.11	30,30,30,30	0
55	MG	1A	3523	1/1	0.93	0.40	70,70,70,70	0
55	MG	1A	3905	1/1	0.93	0.09	58,58,58,58	0
55	MG	2A	3278	1/1	0.93	0.13	53,53,53,53	0
55	MG	1a	3205	1/1	0.93	0.06	78,78,78,78	0
55	MG	2A	3701	1/1	0.93	0.09	59,59,59,59	0
55	MG	2A	3510	1/1	0.93	0.12	82,82,82,82	0
55	MG	1Q	203	1/1	0.93	0.19	49,49,49,49	0
55	MG	1Q	204	1/1	0.93	0.16	51,51,51,51	0
55	MG	2A	3293	1/1	0.93	0.30	72,72,72,72	0
55	MG	2a	1613	1/1	0.93	0.09	50,50,50,50	0
55	MG	2A	3514	1/1	0.93	0.30	50,50,50,50	0
55	MG	2A	3518	1/1	0.93	0.20	60,60,60,60	0
55	MG	2A	3295	1/1	0.93	0.10	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3649	1/1	0.93	0.39	52,52,52,52	0
55	MG	1A	3650	1/1	0.93	0.24	45,45,45,45	0
55	MG	1A	3652	1/1	0.93	0.08	67,67,67,67	0
55	MG	2A	3723	1/1	0.93	0.07	70,70,70,70	0
55	MG	1U	201	1/1	0.93	0.30	56,56,56,56	0
55	MG	1A	3100	1/1	0.93	0.33	31,31,31,31	0
55	MG	1a	3219	1/1	0.93	0.22	68,68,68,68	0
55	MG	1A	3017	1/1	0.93	0.25	31,31,31,31	0
55	MG	1A	3042	1/1	0.93	0.23	32,32,32,32	0
55	MG	1a	3224	1/1	0.93	0.25	60,60,60,60	0
55	MG	1A	3479	1/1	0.93	0.11	31,31,31,31	0
55	MG	1Y	502	1/1	0.93	0.07	68,68,68,68	0
55	MG	1A	3735	1/1	0.93	0.29	79,79,79,79	0
55	MG	2A	3535	1/1	0.93	0.08	67,67,67,67	0
55	MG	1A	3088	1/1	0.93	0.50	34,34,34,34	0
55	MG	1A	3355	1/1	0.93	0.17	22,22,22,22	0
55	MG	2A	3746	1/1	0.93	0.07	73,73,73,73	0
55	MG	1A	3483	1/1	0.93	0.32	56,56,56,56	0
55	MG	2A	3334	1/1	0.93	0.25	71,71,71,71	0
55	MG	1d	506	1/1	0.93	0.16	86,86,86,86	0
55	MG	2A	3750	1/1	0.93	0.14	60,60,60,60	0
55	MG	2A	3751	1/1	0.93	0.20	67,67,67,67	0
55	MG	1a	3081	1/1	0.93	0.23	76,76,76,76	0
55	MG	1A	3590	1/1	0.93	0.31	77,77,77,77	0
55	MG	1A	3485	1/1	0.93	0.30	56,56,56,56	0
55	MG	2A	3341	1/1	0.93	0.04	75,75,75,75	0
55	MG	1A	3750	1/1	0.93	0.21	55,55,55,55	0
55	MG	2A	3759	1/1	0.93	0.10	84,84,84,84	0
55	MG	1t	3001	1/1	0.93	0.21	64,64,64,64	0
55	MG	1A	3019	1/1	0.93	0.45	43,43,43,43	0
55	MG	2a	1660	1/1	0.93	0.15	74,74,74,74	0
55	MG	1A	3673	1/1	0.93	0.14	29,29,29,29	0
55	MG	1A	3595	1/1	0.93	0.43	35,35,35,35	0
55	MG	2a	1665	1/1	0.93	0.35	65,65,65,65	0
55	MG	2A	3354	1/1	0.93	0.19	41,41,41,41	0
55	MG	1a	3102	1/1	0.93	0.09	48,48,48,48	0
55	MG	2a	1675	1/1	0.93	0.22	83,83,83,83	0
55	MG	1A	3676	1/1	0.93	0.15	57,57,57,57	0
55	MG	2a	1677	1/1	0.93	0.16	61,61,61,61	0
55	MG	2a	1678	1/1	0.93	0.18	75,75,75,75	0
55	MG	2a	1681	1/1	0.93	0.10	53,53,53,53	0
55	MG	1a	3107	1/1	0.93	0.22	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3677	1/1	0.93	0.24	38,38,38,38	0
55	MG	2a	1685	1/1	0.93	0.09	77,77,77,77	0
55	MG	1A	3430	1/1	0.93	0.11	54,54,54,54	0
55	MG	2a	1688	1/1	0.93	0.09	58,58,58,58	0
55	MG	2a	1690	1/1	0.93	0.22	83,83,83,83	0
55	MG	2a	1691	1/1	0.93	0.18	64,64,64,64	0
55	MG	1A	3941	1/1	0.93	0.20	54,54,54,54	0
55	MG	2A	3780	1/1	0.93	0.08	54,54,54,54	0
55	MG	1A	3540	1/1	0.93	0.08	80,80,80,80	0
55	MG	1A	3490	1/1	0.93	0.21	50,50,50,50	0
55	MG	2a	1706	1/1	0.93	0.24	90,90,90,90	0
55	MG	2A	3017	1/1	0.93	0.37	65,65,65,65	0
55	MG	1a	3003	1/1	0.93	0.21	81,81,81,81	0
55	MG	1A	3543	1/1	0.93	0.30	39,39,39,39	0
55	MG	2A	3789	1/1	0.93	0.05	68,68,68,68	0
55	MG	2A	3024	1/1	0.93	0.76	60,60,60,60	0
55	MG	2A	3573	1/1	0.93	0.06	73,73,73,73	0
55	MG	1A	3770	1/1	0.93	0.05	64,64,64,64	0
55	MG	2A	3797	1/1	0.93	0.33	88,88,88,88	0
55	MG	1a	3006	1/1	0.93	0.16	72,72,72,72	0
55	MG	2A	3577	1/1	0.93	0.10	51,51,51,51	0
55	MG	1A	3864	1/1	0.93	0.05	53,53,53,53	0
55	MG	2A	3402	1/1	0.93	0.10	80,80,80,80	0
55	MG	1A	3358	1/1	0.93	0.13	24,24,24,24	0
55	MG	1a	3134	1/1	0.93	0.18	73,73,73,73	0
55	MG	1a	3010	1/1	0.93	0.25	60,60,60,60	0
55	MG	2A	3407	1/1	0.93	0.21	70,70,70,70	0
55	MG	2a	1728	1/1	0.93	0.18	81,81,81,81	0
55	MG	2A	3586	1/1	0.93	0.14	89,89,89,89	0
55	MG	2A	3409	1/1	0.93	0.10	88,88,88,88	0
55	MG	1A	3292	1/1	0.93	0.07	34,34,34,34	0
55	MG	1B	210	1/1	0.93	0.21	60,60,60,60	0
55	MG	1B	211	1/1	0.93	0.06	59,59,59,59	0
55	MG	1A	3297	1/1	0.93	0.25	26,26,26,26	0
55	MG	1A	3124	1/1	0.93	0.18	35,35,35,35	0
55	MG	2A	3040	1/1	0.93	0.18	53,53,53,53	0
55	MG	1a	3145	1/1	0.93	0.16	79,79,79,79	0
55	MG	2A	3601	1/1	0.93	0.13	59,59,59,59	0
55	MG	1a	3021	1/1	0.93	0.31	68,68,68,68	0
55	MG	1A	3053	1/1	0.93	0.38	32,32,32,32	0
55	MG	1B	219	1/1	0.93	0.13	47,47,47,47	0
55	MG	1A	3875	1/1	0.93	0.40	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2a	1749	1/1	0.93	0.04	72,72,72,72	0
55	MG	2A	3428	1/1	0.93	0.09	68,68,68,68	0
55	MG	2A	3048	1/1	0.93	0.14	46,46,46,46	0
55	MG	1A	3012	1/1	0.93	0.18	30,30,30,30	0
55	MG	1A	3617	1/1	0.93	0.42	47,47,47,47	0
55	MG	1A	3698	1/1	0.93	0.12	48,48,48,48	0
55	MG	1A	3310	1/1	0.93	0.15	64,64,64,64	0
55	MG	1A	3010	1/1	0.93	0.49	46,46,46,46	0
55	MG	2a	1760	1/1	0.93	0.23	71,71,71,71	0
55	MG	2a	1762	1/1	0.93	0.12	60,60,60,60	0
55	MG	2A	3837	1/1	0.93	0.77	53,53,53,53	0
55	MG	1D	302	1/1	0.93	0.33	44,44,44,44	0
55	MG	2A	3623	1/1	0.93	0.20	71,71,71,71	0
55	MG	2A	3056	1/1	0.93	0.22	47,47,47,47	0
55	MG	1a	3162	1/1	0.93	0.05	72,72,72,72	0
55	MG	1A	3222	1/1	0.93	0.12	46,46,46,46	0
55	MG	2B	3008	1/1	0.93	0.12	84,84,84,84	0
55	MG	2A	3447	1/1	0.93	0.39	47,47,47,47	0
55	MG	1a	3034	1/1	0.93	0.32	74,74,74,74	0
55	MG	1D	304	1/1	0.93	0.07	56,56,56,56	0
55	MG	2A	3061	1/1	0.93	0.87	71,71,71,71	0
55	MG	1A	3624	1/1	0.93	0.14	53,53,53,53	0
55	MG	1A	3884	1/1	0.93	0.12	22,22,22,22	0
55	MG	1A	3208	1/1	0.93	0.12	70,70,70,70	0
55	MG	2A	3214	1/1	0.93	0.16	76,76,76,76	0
55	MG	2A	3460	1/1	0.93	0.17	44,44,44,44	0
55	MG	1A	3707	1/1	0.93	0.18	55,55,55,55	0
55	MG	1a	3172	1/1	0.93	0.18	75,75,75,75	0
55	MG	2D	306	1/1	0.93	1.21	64,64,64,64	0
55	MG	2A	3225	1/1	0.93	0.11	52,52,52,52	0
55	MG	1A	3512	1/1	0.93	0.16	37,37,37,37	0
55	MG	2A	3468	1/1	0.93	0.15	64,64,64,64	0
55	MG	2F	302	1/1	0.93	0.26	58,58,58,58	0
55	MG	1A	3560	1/1	0.93	0.25	24,24,24,24	0
55	MG	1A	3114	1/1	0.93	0.08	59,59,59,59	0
55	MG	2A	3471	1/1	0.93	0.10	72,72,72,72	0
55	MG	2A	3233	1/1	0.93	0.19	48,48,48,48	0
55	MG	2A	3652	1/1	0.93	0.33	58,58,58,58	0
55	MG	1A	3634	1/1	0.93	0.13	44,44,44,44	0
55	MG	1A	3892	1/1	0.93	0.16	59,59,59,59	0
55	MG	2A	3657	1/1	0.93	0.09	55,55,55,55	0
55	MG	1A	3227	1/1	0.93	0.34	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1a	3182	1/1	0.93	0.65	76,76,76,76	0
55	MG	1F	304	1/1	0.93	0.67	41,41,41,41	0
55	MG	1A	3492	1/1	0.94	0.23	68,68,68,68	0
55	MG	2A	3018	1/1	0.94	0.80	48,48,48,48	0
55	MG	2A	3421	1/1	0.94	0.13	52,52,52,52	0
55	MG	1a	3109	1/1	0.94	0.30	60,60,60,60	0
55	MG	1A	3400	1/1	0.94	0.18	44,44,44,44	0
55	MG	1A	3401	1/1	0.94	0.12	43,43,43,43	0
55	MG	2A	3426	1/1	0.94	0.12	62,62,62,62	0
55	MG	2A	3175	1/1	0.94	0.26	50,50,50,50	0
55	MG	1a	3115	1/1	0.94	0.58	71,71,71,71	0
55	MG	2A	3430	1/1	0.94	0.30	54,54,54,54	0
55	MG	1a	3116	1/1	0.94	0.55	80,80,80,80	0
55	MG	2Q	201	1/1	0.94	0.05	77,77,77,77	0
55	MG	1A	3570	1/1	0.94	0.27	46,46,46,46	0
55	MG	2Q	203	1/1	0.94	0.34	55,55,55,55	0
55	MG	1a	3119	1/1	0.94	0.14	78,78,78,78	0
55	MG	2A	3436	1/1	0.94	0.12	82,82,82,82	0
55	MG	2S	201	1/1	0.94	0.52	70,70,70,70	0
55	MG	1A	3497	1/1	0.94	0.21	70,70,70,70	0
55	MG	1A	3256	1/1	0.94	0.35	47,47,47,47	0
55	MG	1A	3056	1/1	0.94	0.23	47,47,47,47	0
55	MG	1A	3794	1/1	0.94	0.26	46,46,46,46	0
55	MG	2A	3443	1/1	0.94	0.17	33,33,33,33	0
55	MG	2A	3186	1/1	0.94	0.40	72,72,72,72	0
55	MG	2A	3187	1/1	0.94	0.17	41,41,41,41	0
55	MG	1A	3033	1/1	0.94	0.42	52,52,52,52	0
55	MG	1A	3233	1/1	0.94	0.23	49,49,49,49	0
55	MG	2A	3191	1/1	0.94	0.20	64,64,64,64	0
55	MG	1A	3578	1/1	0.94	0.21	68,68,68,68	0
55	MG	2A	3453	1/1	0.94	0.12	74,74,74,74	0
55	MG	1A	3503	1/1	0.94	0.20	42,42,42,42	0
55	MG	1A	3580	1/1	0.94	0.24	70,70,70,70	0
55	MG	1A	3915	1/1	0.94	0.27	64,64,64,64	0
55	MG	1A	3408	1/1	0.94	0.21	43,43,43,43	0
55	MG	1A	3140	1/1	0.94	0.36	38,38,38,38	0
55	MG	2A	3198	1/1	0.94	0.23	19,19,19,19	0
55	MG	2A	3199	1/1	0.94	0.61	54,54,54,54	0
55	MG	1A	3506	1/1	0.94	0.18	51,51,51,51	0
55	MG	1a	3141	1/1	0.94	0.12	78,78,78,78	0
55	MG	1a	3002	1/1	0.94	0.21	44,44,44,44	0
55	MG	2A	3466	1/1	0.94	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3587	1/1	0.94	0.12	35,35,35,35	0
55	MG	1A	3420	1/1	0.94	0.17	37,37,37,37	0
55	MG	2A	3683	1/1	0.94	0.08	68,68,68,68	0
55	MG	2A	3052	1/1	0.94	0.23	59,59,59,59	0
55	MG	1A	3693	1/1	0.94	0.09	38,38,38,38	0
55	MG	2A	3687	1/1	0.94	0.18	46,46,46,46	0
55	MG	2A	3213	1/1	0.94	0.13	36,36,36,36	0
55	MG	1A	3262	1/1	0.94	0.15	41,41,41,41	0
55	MG	2a	1617	1/1	0.94	0.21	67,67,67,67	0
55	MG	2A	3219	1/1	0.94	0.14	64,64,64,64	0
55	MG	1A	3592	1/1	0.94	0.17	27,27,27,27	0
55	MG	1A	3930	1/1	0.94	0.22	25,25,25,25	0
55	MG	2A	3478	1/1	0.94	0.23	55,55,55,55	0
55	MG	2a	1622	1/1	0.94	0.39	61,61,61,61	0
55	MG	1A	3081	1/1	0.94	0.37	41,41,41,41	0
55	MG	2a	1626	1/1	0.94	0.51	68,68,68,68	0
55	MG	2a	1629	1/1	0.94	0.21	61,61,61,61	0
55	MG	2A	3227	1/1	0.94	0.28	50,50,50,50	0
55	MG	1a	3012	1/1	0.94	0.22	28,28,28,28	0
55	MG	2A	3704	1/1	0.94	0.08	57,57,57,57	0
55	MG	1A	3264	1/1	0.94	0.16	73,73,73,73	0
55	MG	1a	3014	1/1	0.94	0.17	67,67,67,67	0
55	MG	2A	3232	1/1	0.94	0.07	70,70,70,70	0
55	MG	2A	3709	1/1	0.94	0.12	49,49,49,49	0
55	MG	1a	3155	1/1	0.94	0.05	76,76,76,76	0
55	MG	1a	3016	1/1	0.94	0.24	77,77,77,77	0
55	MG	1a	3158	1/1	0.94	0.08	78,78,78,78	0
55	MG	2A	3239	1/1	0.94	0.18	38,38,38,38	0
55	MG	1a	3159	1/1	0.94	0.13	79,79,79,79	0
55	MG	1A	3265	1/1	0.94	0.17	81,81,81,81	0
55	MG	2A	3722	1/1	0.94	0.07	69,69,69,69	0
55	MG	2A	3496	1/1	0.94	0.16	85,85,85,85	0
55	MG	2A	3070	1/1	0.94	0.58	52,52,52,52	0
55	MG	1A	3516	1/1	0.94	0.15	77,77,77,77	0
55	MG	2A	3249	1/1	0.94	0.07	68,68,68,68	0
55	MG	1A	3341	1/1	0.94	0.15	31,31,31,31	0
55	MG	2A	3252	1/1	0.94	0.34	54,54,54,54	0
55	MG	1A	3599	1/1	0.94	0.54	46,46,46,46	0
55	MG	2A	3734	1/1	0.94	0.04	67,67,67,67	0
55	MG	2A	3735	1/1	0.94	0.16	55,55,55,55	0
55	MG	1A	3103	1/1	0.94	0.52	41,41,41,41	0
55	MG	1A	3709	1/1	0.94	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3345	1/1	0.94	0.14	24,24,24,24	0
55	MG	2A	3257	1/1	0.94	0.22	49,49,49,49	0
55	MG	1A	3835	1/1	0.94	0.07	51,51,51,51	0
55	MG	2a	1663	1/1	0.94	0.20	64,64,64,64	0
55	MG	1A	3347	1/1	0.94	0.23	28,28,28,28	0
55	MG	2a	1666	1/1	0.94	0.08	74,74,74,74	0
55	MG	1A	3605	1/1	0.94	0.05	63,63,63,63	0
55	MG	2a	1668	1/1	0.94	0.13	63,63,63,63	0
55	MG	1A	3122	1/1	0.94	0.58	27,27,27,27	0
55	MG	2a	1672	1/1	0.94	0.04	75,75,75,75	0
55	MG	1A	3351	1/1	0.94	0.08	66,66,66,66	0
55	MG	2A	3088	1/1	0.94	0.08	73,73,73,73	0
55	MG	1A	3524	1/1	0.94	0.17	55,55,55,55	0
55	MG	1A	3841	1/1	0.94	0.08	68,68,68,68	0
55	MG	2a	1679	1/1	0.94	0.43	64,64,64,64	0
55	MG	1A	3842	1/1	0.94	0.03	68,68,68,68	0
55	MG	1A	3450	1/1	0.94	0.31	71,71,71,71	0
55	MG	2A	3279	1/1	0.94	0.08	58,58,58,58	0
55	MG	2A	3755	1/1	0.94	0.20	63,63,63,63	0
55	MG	2A	3281	1/1	0.94	0.17	39,39,39,39	0
55	MG	2A	3283	1/1	0.94	0.15	47,47,47,47	0
55	MG	1a	3181	1/1	0.94	0.11	76,76,76,76	0
55	MG	1A	3612	1/1	0.94	0.12	77,77,77,77	0
55	MG	2A	3763	1/1	0.94	0.17	41,41,41,41	0
55	MG	2a	1695	1/1	0.94	0.31	65,65,65,65	0
55	MG	2A	3531	1/1	0.94	0.09	78,78,78,78	0
55	MG	1A	3847	1/1	0.94	0.14	61,61,61,61	0
55	MG	1A	3071	1/1	0.94	0.21	32,32,32,32	0
55	MG	2A	3099	1/1	0.94	0.23	52,52,52,52	0
55	MG	1A	3045	1/1	0.94	0.22	37,37,37,37	0
55	MG	1A	3851	1/1	0.94	0.08	29,29,29,29	0
55	MG	1A	3109	1/1	0.94	0.25	41,41,41,41	0
55	MG	1a	3042	1/1	0.94	0.20	63,63,63,63	0
55	MG	2a	1711	1/1	0.94	1.00	82,82,82,82	0
55	MG	1A	3128	1/1	0.94	0.17	33,33,33,33	0
55	MG	2a	1713	1/1	0.94	0.06	68,68,68,68	0
55	MG	1A	3726	1/1	0.94	0.28	39,39,39,39	0
55	MG	1A	3460	1/1	0.94	0.07	47,47,47,47	0
55	MG	1a	3047	1/1	0.94	0.15	64,64,64,64	0
55	MG	2A	3111	1/1	0.94	0.58	57,57,57,57	0
55	MG	2a	1720	1/1	0.94	0.18	66,66,66,66	0
55	MG	1A	3278	1/1	0.94	0.10	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3546	1/1	0.94	0.15	43,43,43,43	0
55	MG	1A	3046	1/1	0.94	0.24	13,13,13,13	0
55	MG	2A	3325	1/1	0.94	0.58	68,68,68,68	0
55	MG	1A	3194	1/1	0.94	0.16	54,54,54,54	0
55	MG	2A	3792	1/1	0.94	0.16	77,77,77,77	0
55	MG	1a	3204	1/1	0.94	0.05	70,70,70,70	0
55	MG	2A	3117	1/1	0.94	0.22	56,56,56,56	0
55	MG	1A	3469	1/1	0.94	0.16	62,62,62,62	0
55	MG	2A	3333	1/1	0.94	0.08	69,69,69,69	0
55	MG	1A	3016	1/1	0.94	0.26	18,18,18,18	0
55	MG	2A	3335	1/1	0.94	0.11	70,70,70,70	0
55	MG	2A	3557	1/1	0.94	0.07	55,55,55,55	0
55	MG	1D	309	1/1	0.94	0.23	31,31,31,31	0
55	MG	2A	3125	1/1	0.94	0.18	66,66,66,66	0
55	MG	2a	1736	1/1	0.94	0.34	74,74,74,74	0
55	MG	1A	3471	1/1	0.94	0.08	67,67,67,67	0
55	MG	2a	1738	1/1	0.94	0.05	77,77,77,77	0
55	MG	1A	3196	1/1	0.94	0.11	32,32,32,32	0
55	MG	1A	3740	1/1	0.94	0.09	63,63,63,63	0
55	MG	1E	301	1/1	0.94	0.36	40,40,40,40	0
55	MG	1A	3375	1/1	0.94	0.11	69,69,69,69	0
55	MG	1A	3742	1/1	0.94	0.12	55,55,55,55	0
55	MG	1a	3220	1/1	0.94	0.10	60,60,60,60	0
55	MG	1A	3076	1/1	0.94	0.48	43,43,43,43	0
55	MG	2A	3350	1/1	0.94	0.22	54,54,54,54	0
55	MG	1A	3872	1/1	0.94	0.12	32,32,32,32	0
55	MG	1F	303	1/1	0.94	0.28	44,44,44,44	0
55	MG	2A	3356	1/1	0.94	0.21	51,51,51,51	0
55	MG	1A	3873	1/1	0.94	0.11	59,59,59,59	0
55	MG	1A	3745	1/1	0.94	0.16	30,30,30,30	0
55	MG	1A	3746	1/1	0.94	0.05	52,52,52,52	0
55	MG	2A	3363	1/1	0.94	0.24	43,43,43,43	0
55	MG	2A	3364	1/1	0.94	0.07	34,34,34,34	0
55	MG	2a	1763	1/1	0.94	0.10	55,55,55,55	0
55	MG	2A	3373	1/1	0.94	0.15	76,76,76,76	0
55	MG	1A	3290	1/1	0.94	0.17	52,52,52,52	0
55	MG	1A	3018	1/1	0.94	0.19	30,30,30,30	0
55	MG	1A	3645	1/1	0.94	0.24	35,35,35,35	0
55	MG	2A	3833	1/1	0.94	0.19	57,57,57,57	0
55	MG	2A	3379	1/1	0.94	0.07	76,76,76,76	0
55	MG	1A	3294	1/1	0.94	0.13	25,25,25,25	0
55	MG	1A	3390	1/1	0.94	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3390	1/1	0.94	0.10	48,48,48,48	0
55	MG	2A	3598	1/1	0.94	0.15	70,70,70,70	0
55	MG	1A	3481	1/1	0.94	0.14	35,35,35,35	0
55	MG	1A	3251	1/1	0.94	0.30	34,34,34,34	0
55	MG	1P	201	1/1	0.94	0.23	30,30,30,30	0
55	MG	2a	1782	1/1	0.94	0.16	75,75,75,75	0
55	MG	1A	3393	1/1	0.94	0.17	48,48,48,48	0
55	MG	2B	3009	1/1	0.94	0.12	79,79,79,79	0
55	MG	1A	3653	1/1	0.94	0.15	42,42,42,42	0
55	MG	1A	3200	1/1	0.94	0.31	37,37,37,37	0
55	MG	1a	3082	1/1	0.94	0.24	58,58,58,58	0
55	MG	1A	3761	1/1	0.94	0.61	43,43,43,43	0
55	MG	1A	3486	1/1	0.94	0.30	43,43,43,43	0
55	MG	1A	3094	1/1	0.94	0.48	34,34,34,34	0
55	MG	1A	3202	1/1	0.94	0.43	49,49,49,49	0
55	MG	2A	3408	1/1	0.94	0.15	48,48,48,48	0
55	MG	2D	301	1/1	0.94	0.58	49,49,49,49	0
55	MG	2f	8001	1/1	0.94	0.16	56,56,56,56	0
55	MG	1A	3663	1/1	0.94	0.22	68,68,68,68	0
55	MG	2A	3617	1/1	0.94	0.14	35,35,35,35	0
55	MG	2A	3619	1/1	0.94	0.11	57,57,57,57	0
55	MG	2A	3163	1/1	0.94	0.26	60,60,60,60	0
55	MG	2D	307	1/1	0.94	0.41	60,60,60,60	0
55	MG	1A	3562	1/1	0.94	0.23	52,52,52,52	0
55	MG	2o	3001	1/1	0.94	0.13	57,57,57,57	0
55	MG	1A	3043	1/1	0.94	0.33	13,13,13,13	0
55	MG	2E	304	1/1	0.94	0.15	71,71,71,71	0
55	MG	1A	3775	1/1	0.94	0.06	47,47,47,47	0
55	MG	2A	3168	1/1	0.94	0.27	72,72,72,72	0
55	MG	1A	3274	1/1	0.95	0.29	8,8,8,8	0
55	MG	1A	3008	1/1	0.95	0.26	48,48,48,48	0
55	MG	1A	3415	1/1	0.95	0.11	26,26,26,26	0
55	MG	1a	3202	1/1	0.95	0.07	53,53,53,53	0
55	MG	2A	3467	1/1	0.95	0.16	76,76,76,76	0
55	MG	2A	3096	1/1	0.95	0.34	48,48,48,48	0
55	MG	1A	3828	1/1	0.95	0.19	70,70,70,70	0
55	MG	1A	3362	1/1	0.95	0.29	42,42,42,42	0
55	MG	1A	3184	1/1	0.95	0.72	38,38,38,38	0
55	MG	2A	3100	1/1	0.95	0.33	61,61,61,61	0
55	MG	1A	3097	1/1	0.95	0.36	42,42,42,42	0
55	MG	2A	3676	1/1	0.95	0.36	76,76,76,76	0
55	MG	2A	3677	1/1	0.95	0.17	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3429	1/1	0.95	0.12	41,41,41,41	0
55	MG	2A	3679	1/1	0.95	0.05	71,71,71,71	0
55	MG	1A	3153	1/1	0.95	0.47	36,36,36,36	0
55	MG	1A	3916	1/1	0.95	0.87	49,49,49,49	0
55	MG	2A	3477	1/1	0.95	0.12	81,81,81,81	0
55	MG	2A	3261	1/1	0.95	0.29	52,52,52,52	0
55	MG	2A	3262	1/1	0.95	0.19	71,71,71,71	0
55	MG	1A	3917	1/1	0.95	0.41	38,38,38,38	0
55	MG	2A	3264	1/1	0.95	0.16	61,61,61,61	0
55	MG	2A	3265	1/1	0.95	0.40	69,69,69,69	0
55	MG	2A	3106	1/1	0.95	0.31	67,67,67,67	0
55	MG	2a	1606	1/1	0.95	0.45	57,57,57,57	0
55	MG	1X	8001	1/1	0.95	0.11	27,27,27,27	0
55	MG	2A	3108	1/1	0.95	0.10	65,65,65,65	0
55	MG	2A	3269	1/1	0.95	0.18	38,38,38,38	0
55	MG	1A	3373	1/1	0.95	0.33	53,53,53,53	0
55	MG	2A	3274	1/1	0.95	0.16	51,51,51,51	0
55	MG	1a	3080	1/1	0.95	0.17	67,67,67,67	0
55	MG	1A	3601	1/1	0.95	0.07	38,38,38,38	0
55	MG	1A	3025	1/1	0.95	0.31	32,32,32,32	0
55	MG	1A	3675	1/1	0.95	0.12	65,65,65,65	0
55	MG	10	104	1/1	0.95	0.10	73,73,73,73	0
55	MG	1A	3434	1/1	0.95	0.14	46,46,46,46	0
55	MG	2A	3285	1/1	0.95	0.08	46,46,46,46	0
55	MG	2A	3711	1/1	0.95	0.08	67,67,67,67	0
55	MG	1a	3093	1/1	0.95	0.06	68,68,68,68	0
55	MG	2A	3715	1/1	0.95	0.07	63,63,63,63	0
55	MG	2A	3503	1/1	0.95	0.24	58,58,58,58	0
55	MG	1A	3925	1/1	0.95	0.17	42,42,42,42	0
55	MG	2A	3718	1/1	0.95	0.09	78,78,78,78	0
55	MG	1A	3320	1/1	0.95	0.30	52,52,52,52	0
55	MG	1A	3927	1/1	0.95	0.30	34,34,34,34	0
55	MG	1A	3379	1/1	0.95	0.19	67,67,67,67	0
55	MG	2A	3126	1/1	0.95	0.30	62,62,62,62	0
55	MG	1e	3001	1/1	0.95	0.26	61,61,61,61	0
55	MG	1f	8001	1/1	0.95	0.21	61,61,61,61	0
55	MG	15	201	1/1	0.95	0.57	46,46,46,46	0
55	MG	1A	3099	1/1	0.95	0.29	62,62,62,62	0
55	MG	2a	1640	1/1	0.95	0.52	50,50,50,50	0
55	MG	2A	3304	1/1	0.95	0.23	41,41,41,41	0
55	MG	1h	3002	1/1	0.95	0.12	73,73,73,73	0
55	MG	2A	3314	1/1	0.95	0.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3733	1/1	0.95	0.13	65,65,65,65	0
55	MG	1a	3108	1/1	0.95	0.04	75,75,75,75	0
55	MG	1A	3680	1/1	0.95	0.08	53,53,53,53	0
55	MG	15	205	1/1	0.95	0.09	62,62,62,62	0
55	MG	1A	3754	1/1	0.95	0.11	71,71,71,71	0
55	MG	2A	3738	1/1	0.95	0.07	62,62,62,62	0
55	MG	2A	3137	1/1	0.95	0.40	58,58,58,58	0
55	MG	1A	3846	1/1	0.95	0.14	53,53,53,53	0
55	MG	1A	3681	1/1	0.95	0.24	57,57,57,57	0
55	MG	2A	3003	1/1	0.95	0.08	35,35,35,35	0
55	MG	2A	3530	1/1	0.95	0.13	71,71,71,71	0
55	MG	1A	3325	1/1	0.95	0.19	22,22,22,22	0
55	MG	2a	1656	1/1	0.95	0.06	78,78,78,78	0
55	MG	1A	3060	1/1	0.95	0.26	38,38,38,38	0
55	MG	2A	3143	1/1	0.95	0.20	59,59,59,59	0
55	MG	2A	3007	1/1	0.95	0.25	61,61,61,61	0
55	MG	1A	3610	1/1	0.95	0.10	68,68,68,68	0
55	MG	1A	3852	1/1	0.95	0.21	22,22,22,22	0
55	MG	1A	3447	1/1	0.95	0.18	24,24,24,24	0
55	MG	1A	3448	1/1	0.95	0.17	19,19,19,19	0
55	MG	2A	3012	1/1	0.95	0.18	42,42,42,42	0
55	MG	1A	3616	1/1	0.95	0.08	63,63,63,63	0
55	MG	2A	3014	1/1	0.95	0.74	58,58,58,58	0
55	MG	1A	3763	1/1	0.95	0.10	70,70,70,70	0
55	MG	1A	3691	1/1	0.95	0.09	42,42,42,42	0
55	MG	2a	1673	1/1	0.95	0.16	59,59,59,59	0
55	MG	2A	3345	1/1	0.95	0.07	78,78,78,78	0
55	MG	1a	3008	1/1	0.95	0.21	76,76,76,76	0
55	MG	1A	3858	1/1	0.95	0.12	60,60,60,60	0
55	MG	2A	3020	1/1	0.95	0.10	42,42,42,42	0
55	MG	2A	3351	1/1	0.95	0.06	69,69,69,69	0
55	MG	2a	1680	1/1	0.95	0.10	63,63,63,63	0
55	MG	1A	3449	1/1	0.95	0.10	41,41,41,41	0
55	MG	2A	3770	1/1	0.95	0.04	74,74,74,74	0
55	MG	2A	3022	1/1	0.95	0.14	72,72,72,72	0
55	MG	2A	3023	1/1	0.95	0.53	47,47,47,47	0
55	MG	1B	208	1/1	0.95	0.23	68,68,68,68	0
55	MG	1a	3138	1/1	0.95	0.15	66,66,66,66	0
55	MG	1B	209	1/1	0.95	0.23	59,59,59,59	0
55	MG	2A	3361	1/1	0.95	0.15	53,53,53,53	0
55	MG	2a	1692	1/1	0.95	0.23	82,82,82,82	0
55	MG	2A	3781	1/1	0.95	0.12	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3362	1/1	0.95	0.10	56,56,56,56	0
55	MG	1A	3767	1/1	0.95	0.13	52,52,52,52	0
55	MG	2A	3561	1/1	0.95	0.06	82,82,82,82	0
55	MG	1A	3768	1/1	0.95	0.08	58,58,58,58	0
55	MG	2a	1701	1/1	0.95	0.23	85,85,85,85	0
55	MG	2a	1702	1/1	0.95	0.10	72,72,72,72	0
55	MG	2a	1704	1/1	0.95	0.18	76,76,76,76	0
55	MG	2A	3365	1/1	0.95	0.09	81,81,81,81	0
55	MG	2A	3369	1/1	0.95	0.08	81,81,81,81	0
55	MG	2A	3565	1/1	0.95	0.49	70,70,70,70	0
55	MG	2A	3372	1/1	0.95	0.14	54,54,54,54	0
55	MG	1A	3385	1/1	0.95	0.07	69,69,69,69	0
55	MG	1A	3771	1/1	0.95	0.21	38,38,38,38	0
55	MG	2A	3570	1/1	0.95	0.29	54,54,54,54	0
55	MG	2A	3171	1/1	0.95	0.34	45,45,45,45	0
55	MG	2A	3377	1/1	0.95	0.15	54,54,54,54	0
55	MG	2a	1716	1/1	0.95	0.23	75,75,75,75	0
55	MG	1A	3386	1/1	0.95	0.26	49,49,49,49	0
55	MG	1A	3069	1/1	0.95	0.32	34,34,34,34	0
55	MG	1A	3009	1/1	0.95	0.29	32,32,32,32	0
55	MG	2A	3384	1/1	0.95	0.18	37,37,37,37	0
55	MG	2A	3580	1/1	0.95	0.11	71,71,71,71	0
55	MG	1A	3456	1/1	0.95	0.16	49,49,49,49	0
55	MG	2A	3386	1/1	0.95	0.15	63,63,63,63	0
55	MG	2A	3388	1/1	0.95	0.17	47,47,47,47	0
55	MG	1A	3780	1/1	0.95	0.54	34,34,34,34	0
55	MG	2A	3038	1/1	0.95	0.22	54,54,54,54	0
55	MG	1A	3117	1/1	0.95	0.09	61,61,61,61	0
55	MG	1A	3783	1/1	0.95	0.17	44,44,44,44	0
55	MG	1A	3703	1/1	0.95	0.10	42,42,42,42	0
55	MG	1A	3787	1/1	0.95	0.08	48,48,48,48	0
55	MG	1A	3788	1/1	0.95	0.14	28,28,28,28	0
55	MG	1A	3459	1/1	0.95	0.08	65,65,65,65	0
55	MG	2A	3047	1/1	0.95	0.37	45,45,45,45	0
55	MG	2A	3595	1/1	0.95	0.16	52,52,52,52	0
55	MG	1A	3342	1/1	0.95	0.06	29,29,29,29	0
55	MG	2A	3597	1/1	0.95	0.10	47,47,47,47	0
55	MG	1A	3461	1/1	0.95	0.11	27,27,27,27	0
55	MG	2A	3406	1/1	0.95	0.56	81,81,81,81	0
55	MG	1a	3160	1/1	0.95	0.29	67,67,67,67	0
55	MG	2A	3190	1/1	0.95	0.73	66,66,66,66	0
55	MG	2a	1742	1/1	0.95	0.08	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3463	1/1	0.95	0.33	60,60,60,60	0
55	MG	1A	3092	1/1	0.95	0.14	33,33,33,33	0
55	MG	1A	3574	1/1	0.95	0.41	49,49,49,49	0
55	MG	1A	3799	1/1	0.95	0.11	57,57,57,57	0
55	MG	2A	3836	1/1	0.95	0.56	61,61,61,61	0
55	MG	1A	3231	1/1	0.95	0.60	25,25,25,25	0
55	MG	1D	314	1/1	0.95	0.32	77,77,77,77	0
55	MG	1A	3713	1/1	0.95	0.14	75,75,75,75	0
55	MG	1A	3346	1/1	0.95	0.20	69,69,69,69	0
55	MG	2a	1754	1/1	0.95	0.67	78,78,78,78	0
55	MG	2A	3614	1/1	0.95	0.09	56,56,56,56	0
55	MG	1A	3520	1/1	0.95	0.12	33,33,33,33	0
55	MG	2a	1757	1/1	0.95	0.26	66,66,66,66	0
55	MG	2a	1758	1/1	0.95	0.08	74,74,74,74	0
55	MG	1A	3165	1/1	0.95	0.38	41,41,41,41	0
55	MG	2A	3423	1/1	0.95	0.36	51,51,51,51	0
55	MG	2B	3010	1/1	0.95	0.05	73,73,73,73	0
55	MG	2A	3618	1/1	0.95	0.31	68,68,68,68	0
55	MG	1A	3001	1/1	0.95	0.14	38,38,38,38	0
55	MG	1A	3891	1/1	0.95	0.11	84,84,84,84	0
55	MG	2A	3622	1/1	0.95	0.13	52,52,52,52	0
55	MG	1A	3306	1/1	0.95	0.12	43,43,43,43	0
55	MG	2A	3206	1/1	0.95	0.10	64,64,64,64	0
55	MG	1A	3352	1/1	0.95	0.11	34,34,34,34	0
55	MG	2A	3208	1/1	0.95	0.10	80,80,80,80	0
55	MG	2A	3629	1/1	0.95	0.06	73,73,73,73	0
55	MG	2A	3630	1/1	0.95	0.39	56,56,56,56	0
55	MG	1F	306	1/1	0.95	0.20	25,25,25,25	0
55	MG	2A	3067	1/1	0.95	0.42	61,61,61,61	0
55	MG	2D	305	1/1	0.95	0.10	73,73,73,73	0
55	MG	2A	3212	1/1	0.95	0.14	36,36,36,36	0
55	MG	2a	1781	1/1	0.95	0.16	51,51,51,51	0
55	MG	1A	3651	1/1	0.95	0.14	34,34,34,34	0
55	MG	2a	1784	1/1	0.95	0.05	87,87,87,87	0
55	MG	2D	309	1/1	0.95	0.13	57,57,57,57	0
55	MG	1A	3473	1/1	0.95	0.48	32,32,32,32	0
55	MG	2A	3438	1/1	0.95	0.25	66,66,66,66	0
55	MG	2E	303	1/1	0.95	0.18	52,52,52,52	0
55	MG	2A	3215	1/1	0.95	0.31	42,42,42,42	0
55	MG	2A	3217	1/1	0.95	0.10	57,57,57,57	0
55	MG	1A	3896	1/1	0.95	0.48	38,38,38,38	0
55	MG	1A	3271	1/1	0.95	0.34	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3007	1/1	0.95	0.12	38,38,38,38	0
55	MG	2F	306	1/1	0.95	0.39	47,47,47,47	0
55	MG	1G	3003	1/1	0.95	0.09	49,49,49,49	0
55	MG	1A	3309	1/1	0.95	0.14	37,37,37,37	0
55	MG	1a	3187	1/1	0.95	0.07	82,82,82,82	0
55	MG	1A	3901	1/1	0.95	0.47	35,35,35,35	0
55	MG	2A	3081	1/1	0.95	0.32	39,39,39,39	0
55	MG	1A	3822	1/1	0.95	0.10	54,54,54,54	0
55	MG	1a	3190	1/1	0.95	0.07	73,73,73,73	0
55	MG	1a	3061	1/1	0.95	0.26	66,66,66,66	0
55	MG	2A	3235	1/1	0.95	0.08	77,77,77,77	0
55	MG	1N	8002	1/1	0.95	0.21	61,61,61,61	0
56	ZN	1Y	501	1/1	0.95	0.12	61,61,61,61	0
55	MG	2A	3237	1/1	0.95	0.14	45,45,45,45	0
56	ZN	2Y	501	1/1	0.95	0.06	91,91,91,91	0
55	MG	1N	8003	1/1	0.95	0.17	61,61,61,61	0
55	MG	1A	3658	1/1	0.95	0.04	50,50,50,50	0
55	MG	1G	3001	1/1	0.96	0.07	74,74,74,74	0
55	MG	1A	3065	1/1	0.96	0.35	33,33,33,33	0
55	MG	1a	3083	1/1	0.96	0.23	66,66,66,66	0
55	MG	1A	3502	1/1	0.96	0.19	16,16,16,16	0
55	MG	1A	3438	1/1	0.96	0.19	61,61,61,61	0
55	MG	1a	3088	1/1	0.96	0.37	61,61,61,61	0
55	MG	1A	3439	1/1	0.96	0.15	51,51,51,51	0
55	MG	1A	3125	1/1	0.96	0.19	30,30,30,30	0
55	MG	2A	3633	1/1	0.96	0.11	80,80,80,80	0
55	MG	2A	3414	1/1	0.96	0.07	77,77,77,77	0
55	MG	2A	3016	1/1	0.96	0.46	50,50,50,50	0
55	MG	1a	3094	1/1	0.96	0.06	47,47,47,47	0
55	MG	1a	3095	1/1	0.96	0.31	63,63,63,63	0
55	MG	2A	3418	1/1	0.96	0.11	44,44,44,44	0
55	MG	1A	3360	1/1	0.96	0.19	25,25,25,25	0
55	MG	1N	8004	1/1	0.96	0.22	71,71,71,71	0
55	MG	1A	3301	1/1	0.96	0.21	12,12,12,12	0
55	MG	1A	3777	1/1	0.96	0.06	73,73,73,73	0
55	MG	1a	3103	1/1	0.96	0.13	77,77,77,77	0
55	MG	2A	3645	1/1	0.96	0.07	64,64,64,64	0
55	MG	1a	3105	1/1	0.96	0.11	54,54,54,54	0
55	MG	2V	203	1/1	0.96	0.15	73,73,73,73	0
55	MG	1Q	202	1/1	0.96	0.29	51,51,51,51	0
55	MG	2X	101	1/1	0.96	0.30	77,77,77,77	0
55	MG	1A	3778	1/1	0.96	0.12	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3126	1/1	0.96	0.25	23,23,23,23	0
55	MG	1A	3509	1/1	0.96	0.21	31,31,31,31	0
55	MG	1a	3110	1/1	0.96	0.16	54,54,54,54	0
55	MG	1a	3112	1/1	0.96	0.24	85,85,85,85	0
55	MG	2A	3031	1/1	0.96	0.15	64,64,64,64	0
55	MG	21	101	1/1	0.96	0.12	66,66,66,66	0
55	MG	2A	3654	1/1	0.96	0.05	34,34,34,34	0
55	MG	2A	3433	1/1	0.96	0.19	81,81,81,81	0
55	MG	1A	3066	1/1	0.96	0.28	39,39,39,39	0
55	MG	1A	3785	1/1	0.96	0.17	24,24,24,24	0
55	MG	2A	3659	1/1	0.96	0.07	73,73,73,73	0
55	MG	1A	3513	1/1	0.96	0.16	53,53,53,53	0
55	MG	1A	3589	1/1	0.96	0.10	28,28,28,28	0
55	MG	2A	3205	1/1	0.96	0.15	44,44,44,44	0
55	MG	2A	3036	1/1	0.96	0.52	38,38,38,38	0
55	MG	1A	3023	1/1	0.96	0.15	21,21,21,21	0
55	MG	2A	3442	1/1	0.96	0.09	62,62,62,62	0
55	MG	1V	201	1/1	0.96	0.10	67,67,67,67	0
55	MG	2A	3039	1/1	0.96	0.23	25,25,25,25	0
55	MG	2A	3210	1/1	0.96	0.15	44,44,44,44	0
55	MG	1A	3591	1/1	0.96	0.08	26,26,26,26	0
55	MG	1A	3684	1/1	0.96	0.23	59,59,59,59	0
55	MG	1A	3040	1/1	0.96	0.19	40,40,40,40	0
55	MG	2a	1611	1/1	0.96	0.36	76,76,76,76	0
55	MG	1a	3128	1/1	0.96	0.20	75,75,75,75	0
55	MG	1A	3210	1/1	0.96	0.52	42,42,42,42	0
55	MG	1A	3451	1/1	0.96	0.16	23,23,23,23	0
55	MG	1A	3189	1/1	0.96	0.11	69,69,69,69	0
55	MG	1A	3795	1/1	0.96	0.13	48,48,48,48	0
55	MG	1A	3797	1/1	0.96	0.13	50,50,50,50	0
55	MG	2A	3224	1/1	0.96	0.15	55,55,55,55	0
55	MG	1A	3377	1/1	0.96	0.14	47,47,47,47	0
55	MG	2A	3226	1/1	0.96	0.12	70,70,70,70	0
55	MG	1A	3266	1/1	0.96	0.19	34,34,34,34	0
55	MG	1A	3908	1/1	0.96	0.24	40,40,40,40	0
55	MG	2a	1623	1/1	0.96	0.65	60,60,60,60	0
55	MG	1a	3137	1/1	0.96	0.29	63,63,63,63	0
55	MG	2a	1625	1/1	0.96	0.28	49,49,49,49	0
55	MG	1A	3313	1/1	0.96	0.22	39,39,39,39	0
55	MG	2a	1627	1/1	0.96	0.17	54,54,54,54	0
55	MG	1A	3694	1/1	0.96	0.24	46,46,46,46	0
55	MG	2A	3692	1/1	0.96	0.06	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3314	1/1	0.96	0.09	53,53,53,53	0
55	MG	2a	1632	1/1	0.96	0.46	73,73,73,73	0
55	MG	1A	3212	1/1	0.96	0.45	39,39,39,39	0
55	MG	1A	3027	1/1	0.96	0.17	31,31,31,31	0
55	MG	2A	3697	1/1	0.96	0.05	53,53,53,53	0
55	MG	1A	3808	1/1	0.96	0.23	19,19,19,19	0
55	MG	1A	3149	1/1	0.96	0.18	49,49,49,49	0
55	MG	17	102	1/1	0.96	0.15	55,55,55,55	0
55	MG	2A	3703	1/1	0.96	0.25	91,91,91,91	0
55	MG	1A	3918	1/1	0.96	0.22	28,28,28,28	0
55	MG	2A	3241	1/1	0.96	0.33	44,44,44,44	0
55	MG	1A	3810	1/1	0.96	0.06	63,63,63,63	0
55	MG	2A	3064	1/1	0.96	0.61	54,54,54,54	0
55	MG	2A	3708	1/1	0.96	0.12	69,69,69,69	0
55	MG	1A	3811	1/1	0.96	0.11	35,35,35,35	0
55	MG	2A	3710	1/1	0.96	0.14	62,62,62,62	0
55	MG	2A	3246	1/1	0.96	0.03	71,71,71,71	0
55	MG	2A	3247	1/1	0.96	0.20	38,38,38,38	0
55	MG	2A	3714	1/1	0.96	0.11	52,52,52,52	0
55	MG	19	101	1/1	0.96	0.39	52,52,52,52	0
55	MG	1A	3462	1/1	0.96	0.58	33,33,33,33	0
55	MG	2A	3069	1/1	0.96	0.23	54,54,54,54	0
55	MG	1A	3702	1/1	0.96	0.19	31,31,31,31	0
55	MG	2A	3071	1/1	0.96	0.28	38,38,38,38	0
55	MG	1A	3272	1/1	0.96	0.20	23,23,23,23	0
55	MG	1A	3464	1/1	0.96	0.22	61,61,61,61	0
55	MG	2a	1658	1/1	0.96	0.14	58,58,58,58	0
55	MG	1A	3818	1/1	0.96	0.09	52,52,52,52	0
55	MG	2A	3491	1/1	0.96	0.13	49,49,49,49	0
55	MG	1A	3819	1/1	0.96	0.52	45,45,45,45	0
55	MG	1A	3242	1/1	0.96	0.65	46,46,46,46	0
55	MG	1A	3324	1/1	0.96	0.17	24,24,24,24	0
55	MG	2A	3497	1/1	0.96	0.13	39,39,39,39	0
55	MG	1A	3070	1/1	0.96	0.22	37,37,37,37	0
55	MG	2A	3079	1/1	0.96	0.31	60,60,60,60	0
55	MG	1A	3708	1/1	0.96	0.23	51,51,51,51	0
55	MG	1A	3533	1/1	0.96	0.17	41,41,41,41	0
55	MG	2A	3082	1/1	0.96	0.30	60,60,60,60	0
55	MG	1a	3011	1/1	0.96	0.15	74,74,74,74	0
55	MG	2A	3504	1/1	0.96	0.24	58,58,58,58	0
55	MG	1A	3614	1/1	0.96	0.03	50,50,50,50	0
55	MG	2A	3739	1/1	0.96	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3936	1/1	0.96	0.28	55,55,55,55	0
55	MG	2A	3507	1/1	0.96	0.57	62,62,62,62	0
55	MG	1a	3167	1/1	0.96	0.09	79,79,79,79	0
55	MG	1A	3327	1/1	0.96	0.10	43,43,43,43	0
55	MG	1A	3005	1/1	0.96	0.16	22,22,22,22	0
55	MG	1A	3939	1/1	0.96	0.62	39,39,39,39	0
55	MG	2a	1684	1/1	0.96	0.19	64,64,64,64	0
55	MG	1a	3171	1/1	0.96	0.11	54,54,54,54	0
55	MG	2A	3093	1/1	0.96	0.50	56,56,56,56	0
55	MG	2a	1687	1/1	0.96	0.30	58,58,58,58	0
55	MG	2A	3280	1/1	0.96	0.15	35,35,35,35	0
55	MG	2a	1689	1/1	0.96	0.16	63,63,63,63	0
55	MG	2A	3515	1/1	0.96	0.09	50,50,50,50	0
55	MG	1A	3829	1/1	0.96	0.34	67,67,67,67	0
55	MG	1A	3134	1/1	0.96	0.12	40,40,40,40	0
55	MG	1A	3619	1/1	0.96	0.20	44,44,44,44	0
55	MG	1A	3943	1/1	0.96	0.30	37,37,37,37	0
55	MG	1A	3059	1/1	0.96	0.20	58,58,58,58	0
55	MG	1a	3178	1/1	0.96	0.07	70,70,70,70	0
55	MG	1A	3336	1/1	0.96	0.17	19,19,19,19	0
55	MG	1a	3025	1/1	0.96	0.08	51,51,51,51	0
55	MG	1B	202	1/1	0.96	0.21	60,60,60,60	0
55	MG	2a	1703	1/1	0.96	0.09	60,60,60,60	0
55	MG	1A	3338	1/1	0.96	0.14	24,24,24,24	0
55	MG	2a	1705	1/1	0.96	0.20	75,75,75,75	0
55	MG	2A	3298	1/1	0.96	0.17	37,37,37,37	0
55	MG	1A	3544	1/1	0.96	0.27	30,30,30,30	0
55	MG	2A	3767	1/1	0.96	0.06	69,69,69,69	0
55	MG	2A	3301	1/1	0.96	0.08	85,85,85,85	0
55	MG	1A	3627	1/1	0.96	0.15	49,49,49,49	0
55	MG	1A	3475	1/1	0.96	0.08	25,25,25,25	0
55	MG	1A	3339	1/1	0.96	0.12	23,23,23,23	0
55	MG	1A	3630	1/1	0.96	0.10	60,60,60,60	0
55	MG	2A	3306	1/1	0.96	0.33	62,62,62,62	0
55	MG	2A	3312	1/1	0.96	0.14	62,62,62,62	0
55	MG	2A	3313	1/1	0.96	0.20	65,65,65,65	0
55	MG	2A	3778	1/1	0.96	0.24	51,51,51,51	0
55	MG	2A	3779	1/1	0.96	0.15	36,36,36,36	0
55	MG	1A	3631	1/1	0.96	0.26	81,81,81,81	0
55	MG	1A	3727	1/1	0.96	0.09	48,48,48,48	0
55	MG	1A	3403	1/1	0.96	0.14	48,48,48,48	0
55	MG	2A	3317	1/1	0.96	0.05	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3543	1/1	0.96	0.04	85,85,85,85	0
55	MG	1a	3192	1/1	0.96	0.15	64,64,64,64	0
55	MG	1B	214	1/1	0.96	0.11	50,50,50,50	0
55	MG	2A	3788	1/1	0.96	0.19	66,66,66,66	0
55	MG	1A	3155	1/1	0.96	0.74	60,60,60,60	0
55	MG	2A	3323	1/1	0.96	0.11	59,59,59,59	0
55	MG	1a	3195	1/1	0.96	0.14	68,68,68,68	0
55	MG	2A	3116	1/1	0.96	0.21	56,56,56,56	0
55	MG	1A	3279	1/1	0.96	0.12	55,55,55,55	0
55	MG	1B	218	1/1	0.96	0.08	49,49,49,49	0
55	MG	2A	3331	1/1	0.96	0.18	45,45,45,45	0
55	MG	1A	3343	1/1	0.96	0.26	54,54,54,54	0
55	MG	2A	3120	1/1	0.96	0.07	75,75,75,75	0
55	MG	2A	3121	1/1	0.96	0.23	46,46,46,46	0
55	MG	1A	3637	1/1	0.96	0.14	45,45,45,45	0
55	MG	2a	1739	1/1	0.96	0.13	81,81,81,81	0
55	MG	1A	3407	1/1	0.96	0.12	58,58,58,58	0
55	MG	1B	223	1/1	0.96	0.32	61,61,61,61	0
55	MG	2A	3560	1/1	0.96	0.08	66,66,66,66	0
55	MG	2a	1743	1/1	0.96	0.32	65,65,65,65	0
55	MG	1a	3203	1/1	0.96	0.16	64,64,64,64	0
55	MG	2A	3339	1/1	0.96	0.17	37,37,37,37	0
55	MG	1a	3045	1/1	0.96	0.33	63,63,63,63	0
55	MG	1A	3249	1/1	0.96	0.23	10,10,10,10	0
55	MG	1A	3640	1/1	0.96	0.44	37,37,37,37	0
55	MG	1a	3209	1/1	0.96	0.14	56,56,56,56	0
55	MG	1A	3641	1/1	0.96	0.13	41,41,41,41	0
55	MG	2A	3817	1/1	0.96	1.18	56,56,56,56	0
55	MG	1a	3211	1/1	0.96	0.28	65,65,65,65	0
55	MG	2A	3346	1/1	0.96	0.05	77,77,77,77	0
55	MG	2A	3820	1/1	0.96	0.56	51,51,51,51	0
55	MG	1a	3212	1/1	0.96	0.05	56,56,56,56	0
55	MG	1A	3197	1/1	0.96	0.41	31,31,31,31	0
55	MG	2A	3349	1/1	0.96	0.14	80,80,80,80	0
55	MG	2A	3575	1/1	0.96	0.16	52,52,52,52	0
55	MG	1A	3411	1/1	0.96	0.04	48,48,48,48	0
55	MG	2a	1761	1/1	0.96	0.15	68,68,68,68	0
55	MG	2A	3826	1/1	0.96	1.08	56,56,56,56	0
55	MG	1A	3743	1/1	0.96	0.04	58,58,58,58	0
55	MG	2A	3828	1/1	0.96	0.69	65,65,65,65	0
55	MG	2A	3352	1/1	0.96	0.20	29,29,29,29	0
55	MG	2a	1766	1/1	0.96	0.25	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3555	1/1	0.96	0.12	28,28,28,28	0
55	MG	1A	3646	1/1	0.96	0.16	49,49,49,49	0
55	MG	2a	1770	1/1	0.96	0.06	61,61,61,61	0
55	MG	1A	3284	1/1	0.96	0.11	64,64,64,64	0
55	MG	1A	3559	1/1	0.96	0.18	56,56,56,56	0
55	MG	1a	3221	1/1	0.96	0.44	79,79,79,79	0
55	MG	1A	3107	1/1	0.96	0.23	25,25,25,25	0
55	MG	2A	3145	1/1	0.96	0.13	75,75,75,75	0
55	MG	1A	3158	1/1	0.96	0.13	31,31,31,31	0
55	MG	1D	311	1/1	0.96	0.09	61,61,61,61	0
55	MG	1a	3059	1/1	0.96	0.16	78,78,78,78	0
55	MG	1A	3349	1/1	0.96	0.38	62,62,62,62	0
55	MG	2A	3592	1/1	0.96	0.10	80,80,80,80	0
55	MG	2B	3006	1/1	0.96	0.44	80,80,80,80	0
55	MG	2a	1783	1/1	0.96	0.07	59,59,59,59	0
55	MG	1b	3001	1/1	0.96	0.07	71,71,71,71	0
55	MG	1A	3753	1/1	0.96	0.05	50,50,50,50	0
55	MG	1a	3062	1/1	0.96	0.62	81,81,81,81	0
55	MG	1A	3563	1/1	0.96	0.15	29,29,29,29	0
55	MG	1A	3564	1/1	0.96	0.13	28,28,28,28	0
55	MG	2A	3156	1/1	0.96	0.27	58,58,58,58	0
55	MG	1E	302	1/1	0.96	0.19	26,26,26,26	0
55	MG	2A	3600	1/1	0.96	0.38	53,53,53,53	0
55	MG	2a	1793	1/1	0.96	0.14	56,56,56,56	0
55	MG	2a	1794	1/1	0.96	0.06	74,74,74,74	0
55	MG	2a	1795	1/1	0.96	0.37	80,80,80,80	0
55	MG	2a	1796	1/1	0.96	0.12	58,58,58,58	0
55	MG	1A	3428	1/1	0.96	0.14	18,18,18,18	0
55	MG	1A	3867	1/1	0.96	0.34	45,45,45,45	0
55	MG	1A	3868	1/1	0.96	0.12	27,27,27,27	0
55	MG	2e	201	1/1	0.96	0.15	71,71,71,71	0
55	MG	1A	3656	1/1	0.96	0.11	57,57,57,57	0
55	MG	1A	3108	1/1	0.96	0.21	32,32,32,32	0
55	MG	2A	3387	1/1	0.96	0.08	58,58,58,58	0
55	MG	1A	3494	1/1	0.96	0.09	48,48,48,48	0
55	MG	1A	3082	1/1	0.96	0.76	47,47,47,47	0
55	MG	2A	3392	1/1	0.96	0.13	55,55,55,55	0
55	MG	1A	3291	1/1	0.96	0.10	72,72,72,72	0
55	MG	2A	3394	1/1	0.96	0.15	49,49,49,49	0
55	MG	1A	3762	1/1	0.96	0.17	19,19,19,19	0
55	MG	1a	3075	1/1	0.96	0.23	57,57,57,57	0
55	MG	1A	3096	1/1	0.96	0.35	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3181	1/1	0.96	0.42	43,43,43,43	0
56	ZN	1n	501	1/1	0.96	0.13	85,85,85,85	0
55	MG	1A	3573	1/1	0.96	0.19	21,21,21,21	0
55	MG	1A	3435	1/1	0.96	0.09	44,44,44,44	0
56	ZN	2n	501	1/1	0.96	0.06	94,94,94,94	0
55	MG	1F	312	1/1	0.96	0.11	47,47,47,47	0
55	MG	1A	3484	1/1	0.97	0.20	69,69,69,69	0
55	MG	2A	3353	1/1	0.97	0.06	70,70,70,70	0
55	MG	2A	3806	1/1	0.97	0.26	47,47,47,47	0
55	MG	2A	3807	1/1	0.97	0.43	57,57,57,57	0
55	MG	2A	3218	1/1	0.97	0.34	23,23,23,23	0
55	MG	1A	3230	1/1	0.97	0.67	35,35,35,35	0
55	MG	2A	3220	1/1	0.97	0.31	49,49,49,49	0
55	MG	1A	3157	1/1	0.97	0.20	33,33,33,33	0
55	MG	1A	3715	1/1	0.97	0.06	51,51,51,51	0
55	MG	1A	3716	1/1	0.97	0.12	31,31,31,31	0
55	MG	1A	3539	1/1	0.97	0.52	35,35,35,35	0
55	MG	1A	3389	1/1	0.97	0.18	21,21,21,21	0
55	MG	1A	3350	1/1	0.97	0.13	26,26,26,26	0
55	MG	2a	1664	1/1	0.97	0.34	68,68,68,68	0
55	MG	1A	3321	1/1	0.97	0.25	49,49,49,49	0
55	MG	1A	3597	1/1	0.97	0.05	49,49,49,49	0
55	MG	2A	3366	1/1	0.97	0.20	35,35,35,35	0
55	MG	2A	3230	1/1	0.97	0.18	44,44,44,44	0
55	MG	2a	1669	1/1	0.97	0.07	49,49,49,49	0
55	MG	2a	1670	1/1	0.97	0.10	49,49,49,49	0
55	MG	1A	3491	1/1	0.97	0.15	42,42,42,42	0
55	MG	1A	3075	1/1	0.97	0.47	33,33,33,33	0
55	MG	2A	3122	1/1	0.97	0.28	46,46,46,46	0
55	MG	2a	1674	1/1	0.97	0.19	71,71,71,71	0
55	MG	2A	3517	1/1	0.97	0.13	80,80,80,80	0
55	MG	2A	3123	1/1	0.97	0.22	52,52,52,52	0
55	MG	1A	3446	1/1	0.97	0.16	24,24,24,24	0
55	MG	1B	205	1/1	0.97	0.10	54,54,54,54	0
55	MG	1A	3798	1/1	0.97	0.14	46,46,46,46	0
55	MG	2A	3667	1/1	0.97	0.15	64,64,64,64	0
55	MG	1A	3323	1/1	0.97	0.07	29,29,29,29	0
55	MG	2A	3670	1/1	0.97	0.04	76,76,76,76	0
55	MG	2A	3381	1/1	0.97	0.11	66,66,66,66	0
55	MG	2A	3382	1/1	0.97	0.21	61,61,61,61	0
55	MG	2A	3383	1/1	0.97	0.14	66,66,66,66	0
55	MG	11	101	1/1	0.97	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3527	1/1	0.97	0.20	37,37,37,37	0
55	MG	1A	3020	1/1	0.97	0.42	38,38,38,38	0
55	MG	1A	3664	1/1	0.97	0.25	48,48,48,48	0
55	MG	1A	3356	1/1	0.97	0.14	23,23,23,23	0
55	MG	2B	3004	1/1	0.97	0.12	78,78,78,78	0
55	MG	1A	3666	1/1	0.97	0.23	53,53,53,53	0
55	MG	2a	1693	1/1	0.97	0.33	60,60,60,60	0
55	MG	2A	3389	1/1	0.97	0.18	51,51,51,51	0
55	MG	1B	212	1/1	0.97	0.18	56,56,56,56	0
55	MG	1A	3604	1/1	0.97	0.05	59,59,59,59	0
55	MG	2A	3248	1/1	0.97	0.07	28,28,28,28	0
55	MG	2a	1698	1/1	0.97	0.65	61,61,61,61	0
55	MG	1A	3398	1/1	0.97	0.24	66,66,66,66	0
55	MG	1A	3300	1/1	0.97	0.11	43,43,43,43	0
55	MG	1A	3452	1/1	0.97	0.07	55,55,55,55	0
55	MG	2A	3688	1/1	0.97	0.17	73,73,73,73	0
55	MG	1A	3261	1/1	0.97	0.19	17,17,17,17	0
55	MG	1A	3304	1/1	0.97	0.12	14,14,14,14	0
55	MG	1A	3738	1/1	0.97	0.17	23,23,23,23	0
55	MG	1B	221	1/1	0.97	0.35	79,79,79,79	0
55	MG	1a	3085	1/1	0.97	0.33	66,66,66,66	0
55	MG	1a	3086	1/1	0.97	0.45	64,64,64,64	0
55	MG	2A	3259	1/1	0.97	0.12	89,89,89,89	0
55	MG	2A	3044	1/1	0.97	0.38	38,38,38,38	0
55	MG	2A	3698	1/1	0.97	0.17	40,40,40,40	0
55	MG	2A	3699	1/1	0.97	0.15	37,37,37,37	0
55	MG	1A	3028	1/1	0.97	0.29	37,37,37,37	0
55	MG	2a	1715	1/1	0.97	0.17	81,81,81,81	0
55	MG	1a	3191	1/1	0.97	0.12	49,49,49,49	0
55	MG	2D	308	1/1	0.97	0.25	28,28,28,28	0
55	MG	1A	3815	1/1	0.97	0.16	25,25,25,25	0
55	MG	1A	3331	1/1	0.97	0.19	23,23,23,23	0
55	MG	1A	3365	1/1	0.97	0.22	30,30,30,30	0
55	MG	2A	3413	1/1	0.97	0.13	70,70,70,70	0
55	MG	1A	3368	1/1	0.97	0.11	47,47,47,47	0
55	MG	1A	3121	1/1	0.97	0.43	31,31,31,31	0
55	MG	1A	3370	1/1	0.97	0.21	26,26,26,26	0
55	MG	1a	3198	1/1	0.97	0.08	57,57,57,57	0
55	MG	2F	304	1/1	0.97	0.34	62,62,62,62	0
55	MG	1A	3223	1/1	0.97	0.08	72,72,72,72	0
55	MG	2A	3272	1/1	0.97	0.07	60,60,60,60	0
55	MG	1A	3620	1/1	0.97	0.09	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1D	305	1/1	0.97	0.35	42,42,42,42	0
55	MG	1A	3748	1/1	0.97	0.07	39,39,39,39	0
55	MG	1A	3510	1/1	0.97	0.40	44,44,44,44	0
55	MG	1A	3897	1/1	0.97	0.22	11,11,11,11	0
55	MG	1A	3337	1/1	0.97	0.18	18,18,18,18	0
55	MG	2A	3566	1/1	0.97	0.34	55,55,55,55	0
55	MG	1a	3206	1/1	0.97	0.04	74,74,74,74	0
55	MG	2A	3282	1/1	0.97	0.12	42,42,42,42	0
55	MG	2A	3164	1/1	0.97	0.29	41,41,41,41	0
55	MG	2A	3429	1/1	0.97	0.20	76,76,76,76	0
55	MG	1A	3224	1/1	0.97	0.14	35,35,35,35	0
55	MG	1A	3827	1/1	0.97	0.09	69,69,69,69	0
55	MG	2A	3726	1/1	0.97	0.11	38,38,38,38	0
55	MG	2R	8002	1/1	0.97	0.25	45,45,45,45	0
55	MG	2A	3290	1/1	0.97	0.22	71,71,71,71	0
55	MG	2A	3728	1/1	0.97	0.12	46,46,46,46	0
55	MG	1A	3413	1/1	0.97	0.09	28,28,28,28	0
55	MG	2V	201	1/1	0.97	0.72	54,54,54,54	0
55	MG	2A	3730	1/1	0.97	0.14	51,51,51,51	0
55	MG	1A	3686	1/1	0.97	0.29	55,55,55,55	0
55	MG	1A	3625	1/1	0.97	0.45	44,44,44,44	0
55	MG	2A	3578	1/1	0.97	0.09	61,61,61,61	0
55	MG	2A	3294	1/1	0.97	0.14	45,45,45,45	0
55	MG	1A	3466	1/1	0.97	0.11	53,53,53,53	0
55	MG	2A	3068	1/1	0.97	0.11	65,65,65,65	0
55	MG	1A	3414	1/1	0.97	0.15	31,31,31,31	0
55	MG	1a	3023	1/1	0.97	0.48	53,53,53,53	0
55	MG	1A	3283	1/1	0.97	0.23	40,40,40,40	0
55	MG	1A	3416	1/1	0.97	0.20	31,31,31,31	0
55	MG	1A	3417	1/1	0.97	0.16	37,37,37,37	0
55	MG	1a	3121	1/1	0.97	0.71	72,72,72,72	0
55	MG	1A	3187	1/1	0.97	0.56	35,35,35,35	0
55	MG	2A	3745	1/1	0.97	0.10	65,65,65,65	0
55	MG	1A	3910	1/1	0.97	0.38	36,36,36,36	0
55	MG	1A	3422	1/1	0.97	0.07	68,68,68,68	0
55	MG	2A	3307	1/1	0.97	0.16	63,63,63,63	0
55	MG	2A	3308	1/1	0.97	0.15	58,58,58,58	0
55	MG	2a	1768	1/1	0.97	0.21	74,74,74,74	0
55	MG	2A	3182	1/1	0.97	0.09	80,80,80,80	0
55	MG	1A	3696	1/1	0.97	0.16	25,25,25,25	0
55	MG	1A	3376	1/1	0.97	0.13	13,13,13,13	0
55	MG	1A	3765	1/1	0.97	0.05	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3635	1/1	0.97	0.08	29,29,29,29	0
55	MG	1A	3699	1/1	0.97	0.15	27,27,27,27	0
55	MG	1A	3102	1/1	0.97	0.34	34,34,34,34	0
55	MG	2A	3319	1/1	0.97	0.20	30,30,30,30	0
55	MG	2A	3084	1/1	0.97	0.30	49,49,49,49	0
55	MG	2a	1778	1/1	0.97	0.09	64,64,64,64	0
55	MG	2A	3761	1/1	0.97	0.17	38,38,38,38	0
55	MG	2A	3321	1/1	0.97	0.04	65,65,65,65	0
55	MG	1A	3844	1/1	0.97	0.09	25,25,25,25	0
55	MG	1a	3037	1/1	0.97	0.16	70,70,70,70	0
55	MG	2A	3087	1/1	0.97	0.17	61,61,61,61	0
55	MG	1A	3378	1/1	0.97	0.16	47,47,47,47	0
55	MG	1A	3269	1/1	0.97	0.09	26,26,26,26	0
55	MG	1A	3380	1/1	0.97	0.14	49,49,49,49	0
55	MG	2A	3330	1/1	0.97	0.13	45,45,45,45	0
55	MG	1A	3923	1/1	0.97	0.14	17,17,17,17	0
55	MG	1A	3581	1/1	0.97	0.22	39,39,39,39	0
55	MG	1a	3142	1/1	0.97	0.15	86,86,86,86	0
55	MG	1k	201	1/1	0.97	0.23	50,50,50,50	0
55	MG	1A	3381	1/1	0.97	0.17	23,23,23,23	0
55	MG	2A	3775	1/1	0.97	0.12	63,63,63,63	0
55	MG	1A	3850	1/1	0.97	0.12	23,23,23,23	0
55	MG	2A	3620	1/1	0.97	0.12	40,40,40,40	0
55	MG	2a	1797	1/1	0.97	0.09	75,75,75,75	0
55	MG	1A	3003	1/1	0.97	0.10	20,20,20,20	0
55	MG	1A	3776	1/1	0.97	0.06	43,43,43,43	0
55	MG	2A	3204	1/1	0.97	0.71	58,58,58,58	0
55	MG	2A	3482	1/1	0.97	0.66	56,56,56,56	0
55	MG	1a	3147	1/1	0.97	0.13	73,73,73,73	0
55	MG	2A	3784	1/1	0.97	0.16	64,64,64,64	0
55	MG	1A	3015	1/1	0.97	0.29	30,30,30,30	0
55	MG	2A	3628	1/1	0.97	0.22	57,57,57,57	0
55	MG	1A	3229	1/1	0.97	0.15	41,41,41,41	0
55	MG	1Q	201	1/1	0.97	0.12	51,51,51,51	0
55	MG	1A	3779	1/1	0.97	0.04	57,57,57,57	0
55	MG	2A	3006	1/1	0.97	0.13	40,40,40,40	0
55	MG	1A	3318	1/1	0.97	0.14	70,70,70,70	0
55	MG	1A	3933	1/1	0.97	0.15	28,28,28,28	0
55	MG	1A	3437	1/1	0.97	0.09	66,66,66,66	0
55	MG	1A	3935	1/1	0.97	0.14	27,27,27,27	0
55	MG	2A	3494	1/1	0.97	0.09	59,59,59,59	0
55	MG	2A	3495	1/1	0.97	0.16	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3639	1/1	0.97	0.19	79,79,79,79	0
56	ZN	25	103	1/1	0.97	0.08	64,64,64,64	0
55	MG	1a	3156	1/1	0.97	0.14	70,70,70,70	0
55	MG	2A	3216	1/1	0.97	0.14	37,37,37,37	0
55	MG	1a	3100	1/1	0.98	0.38	62,62,62,62	0
55	MG	1A	3731	1/1	0.98	0.09	25,25,25,25	0
55	MG	2A	3758	1/1	0.98	0.06	78,78,78,78	0
55	MG	1A	3796	1/1	0.98	0.08	33,33,33,33	0
55	MG	2A	3760	1/1	0.98	0.07	42,42,42,42	0
55	MG	1A	3303	1/1	0.98	0.20	16,16,16,16	0
55	MG	1a	3104	1/1	0.98	0.24	80,80,80,80	0
55	MG	1A	3618	1/1	0.98	0.07	51,51,51,51	0
55	MG	2a	1700	1/1	0.98	0.15	68,68,68,68	0
55	MG	1A	3154	1/1	0.98	0.39	31,31,31,31	0
55	MG	2A	3311	1/1	0.98	0.12	48,48,48,48	0
55	MG	1G	3002	1/1	0.98	0.09	67,67,67,67	0
55	MG	1A	3305	1/1	0.98	0.06	68,68,68,68	0
55	MG	1A	3801	1/1	0.98	0.16	32,32,32,32	0
55	MG	1A	3736	1/1	0.98	0.09	20,20,20,20	0
55	MG	1A	3569	1/1	0.98	0.45	48,48,48,48	0
55	MG	1A	3445	1/1	0.98	0.21	24,24,24,24	0
55	MG	1A	3129	1/1	0.98	0.26	33,33,33,33	0
55	MG	1A	3871	1/1	0.98	0.12	16,16,16,16	0
55	MG	1A	3525	1/1	0.98	0.13	27,27,27,27	0
55	MG	1A	3807	1/1	0.98	0.07	17,17,17,17	0
55	MG	2A	3776	1/1	0.98	0.07	44,44,44,44	0
55	MG	1a	3118	1/1	0.98	0.06	68,68,68,68	0
55	MG	2A	3222	1/1	0.98	0.16	56,56,56,56	0
55	MG	1A	3288	1/1	0.98	0.09	62,62,62,62	0
55	MG	1A	3626	1/1	0.98	0.06	42,42,42,42	0
55	MG	1a	3207	1/1	0.98	0.17	77,77,77,77	0
55	MG	2A	3663	1/1	0.98	0.12	53,53,53,53	0
55	MG	2A	3328	1/1	0.98	0.19	63,63,63,63	0
55	MG	1A	3326	1/1	0.98	0.11	28,28,28,28	0
55	MG	1a	3122	1/1	0.98	0.28	67,67,67,67	0
55	MG	1a	3123	1/1	0.98	0.23	79,79,79,79	0
55	MG	2A	3551	1/1	0.98	0.10	62,62,62,62	0
55	MG	1A	3487	1/1	0.98	0.10	32,32,32,32	0
55	MG	1a	3125	1/1	0.98	0.34	78,78,78,78	0
55	MG	2A	3790	1/1	0.98	0.12	39,39,39,39	0
55	MG	1B	201	1/1	0.98	0.70	48,48,48,48	0
55	MG	1A	3141	1/1	0.98	0.54	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3793	1/1	0.98	0.21	53,53,53,53	0
55	MG	1A	3879	1/1	0.98	0.11	47,47,47,47	0
55	MG	2a	1605	1/1	0.98	0.09	53,53,53,53	0
55	MG	1A	3813	1/1	0.98	0.12	22,22,22,22	0
55	MG	2A	3796	1/1	0.98	0.15	78,78,78,78	0
55	MG	1A	3410	1/1	0.98	0.18	8,8,8,8	0
55	MG	1A	3687	1/1	0.98	0.15	25,25,25,25	0
55	MG	1A	3086	1/1	0.98	0.10	55,55,55,55	0
55	MG	2A	3449	1/1	0.98	0.18	34,34,34,34	0
55	MG	2A	3238	1/1	0.98	0.17	46,46,46,46	0
55	MG	1A	3412	1/1	0.98	0.21	22,22,22,22	0
55	MG	1A	3751	1/1	0.98	0.08	24,24,24,24	0
55	MG	1A	3106	1/1	0.98	0.32	34,34,34,34	0
55	MG	1A	3354	1/1	0.98	0.14	26,26,26,26	0
55	MG	1A	3535	1/1	0.98	0.28	38,38,38,38	0
55	MG	2a	1745	1/1	0.98	0.04	77,77,77,77	0
55	MG	1A	3175	1/1	0.98	0.17	47,47,47,47	0
55	MG	2A	3459	1/1	0.98	0.06	64,64,64,64	0
55	MG	2A	3245	1/1	0.98	0.30	35,35,35,35	0
55	MG	1A	3495	1/1	0.98	0.23	66,66,66,66	0
55	MG	1A	3538	1/1	0.98	0.18	22,22,22,22	0
55	MG	1A	3332	1/1	0.98	0.19	23,23,23,23	0
55	MG	1A	3293	1/1	0.98	0.14	19,19,19,19	0
55	MG	1A	3418	1/1	0.98	0.12	34,34,34,34	0
55	MG	1A	3542	1/1	0.98	0.16	37,37,37,37	0
55	MG	2A	3696	1/1	0.98	0.05	61,61,61,61	0
55	MG	1A	3643	1/1	0.98	0.14	22,22,22,22	0
55	MG	1A	3419	1/1	0.98	0.17	28,28,28,28	0
55	MG	2A	3357	1/1	0.98	0.11	53,53,53,53	0
55	MG	13	101	1/1	0.98	0.30	42,42,42,42	0
55	MG	1A	3334	1/1	0.98	0.16	27,27,27,27	0
55	MG	1A	3421	1/1	0.98	0.16	23,23,23,23	0
55	MG	1A	3268	1/1	0.98	0.16	22,22,22,22	0
55	MG	1A	3423	1/1	0.98	0.18	23,23,23,23	0
55	MG	1A	3295	1/1	0.98	0.19	11,11,11,11	0
55	MG	1A	3769	1/1	0.98	0.16	31,31,31,31	0
55	MG	2a	1639	1/1	0.98	0.15	74,74,74,74	0
55	MG	1A	3361	1/1	0.98	0.10	28,28,28,28	0
55	MG	1A	3391	1/1	0.98	0.12	62,62,62,62	0
55	MG	2A	3367	1/1	0.98	0.09	46,46,46,46	0
55	MG	1A	3248	1/1	0.98	0.12	21,21,21,21	0
55	MG	2A	3371	1/1	0.98	0.18	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3363	1/1	0.98	0.15	39,39,39,39	0
55	MG	2A	3713	1/1	0.98	0.04	79,79,79,79	0
55	MG	2A	3176	1/1	0.98	0.61	43,43,43,43	0
55	MG	1A	3654	1/1	0.98	0.15	40,40,40,40	0
55	MG	1A	3364	1/1	0.98	0.12	26,26,26,26	0
55	MG	2B	3001	1/1	0.98	0.21	64,64,64,64	0
55	MG	1A	3137	1/1	0.98	0.22	43,43,43,43	0
55	MG	2A	3270	1/1	0.98	0.10	45,45,45,45	0
55	MG	1A	3911	1/1	0.98	0.21	33,33,33,33	0
55	MG	2A	3490	1/1	0.98	0.11	56,56,56,56	0
55	MG	1A	3511	1/1	0.98	0.12	25,25,25,25	0
55	MG	2A	3273	1/1	0.98	0.13	44,44,44,44	0
55	MG	1A	3556	1/1	0.98	0.13	32,32,32,32	0
55	MG	2A	3275	1/1	0.98	0.25	35,35,35,35	0
55	MG	1A	3557	1/1	0.98	0.23	29,29,29,29	0
55	MG	2a	1787	1/1	0.98	0.05	78,78,78,78	0
55	MG	2A	3607	1/1	0.98	0.06	74,74,74,74	0
55	MG	1A	3660	1/1	0.98	0.12	35,35,35,35	0
55	MG	1A	3366	1/1	0.98	0.25	31,31,31,31	0
55	MG	1A	3662	1/1	0.98	0.09	22,22,22,22	0
55	MG	1A	3397	1/1	0.98	0.26	17,17,17,17	0
55	MG	1A	3340	1/1	0.98	0.11	25,25,25,25	0
55	MG	1E	305	1/1	0.98	0.17	57,57,57,57	0
55	MG	2A	3391	1/1	0.98	0.22	38,38,38,38	0
55	MG	1A	3317	1/1	0.98	0.28	38,38,38,38	0
55	MG	1A	3611	1/1	0.98	0.05	81,81,81,81	0
55	MG	2A	3286	1/1	0.98	0.07	37,37,37,37	0
55	MG	2d	502	1/1	0.98	0.10	70,70,70,70	0
55	MG	1a	3015	1/1	0.98	0.29	71,71,71,71	0
55	MG	2A	3289	1/1	0.98	0.17	40,40,40,40	0
55	MG	1a	3089	1/1	0.98	0.09	52,52,52,52	0
55	MG	1a	3090	1/1	0.98	0.07	39,39,39,39	0
55	MG	2A	3741	1/1	0.98	0.05	70,70,70,70	0
55	MG	2A	3399	1/1	0.98	0.18	51,51,51,51	0
55	MG	1a	3091	1/1	0.98	0.11	40,40,40,40	0
55	MG	2A	3401	1/1	0.98	0.14	40,40,40,40	0
55	MG	2E	302	1/1	0.98	0.15	39,39,39,39	0
55	MG	1A	3091	1/1	0.98	0.32	17,17,17,17	0
55	MG	1A	3613	1/1	0.98	0.14	23,23,23,23	0
55	MG	1A	3083	1/1	0.98	0.06	50,50,50,50	0
55	MG	2A	3516	1/1	0.98	0.10	59,59,59,59	0
55	MG	1A	3440	1/1	0.98	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3302	1/1	0.98	0.12	51,51,51,51	0
56	ZN	16	101	1/1	0.98	0.12	62,62,62,62	0
56	ZN	19	102	1/1	0.98	0.13	68,68,68,68	0
55	MG	1A	3672	1/1	0.98	0.18	35,35,35,35	0
55	MG	1a	3098	1/1	0.98	0.24	59,59,59,59	0
55	MG	2A	3300	1/1	0.98	0.14	42,42,42,42	0
55	MG	2F	308	1/1	0.98	0.38	57,57,57,57	0
56	ZN	29	501	1/1	0.98	0.10	77,77,77,77	0
55	MG	2A	3410	1/1	0.98	0.11	59,59,59,59	0
55	MG	1a	3099	1/1	0.98	0.17	64,64,64,64	0
55	MG	1A	3582	1/1	0.99	0.11	40,40,40,40	0
55	MG	1a	3126	1/1	0.99	0.18	74,74,74,74	0
55	MG	1A	3784	1/1	0.99	0.15	32,32,32,32	0
55	MG	2A	3435	1/1	0.99	0.06	71,71,71,71	0
55	MG	1A	3298	1/1	0.99	0.10	49,49,49,49	0
55	MG	1A	3282	1/1	0.99	0.15	50,50,50,50	0
55	MG	1A	3585	1/1	0.99	0.10	49,49,49,49	0
55	MG	1a	3177	1/1	0.99	0.06	75,75,75,75	0
55	MG	2A	3135	1/1	0.99	0.21	71,71,71,71	0
55	MG	2Q	205	1/1	0.99	0.12	57,57,57,57	0
55	MG	2A	3368	1/1	0.99	0.13	63,63,63,63	0
55	MG	1A	3458	1/1	0.99	0.16	20,20,20,20	0
55	MG	2a	1628	1/1	0.99	0.22	80,80,80,80	0
55	MG	2A	3370	1/1	0.99	0.18	36,36,36,36	0
55	MG	1A	3432	1/1	0.99	0.18	14,14,14,14	0
55	MG	1A	3330	1/1	0.99	0.13	31,31,31,31	0
55	MG	1a	3111	1/1	0.99	0.15	55,55,55,55	0
55	MG	2A	3609	1/1	0.99	0.11	36,36,36,36	0
55	MG	1A	3286	1/1	0.99	0.17	25,25,25,25	0
55	MG	2A	3800	1/1	0.99	0.27	27,27,27,27	0
55	MG	2A	3656	1/1	0.99	0.11	45,45,45,45	0
55	MG	2A	3375	1/1	0.99	0.17	31,31,31,31	0
55	MG	1A	3024	1/1	0.99	0.30	34,34,34,34	0
55	MG	2A	3613	1/1	0.99	0.10	57,57,57,57	0
55	MG	2A	3450	1/1	0.99	0.33	62,62,62,62	0
55	MG	2A	3571	1/1	0.99	0.13	47,47,47,47	0
55	MG	20	104	1/1	0.99	0.07	68,68,68,68	0
55	MG	2A	3451	1/1	0.99	0.07	55,55,55,55	0
55	MG	1A	3296	1/1	0.99	0.20	31,31,31,31	0
55	MG	2A	3309	1/1	0.99	0.17	44,44,44,44	0
55	MG	2A	3310	1/1	0.99	0.21	46,46,46,46	0
55	MG	2A	3251	1/1	0.99	0.17	52,52,52,52	0

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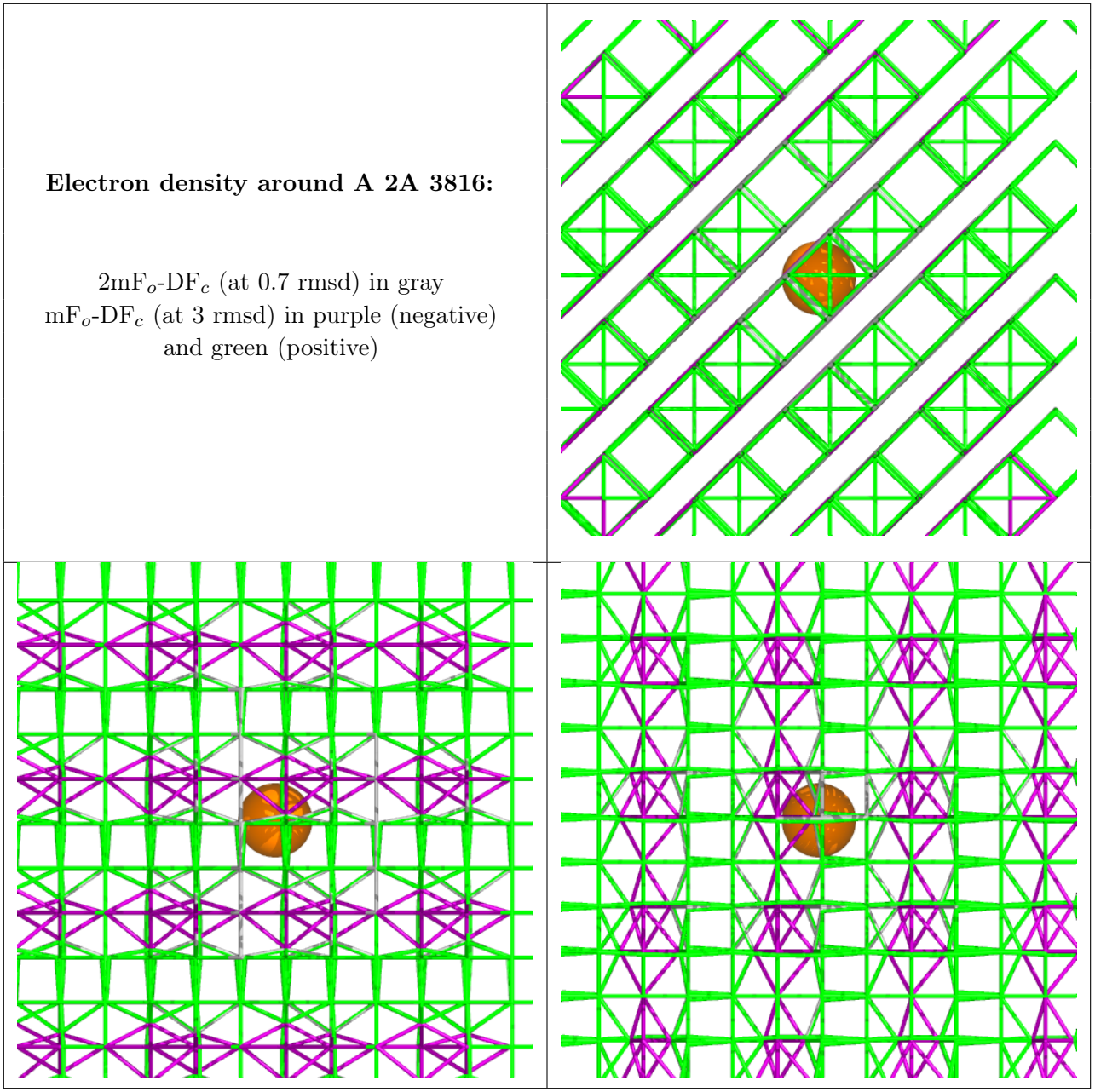
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3424	1/1	0.99	0.10	22,22,22,22	0
55	MG	1A	3739	1/1	0.99	0.08	19,19,19,19	0
55	MG	2A	3669	1/1	0.99	0.14	45,45,45,45	0
55	MG	1A	3085	1/1	0.99	0.22	38,38,38,38	0
55	MG	1A	3367	1/1	0.99	0.09	14,14,14,14	0
55	MG	2A	3625	1/1	0.99	0.06	67,67,67,67	0
55	MG	2A	3284	1/1	0.99	0.10	36,36,36,36	0
55	MG	1A	3427	1/1	0.99	0.14	27,27,27,27	0
55	MG	1a	3214	1/1	0.99	0.06	73,73,73,73	0
55	MG	2A	3287	1/1	0.99	0.21	57,57,57,57	0
55	MG	1A	3335	1/1	0.99	0.14	42,42,42,42	0
56	ZN	15	204	1/1	0.99	0.10	53,53,53,53	0
55	MG	2A	3465	1/1	0.99	0.18	34,34,34,34	0
55	MG	1B	215	1/1	0.99	0.15	50,50,50,50	0
55	MG	1A	3387	1/1	0.99	0.23	47,47,47,47	0
55	MG	1A	3781	1/1	0.99	0.08	36,36,36,36	0
55	MG	2A	3324	1/1	0.99	0.15	37,37,37,37	0
55	MG	2A	3591	1/1	0.99	0.18	56,56,56,56	0
56	ZN	26	101	1/1	0.99	0.12	66,66,66,66	0
55	MG	2A	3153	1/1	0.99	0.16	51,51,51,51	0
55	MG	2A	3685	1/1	0.99	0.34	55,55,55,55	0
57	SF4	1d	501	8/8	0.99	0.12	65,73,78,86	0
57	SF4	2d	501	8/8	0.99	0.09	67,72,87,89	0
55	MG	1A	3710	1/1	0.99	0.23	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A 2A 3816:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.