wwPDB X-ray Structure Validation Summary Report (i)

Sep 2, 2026 – 10:29 PM EDT

PDB ID	:	9Q6Q / pdb_00009q6q
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with pleuromutilin-18 triazole derivative and protein Y at 2.90A resolution
Authors	:	Killam, B.Y.; Kopec, I.; Breiner, L.M.; Hoernig, M.; LoPresti, M.; Abdelsattar, A.S.; Abouelkhair, A.A.; Briganti, A.J.; Slowinski, R.P.; Vogelaar, N.J.; Seleem, M.N.; Brown, A.M.; Lowell, A.N.; Polikanov, Y.S.
Deposited on	:	2025-08-22
Resolution	:	2.90 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 (1)) were used in the production of this report:

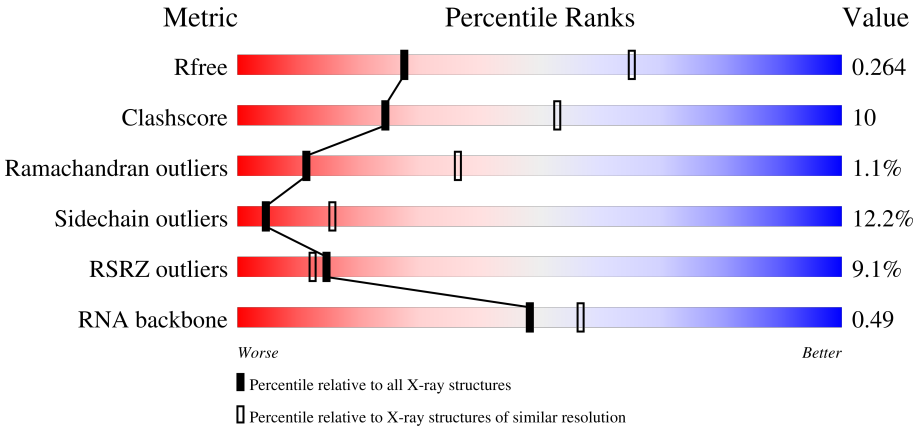
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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% 60% 33% 6%
1	2A	2915	6% 56% 35% 8%
2	1B	121	% 64% 32%
2	2B	121	9% 57% 37% 5%

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Mol	Chain	Length	Quality of chain
3	1D	276	2% 75% 22%
3	2D	276	3% 76% 20%
4	1E	206	67% 26% 6%
4	2E	206	2% 62% 31% 6%
5	1F	210	68% 24% 5%
5	2F	210	3% 59% 30% 8%
6	1G	182	8% 59% 35% 5%
6	2G	182	30% 53% 43%
7	1H	180	2% 71% 23%
7	2H	180	14% 47% 43% 6%
8	1I	148	9% 64% 26% 9%
8	2I	148	9% 70% 25%
9	1N	140	% 74% 22%
9	2N	140	3% 69% 27%
10	1O	122	% 70% 25% 5%
10	2O	122	6% 72% 26%
11	1P	150	3% 71% 27%
11	2P	150	2% 66% 30%
12	1Q	141	2% 75% 21%
12	2Q	141	6% 70% 26%
13	1R	118	65% 30% 5%
13	2R	118	% 57% 40%
14	1S	112	% 70% 24%
14	2S	112	13% 53% 40% 5%
15	1T	146	3% 64% 23% 10%

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Mol	Chain	Length	Quality of chain
15	2T	146	3% 61% 25% 10%
16	1U	118	2% 78% 19%
16	2U	118	4% 73% 22%
17	1V	101	% 75% 20%
17	2V	101	4% 66% 28%
18	1W	113	% 74% 19% 5%
18	2W	113	% 72% 20% 6%
19	1X	96	% 73% 22%
19	2X	96	3% 70% 27%
20	1Y	110	2% 66% 28%
20	2Y	110	20% 58% 35%
21	1Z	206	5% 67% 28%
21	2Z	206	17% 62% 31% 5%
22	10	85	2% 66% 21% 9%
22	20	85	6% 64% 26% 9%
23	11	98	4% 80% 16%
23	21	98	4% 62% 31% 6%
24	12	72	% 71% 24%
24	22	72	15% 64% 28% 6%
25	13	60	2% 73% 20% 5%
25	23	60	2% 60% 32% 7%
26	14	71	15% 51% 37% 8%
26	24	71	51% 54% 31% 11%
27	15	60	3% 72% 23%
27	25	60	2% 72% 25%

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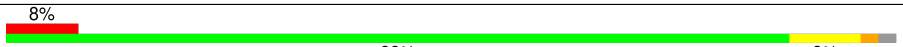
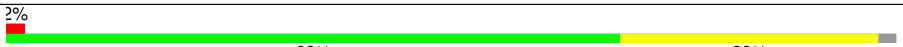
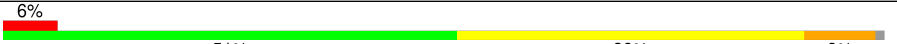
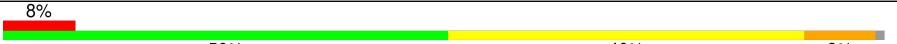
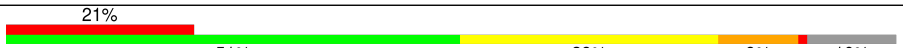
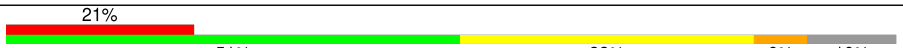
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	53% 41% 48% 10%
41	1j	105	39% 50% 32% 10% 8%
41	2j	105	49% 52% 34% 5% 9%
42	1k	129	9% 56% 27% 5% 12%
42	2k	129	7% 59% 25% 5% 12%
43	1l	132	2% 63% 26% 8%
43	2l	132	6% 61% 27% 5% 8%
44	1m	126	17% 54% 33% 6% 8%
44	2m	126	30% 51% 33% 6% 10%
45	1n	61	36% 41% 49% 8%
45	2n	61	49% 62% 33%
46	1o	89	9% 67% 28%
46	2o	89	3% 64% 31%
47	1p	88	14% 49% 38% 7% 7%
47	2p	88	11% 56% 35% 7%
48	1q	105	5% 62% 30% 6%
48	2q	105	5% 69% 22% 6%
49	1r	88	9% 56% 19% 23%
49	2r	88	6% 52% 22% 23%
50	1s	93	29% 55% 31% 11%
50	2s	93	40% 48% 37% 11%
51	1t	106	21% 61% 25% 9%
51	2t	106	8% 64% 26% 8%
52	1u	27	33% 56% 26% 15%
52	2u	27	48% 63% 22% 15%

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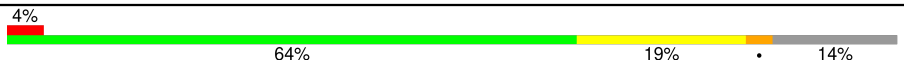
Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3856	-	-	-	X
54	MG	1A	3996	-	-	-	X
54	MG	2A	3706	-	-	-	X

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 297540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1011	Total 1011	Mg 1011	0	0
54	1B	30	Total 30	Mg 30	0	0
54	1D	18	Total 18	Mg 18	0	0
54	1E	9	Total 9	Mg 9	0	0
54	1F	16	Total 16	Mg 16	0	0
54	1G	4	Total 4	Mg 4	0	0
54	1H	3	Total 3	Mg 3	0	0
54	1N	2	Total 2	Mg 2	0	0
54	1O	2	Total 2	Mg 2	0	0
54	1P	6	Total 6	Mg 6	0	0
54	1Q	7	Total 7	Mg 7	0	0
54	1R	8	Total 8	Mg 8	0	0
54	1S	1	Total 1	Mg 1	0	0
54	1T	5	Total 5	Mg 5	0	0
54	1U	5	Total 5	Mg 5	0	0
54	1V	6	Total 6	Mg 6	0	0
54	1W	3	Total 3	Mg 3	0	0
54	1Y	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1Z	1	Total Mg 1 1	0	0
54	10	7	Total Mg 7 7	0	0
54	11	4	Total Mg 4 4	0	0
54	13	3	Total Mg 3 3	0	0
54	15	6	Total Mg 6 6	0	0
54	17	4	Total Mg 4 4	0	0
54	18	4	Total Mg 4 4	0	0
54	19	2	Total Mg 2 2	0	0
54	1a	270	Total Mg 270 270	0	0
54	1b	1	Total Mg 1 1	0	0
54	1d	5	Total Mg 5 5	0	0
54	1e	4	Total Mg 4 4	0	0
54	1f	2	Total Mg 2 2	0	0
54	1g	3	Total Mg 3 3	0	0
54	1h	2	Total Mg 2 2	0	0
54	1i	1	Total Mg 1 1	0	0
54	1l	2	Total Mg 2 2	0	0
54	1m	1	Total Mg 1 1	0	0
54	1n	2	Total Mg 2 2	0	0
54	1o	2	Total Mg 2 2	0	0
54	1p	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1t	2	Total Mg 2 2	0	0
54	1y	5	Total Mg 5 5	0	0
54	2A	732	Total Mg 732 732	0	0
54	2B	20	Total Mg 20 20	0	0
54	2D	7	Total Mg 7 7	0	0
54	2E	8	Total Mg 8 8	0	0
54	2F	4	Total Mg 4 4	0	0
54	2G	3	Total Mg 3 3	0	0
54	2I	1	Total Mg 1 1	0	0
54	2N	1	Total Mg 1 1	0	0
54	2O	1	Total Mg 1 1	0	0
54	2P	3	Total Mg 3 3	0	0
54	2Q	4	Total Mg 4 4	0	0
54	2R	2	Total Mg 2 2	0	0
54	2T	3	Total Mg 3 3	0	0
54	2U	1	Total Mg 1 1	0	0
54	2V	1	Total Mg 1 1	0	0
54	2W	3	Total Mg 3 3	0	0
54	2X	1	Total Mg 1 1	0	0
54	2Y	1	Total Mg 1 1	0	0
54	20	2	Total Mg 2 2	0	0

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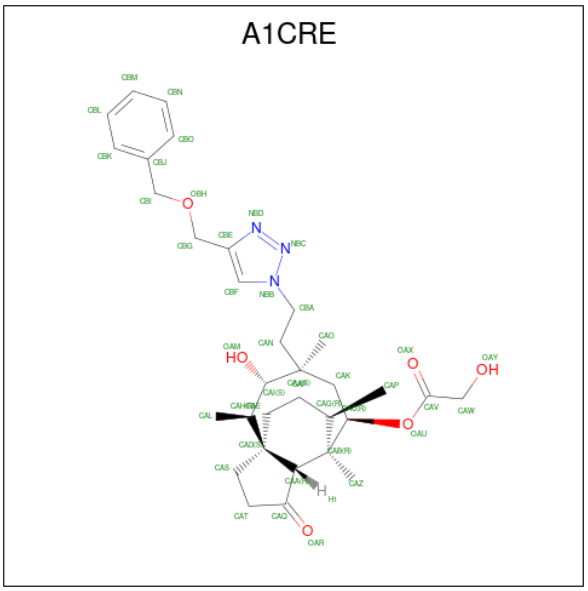
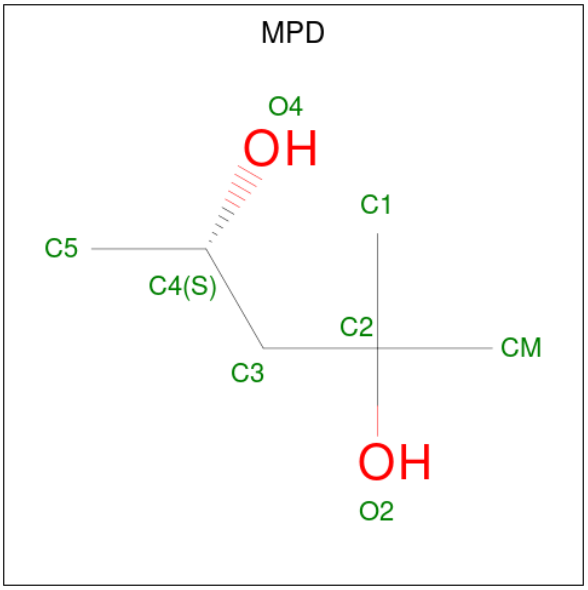
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	21	1	Total Mg 1 1	0	0
54	23	1	Total Mg 1 1	0	0
54	25	3	Total Mg 3 3	0	0
54	27	1	Total Mg 1 1	0	0
54	28	2	Total Mg 2 2	0	0
54	2a	192	Total Mg 192 192	0	0
54	2e	2	Total Mg 2 2	0	0
54	2f	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2k	1	Total Mg 1 1	0	0
54	2l	1	Total Mg 1 1	0	0
54	2o	1	Total Mg 1 1	0	0
54	2q	1	Total Mg 1 1	0	0
54	2r	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0
54	2y	1	Total Mg 1 1	0	0

- Molecule 55 is (3aS,4R,5S,6S,8R,9R,9aR,10R)-6-(2-{4-[(benzyloxy)methyl]-1H-1,2,3-triazol-1-yl}ethyl)-5-hydroxy-4,6,9,10-tetramethyl-1-oxodecahydro-3a,9-propanocyclopenta[8]annulen-8-yl hydroxyacetate (CCD ID: A1CRE) (formula: $C_{32}H_{45}N_3O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1A	1	Total C N O 41 32 3 6	0	0
55	2A	1	Total C N O 41 32 3 6	0	0

- Molecule 56 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



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

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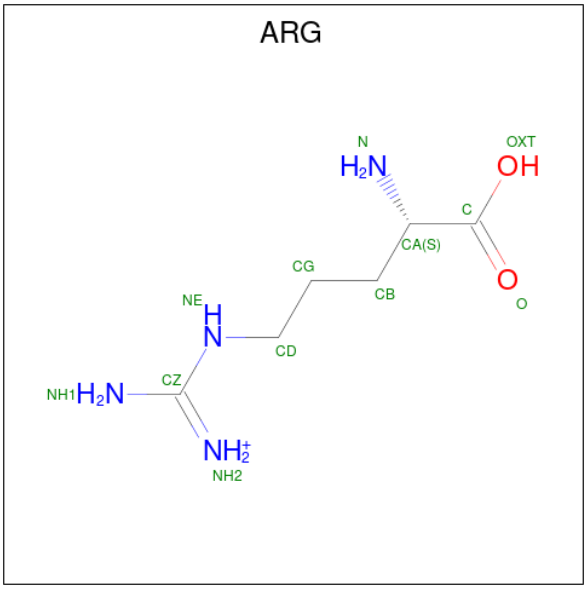
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1a	1	Total C O 8 6 2	0	0
56	1a	1	Total C O 8 6 2	0	0
56	2A	1	Total C O 8 6 2	0	0
56	2A	1	Total C O 8 6 2	0	0
56	2B	1	Total C O 8 6 2	0	0

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



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

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

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

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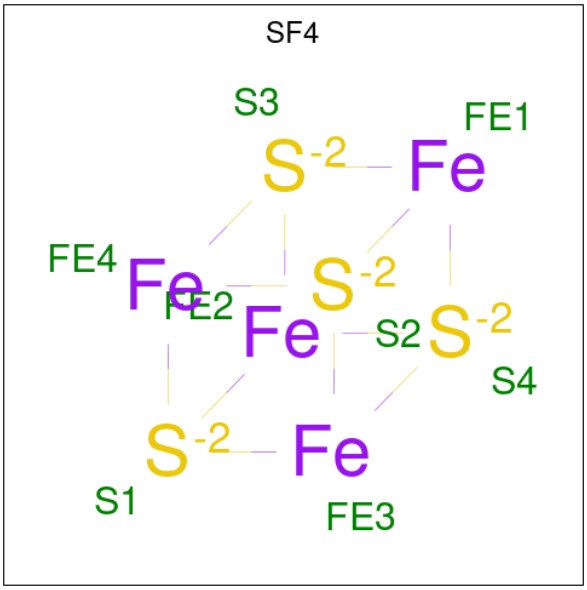
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	15	1	Total Zn 1 1	0	0
58	16	1	Total Zn 1 1	0	0
58	19	1	Total Zn 1 1	0	0
58	1n	1	Total Zn 1 1	0	0
58	2Y	1	Total Zn 1 1	0	0
58	24	1	Total Zn 1 1	0	0
58	25	1	Total Zn 1 1	0	0
58	26	1	Total Zn 1 1	0	0
58	29	1	Total Zn 1 1	0	0
58	2n	1	Total Zn 1 1	0	0

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



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

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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	3794	Total O 3794 3794	0	0
60	1B	98	Total O 98 98	0	0
60	1D	112	Total O 112 112	0	0
60	1E	73	Total O 73 73	0	0
60	1F	61	Total O 61 61	0	0
60	1G	20	Total O 20 20	0	0
60	1H	14	Total O 14 14	0	0
60	1I	8	Total O 8 8	0	0
60	1N	51	Total O 51 51	0	0
60	1O	20	Total O 20 20	0	0
60	1P	64	Total O 64 64	0	0
60	1Q	39	Total O 39 39	0	0
60	1R	30	Total O 30 30	0	0
60	1S	8	Total O 8 8	0	0
60	1T	39	Total O 39 39	0	0
60	1U	39	Total O 39 39	0	0
60	1V	38	Total O 38 38	0	0
60	1W	28	Total O 28 28	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1X	26	Total O 26 26	0	0
60	1Y	15	Total O 15 15	0	0
60	1Z	11	Total O 11 11	0	0
60	10	26	Total O 26 26	0	0
60	11	25	Total O 25 25	0	0
60	12	15	Total O 15 15	0	0
60	13	23	Total O 23 23	0	0
60	14	1	Total O 1 1	0	0
60	15	29	Total O 29 29	0	0
60	16	14	Total O 14 14	0	0
60	17	13	Total O 13 13	0	0
60	18	28	Total O 28 28	0	0
60	19	11	Total O 11 11	0	0
60	1a	532	Total O 532 532	0	0
60	1b	1	Total O 1 1	0	0
60	1d	9	Total O 9 9	0	0
60	1e	6	Total O 6 6	0	0
60	1f	2	Total O 2 2	0	0
60	1g	1	Total O 1 1	0	0
60	1h	2	Total O 2 2	0	0
60	1i	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1j	1	Total O 1 1	0	0
60	1l	5	Total O 5 5	0	0
60	1m	2	Total O 2 2	0	0
60	1o	2	Total O 2 2	0	0
60	1p	3	Total O 3 3	0	0
60	1q	1	Total O 1 1	0	0
60	1r	1	Total O 1 1	0	0
60	1t	1	Total O 1 1	0	0
60	1u	1	Total O 1 1	0	0
60	1y	6	Total O 6 6	0	0
60	2A	2275	Total O 2275 2275	0	0
60	2B	60	Total O 60 60	0	0
60	2D	50	Total O 50 50	0	0
60	2E	29	Total O 29 29	0	0
60	2F	20	Total O 20 20	0	0
60	2G	6	Total O 6 6	0	0
60	2H	3	Total O 3 3	0	0
60	2I	3	Total O 3 3	0	0
60	2N	5	Total O 5 5	0	0
60	2O	15	Total O 15 15	0	0
60	2P	26	Total O 26 26	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2Q	20	Total O 20 20	0	0
60	2R	17	Total O 17 17	0	0
60	2S	5	Total O 5 5	0	0
60	2T	13	Total O 13 13	0	0
60	2U	8	Total O 8 8	0	0
60	2V	7	Total O 7 7	0	0
60	2W	21	Total O 21 21	0	0
60	2X	7	Total O 7 7	0	0
60	2Y	3	Total O 3 3	0	0
60	2Z	13	Total O 13 13	0	0
60	20	12	Total O 12 12	0	0
60	21	19	Total O 19 19	0	0
60	23	3	Total O 3 3	0	0
60	24	1	Total O 1 1	0	0
60	25	11	Total O 11 11	0	0
60	26	5	Total O 5 5	0	0
60	27	11	Total O 11 11	0	0
60	28	14	Total O 14 14	0	0
60	29	1	Total O 1 1	0	0
60	2a	436	Total O 436 436	0	0
60	2d	5	Total O 5 5	0	0

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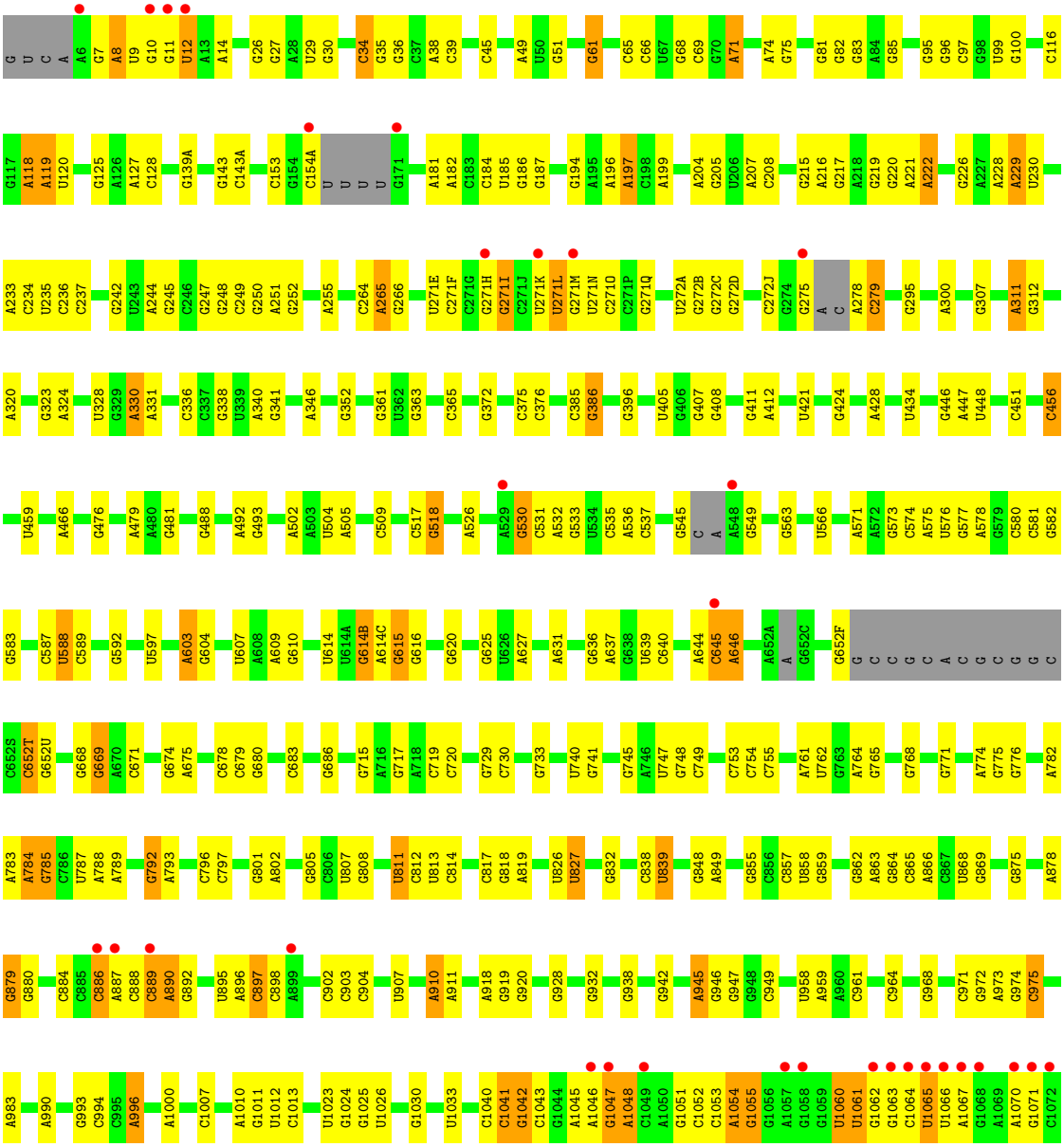
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2e	3	Total O 3 3	0	0
60	2f	2	Total O 2 2	0	0
60	2j	2	Total O 2 2	0	0
60	2l	4	Total O 4 4	0	0
60	2m	1	Total O 1 1	0	0
60	2n	1	Total O 1 1	0	0
60	2o	4	Total O 4 4	0	0
60	2p	4	Total O 4 4	0	0
60	2q	1	Total O 1 1	0	0
60	2r	3	Total O 3 3	0	0
60	2t	1	Total O 1 1	0	0
60	2u	1	Total O 1 1	0	0
60	2y	8	Total O 8 8	0	0

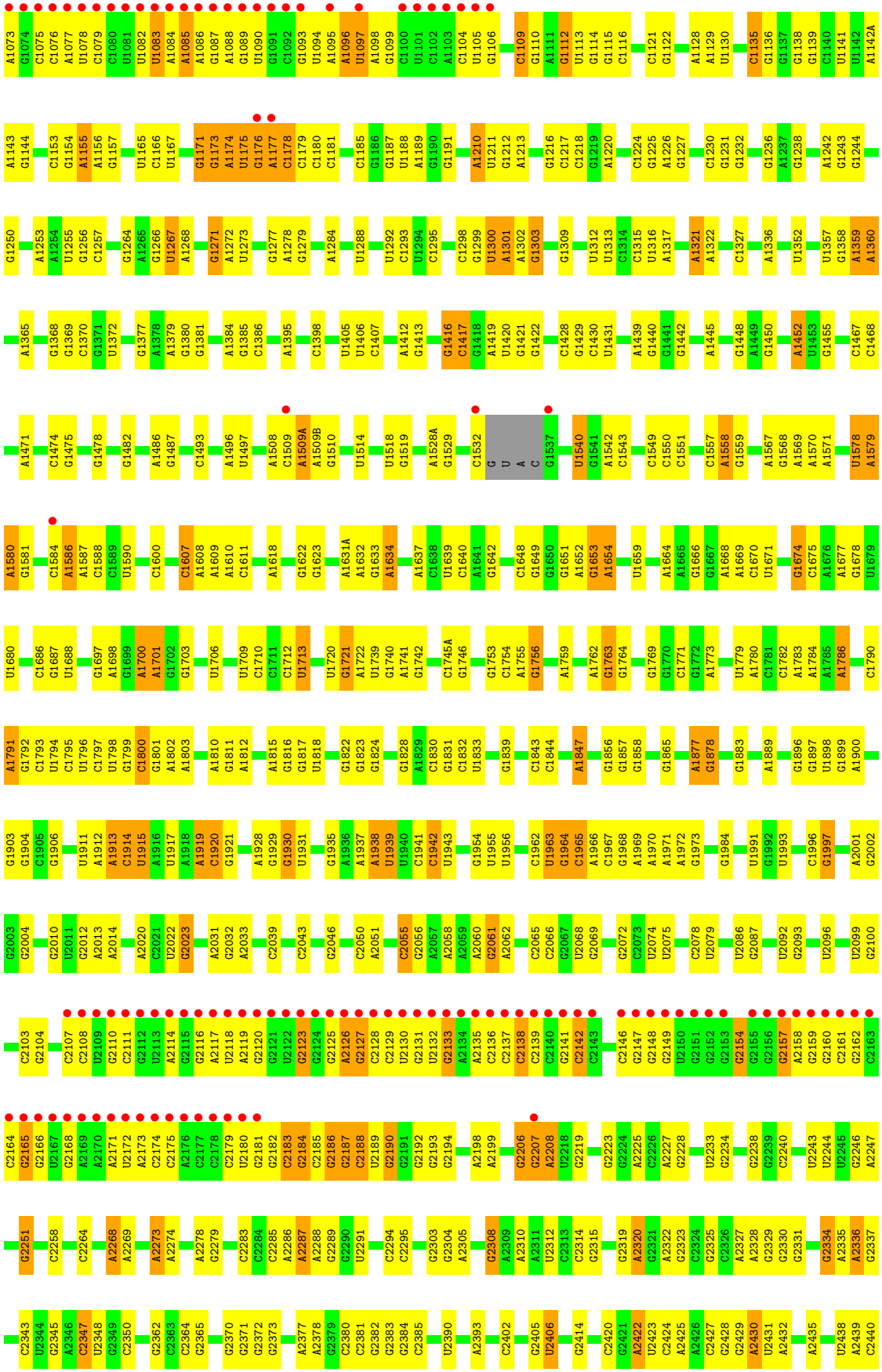
3 Residue-property plots (i)

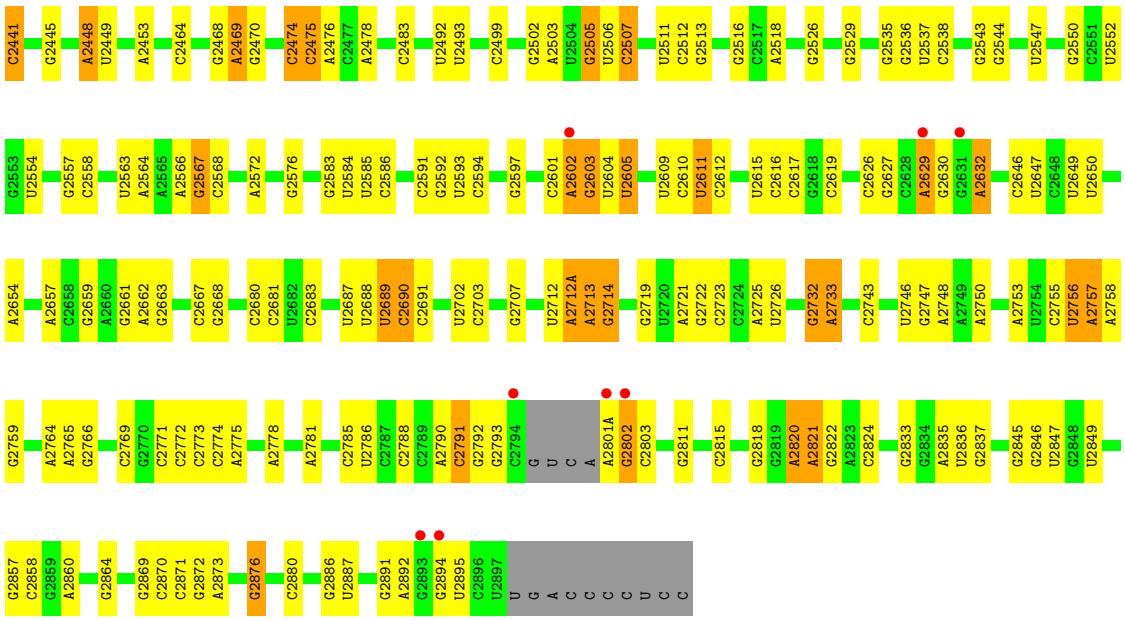
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:

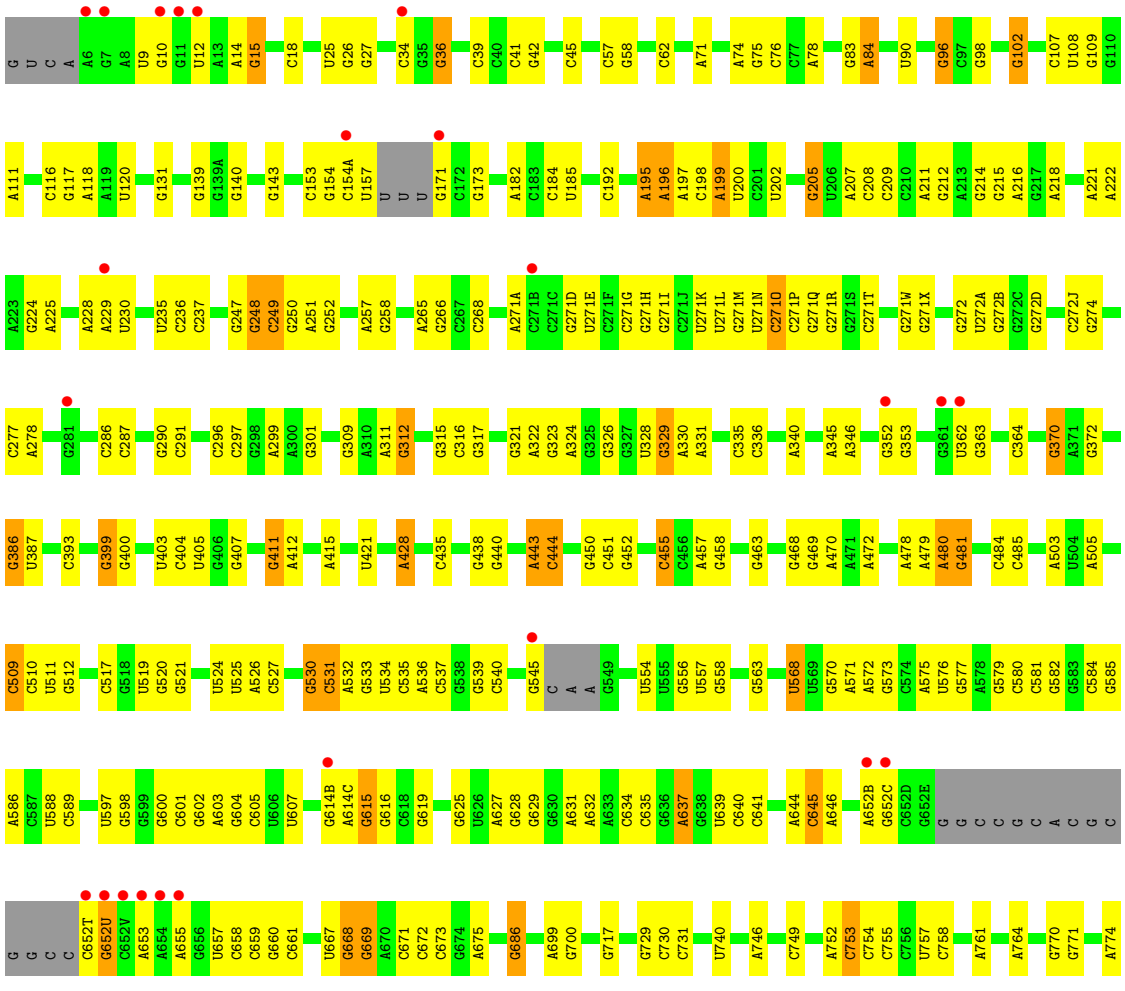


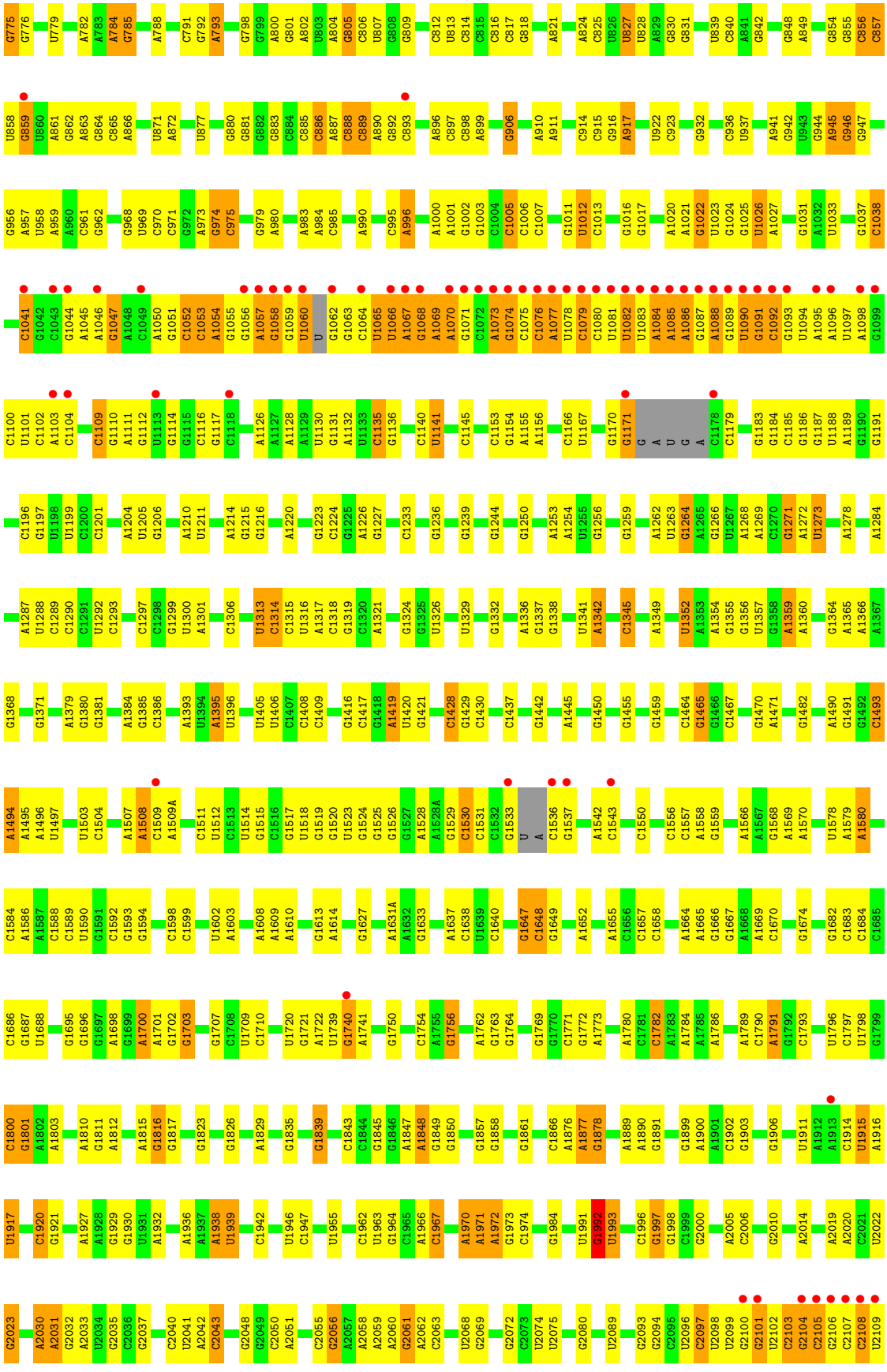


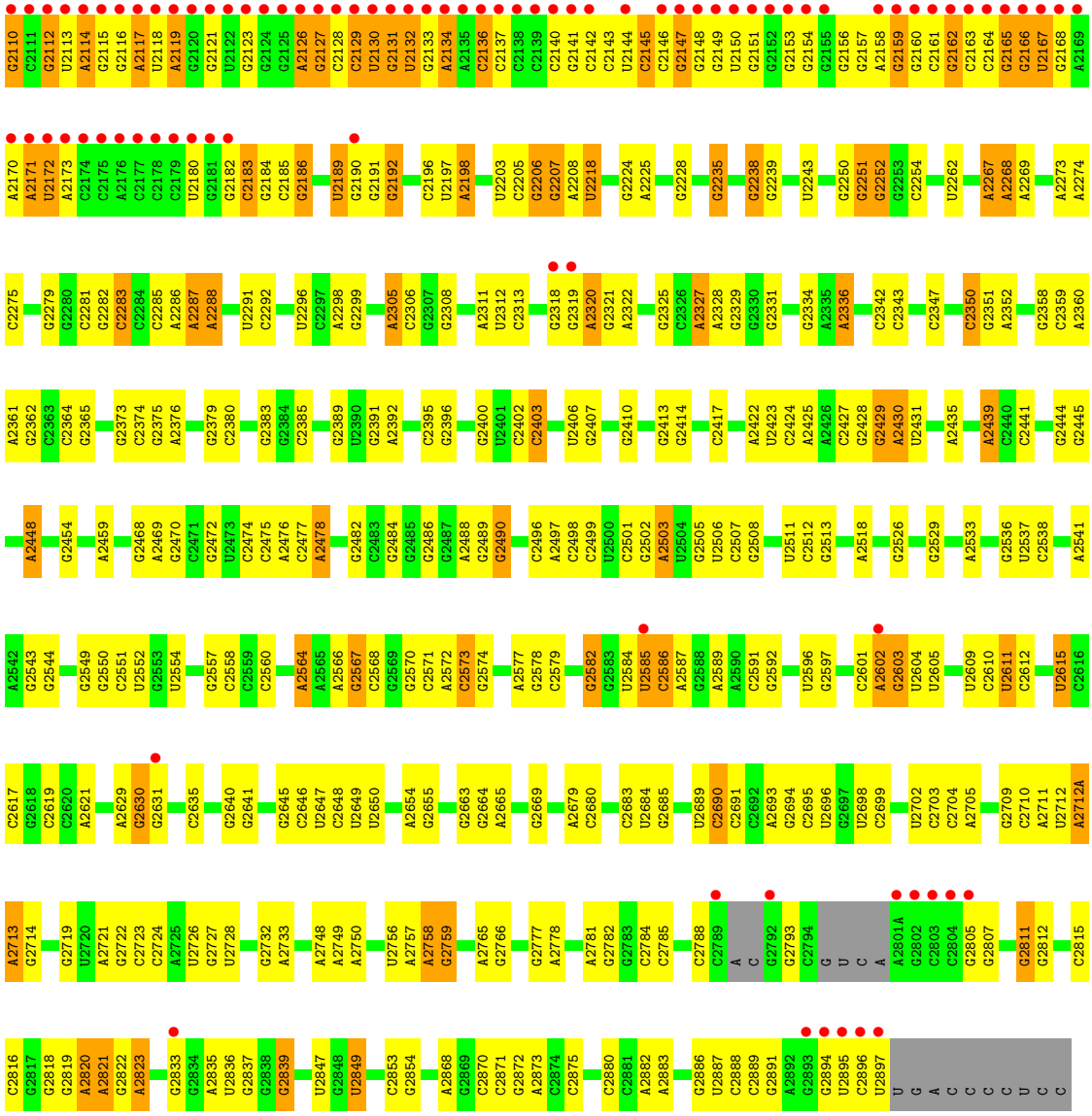


• Molecule 1: 23S Ribosomal RNA

Chain 2A:

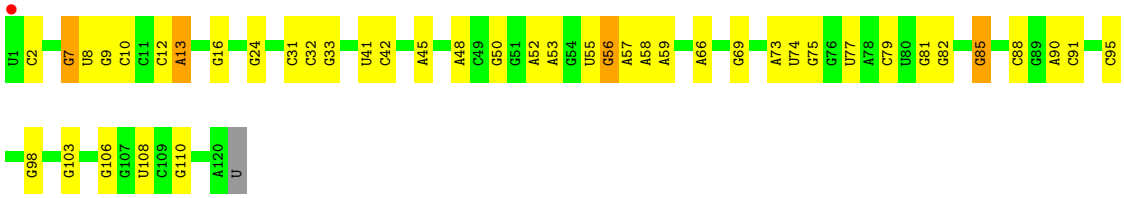






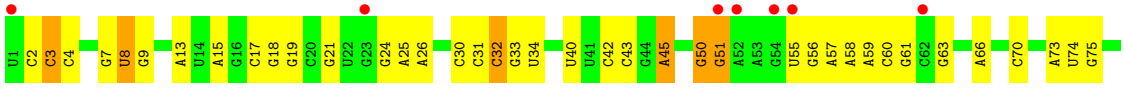
• Molecule 2: 5S Ribosomal RNA

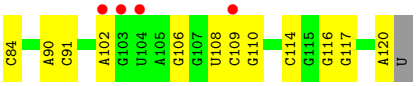
Chain 1B:



• Molecule 2: 5S Ribosomal RNA

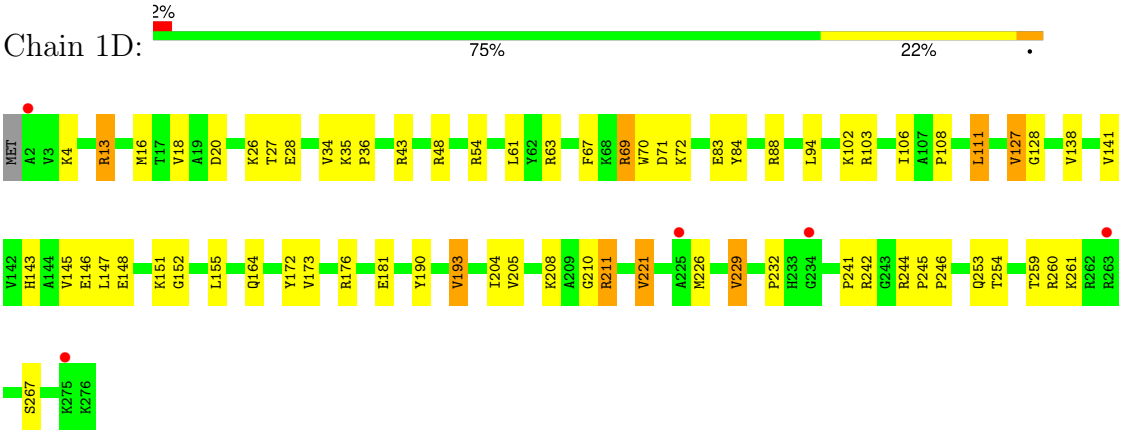
Chain 2B:





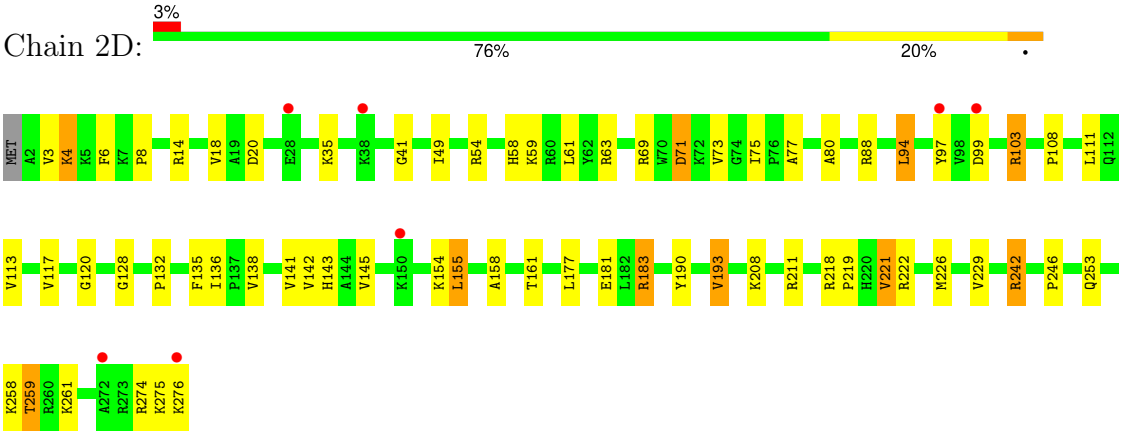
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



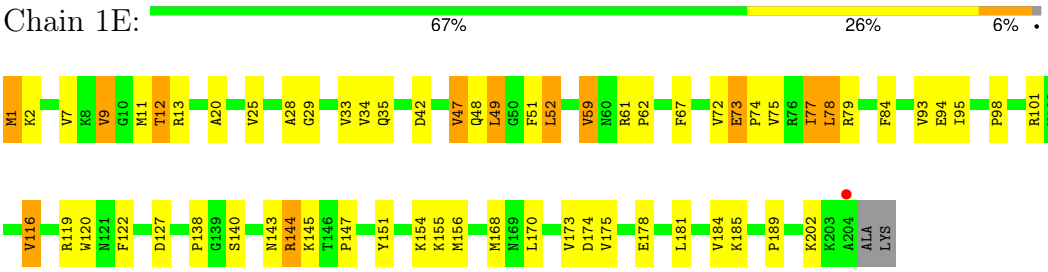
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



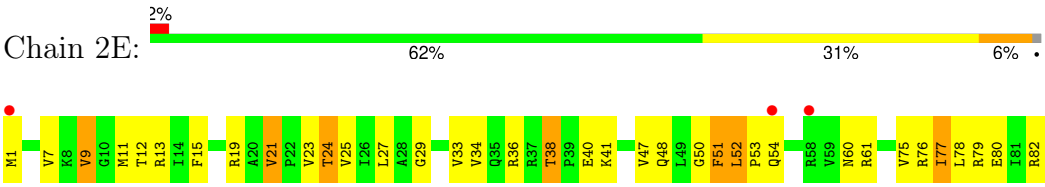
• Molecule 4: 50S ribosomal protein L3

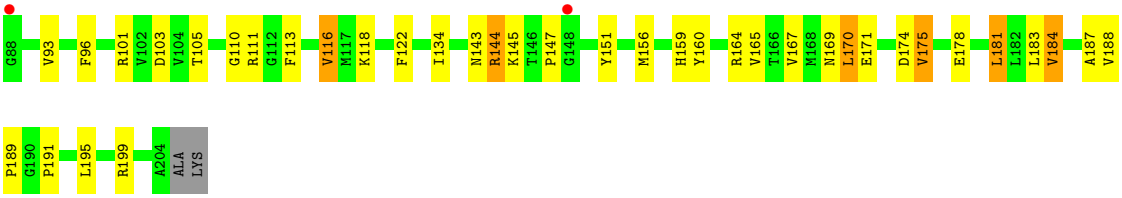
Chain 1E:



• Molecule 4: 50S ribosomal protein L3

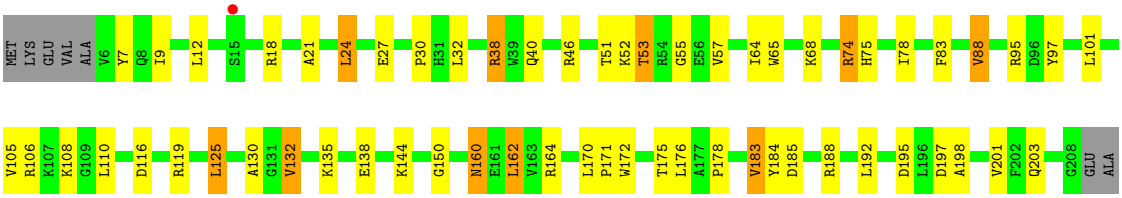
Chain 2E:





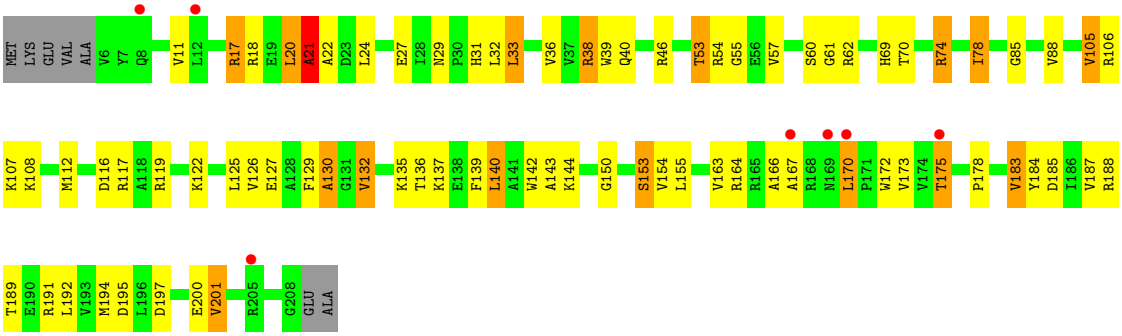
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



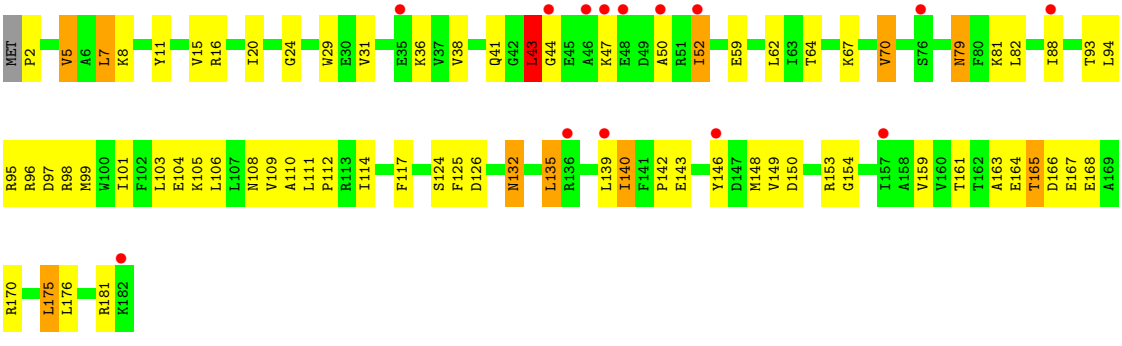
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



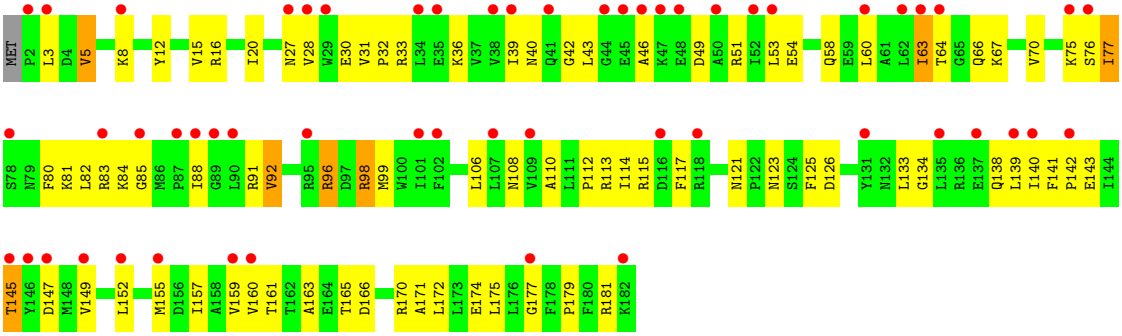
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



• Molecule 6: 50S ribosomal protein L5

Chain 2G:



• Molecule 7: 50S ribosomal protein L6

Chain 1H:

• Molecule 7: 50S ribosomal protein L6

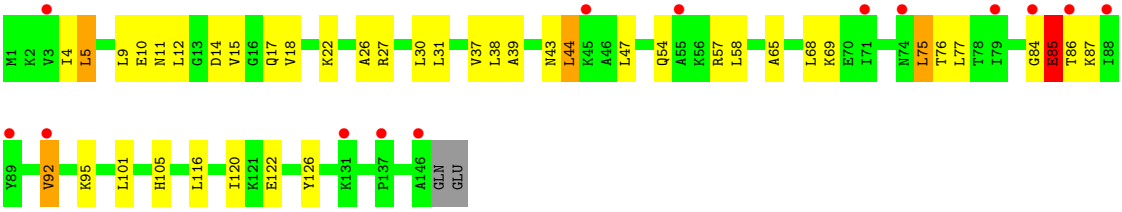
Chain 2H:

• Molecule 8: 50S ribosomal protein L9

Chain 1I:

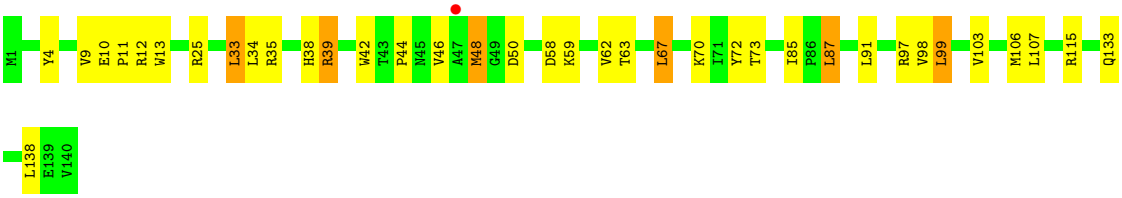
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



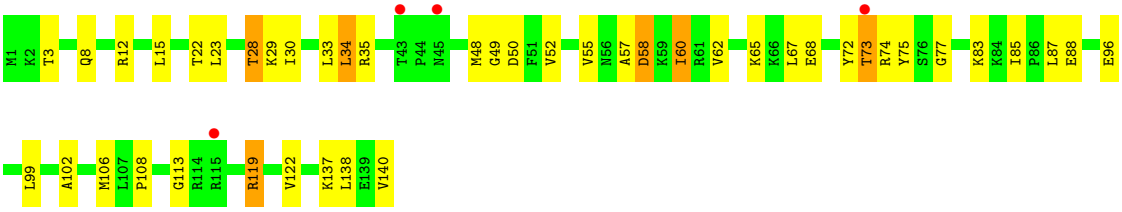
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



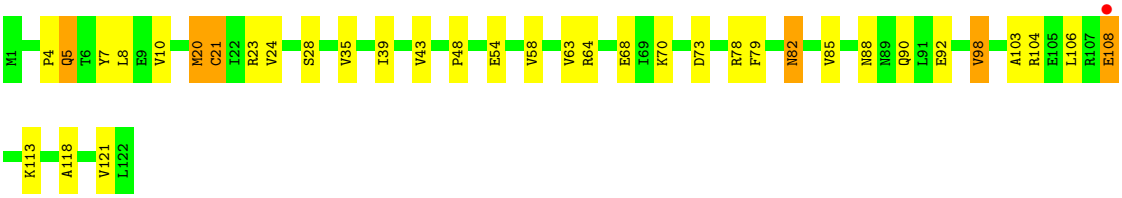
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



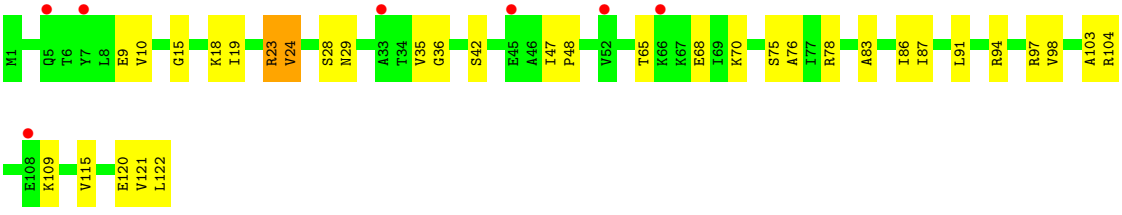
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



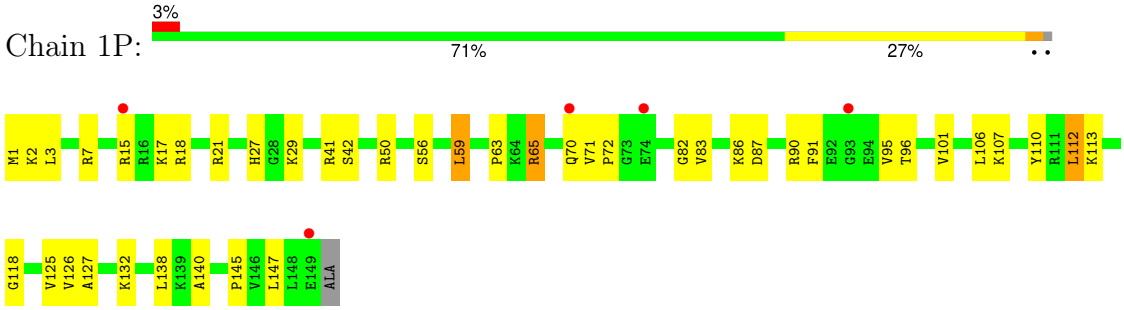
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



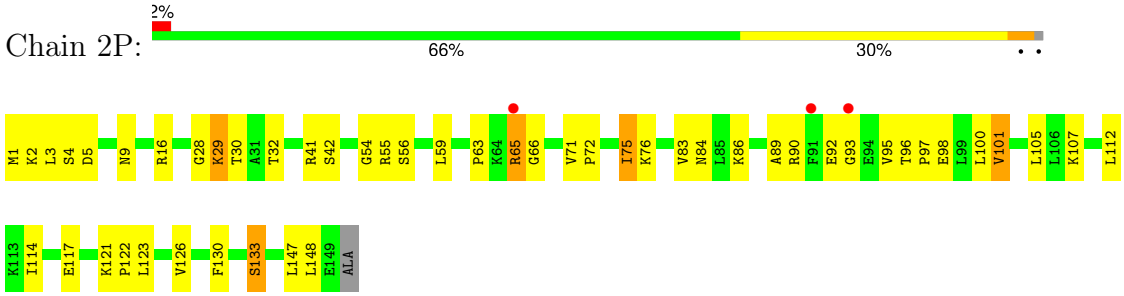
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



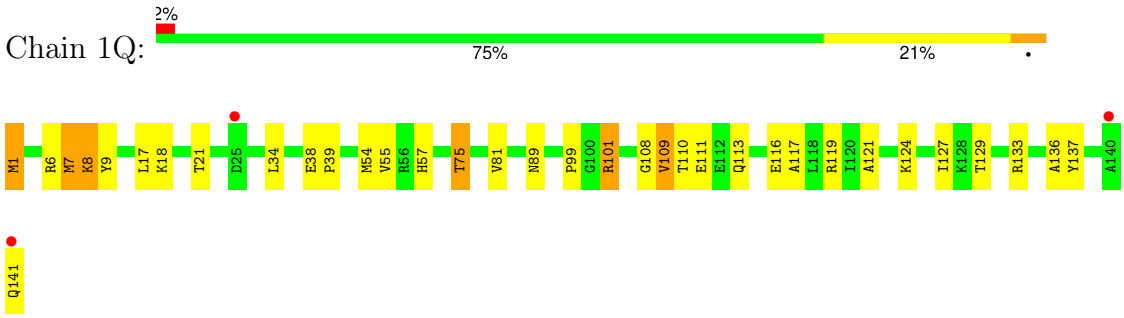
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



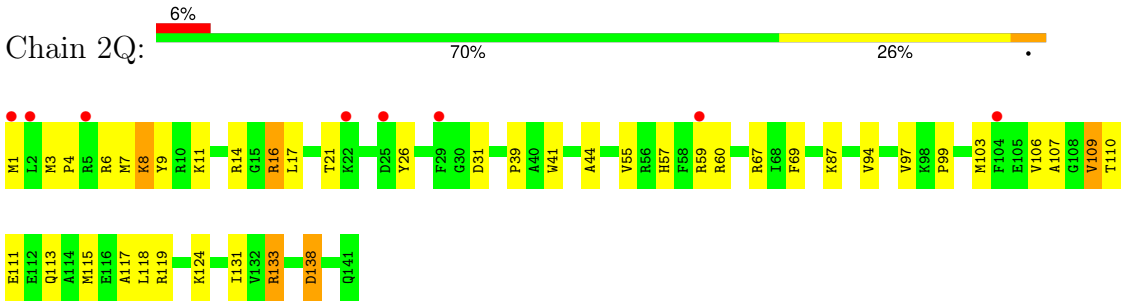
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



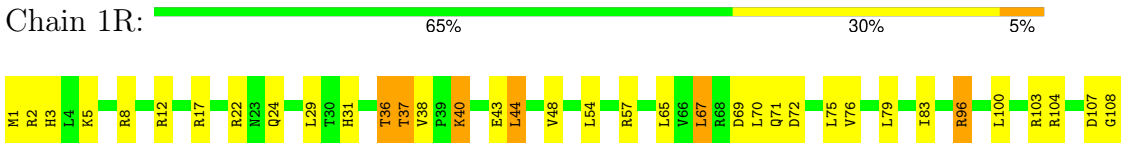
• Molecule 12: 50S ribosomal protein L16

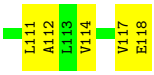
Chain 2Q:



• Molecule 13: 50S ribosomal protein L17

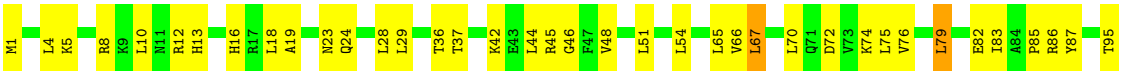
Chain 1R:

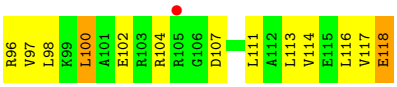




• Molecule 13: 50S ribosomal protein L17

Chain 2R:



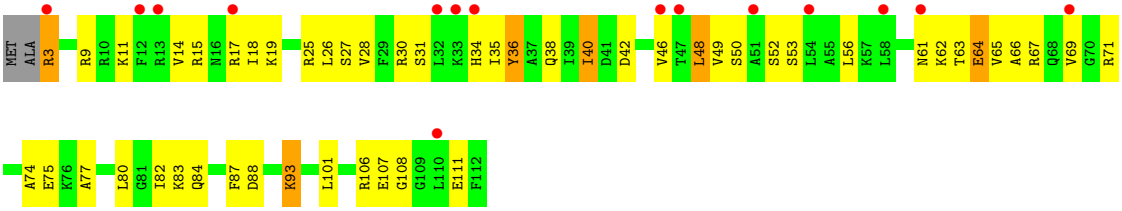


• Molecule 14: 50S ribosomal protein L18

Chain 1S:

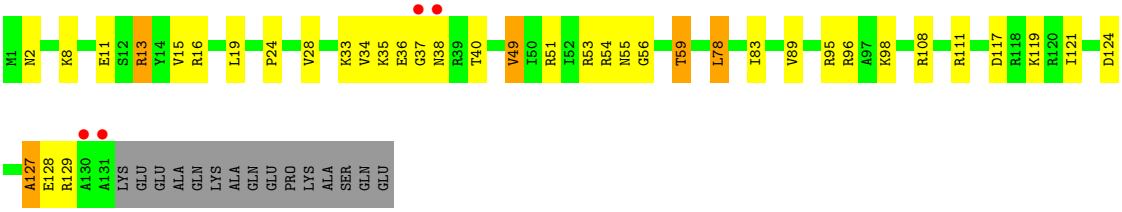
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



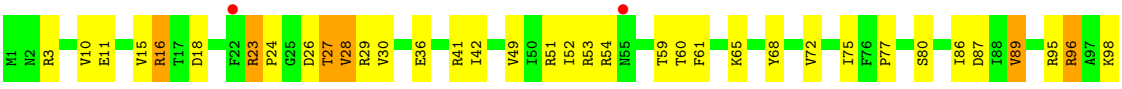
• Molecule 15: 50S ribosomal protein L19

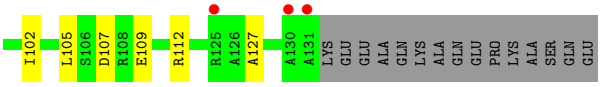
Chain 1T:



• Molecule 15: 50S ribosomal protein L19

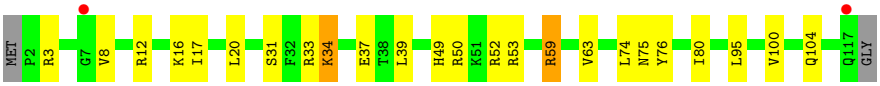
Chain 2T:





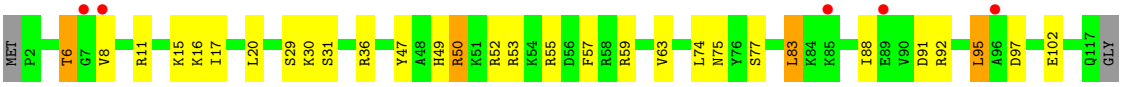
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



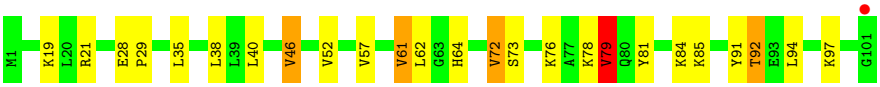
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



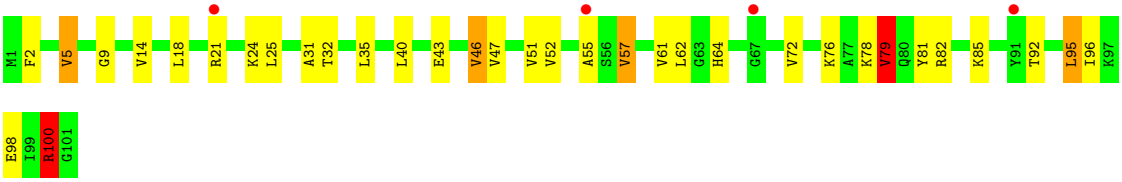
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



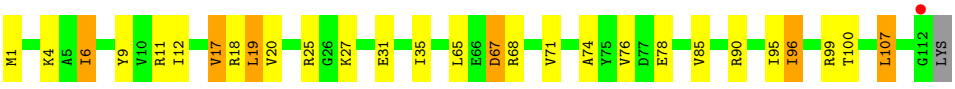
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



• Molecule 18: 50S ribosomal protein L22

Chain 1W:

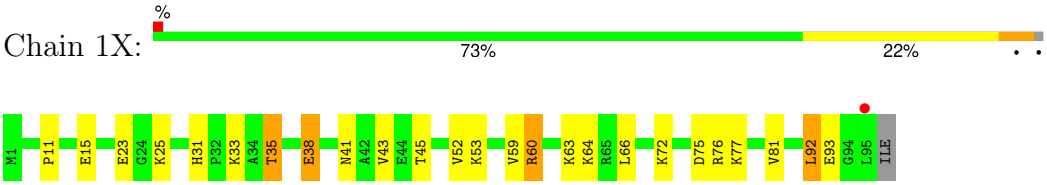


• Molecule 18: 50S ribosomal protein L22

Chain 2W:

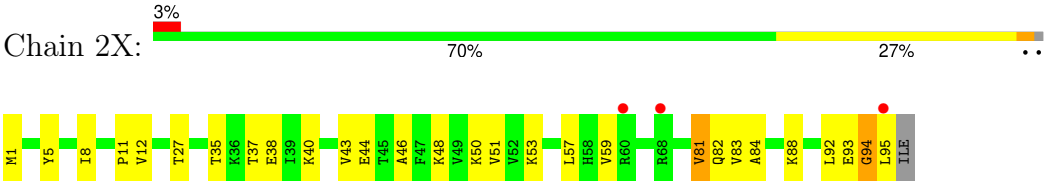
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



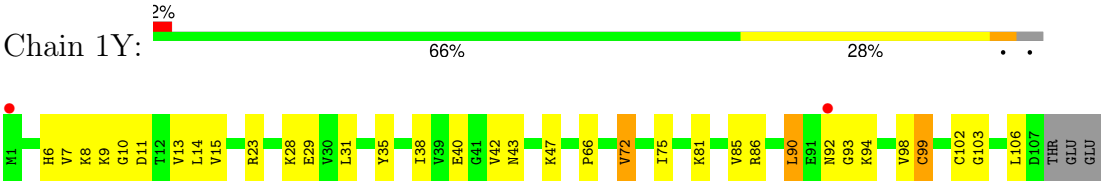
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



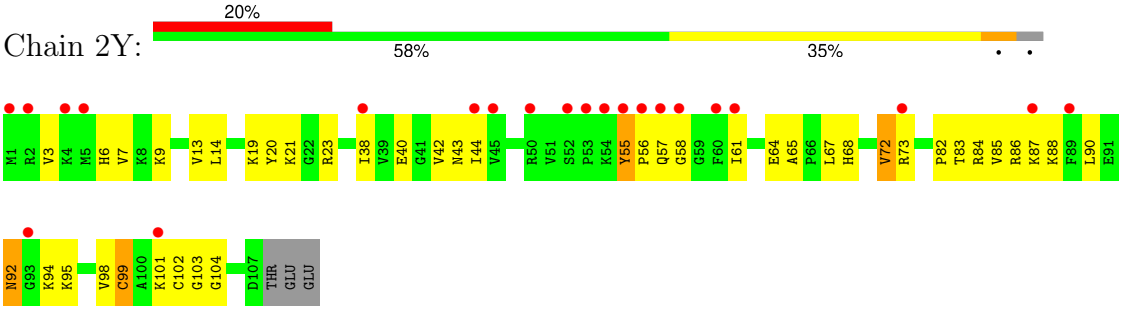
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



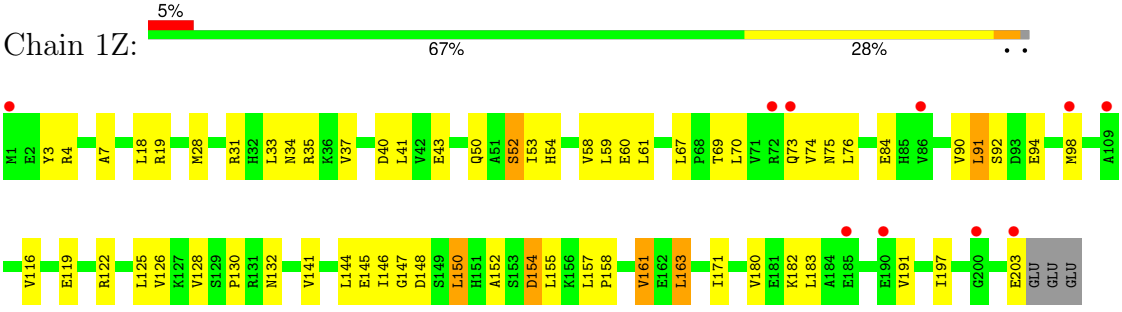
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



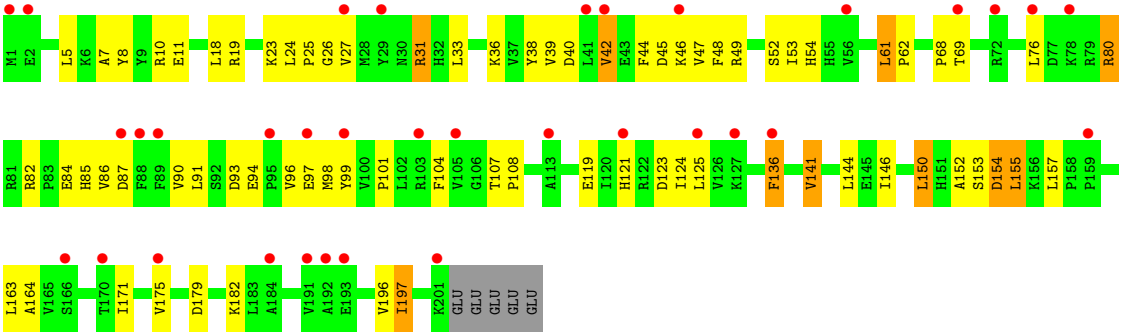
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:

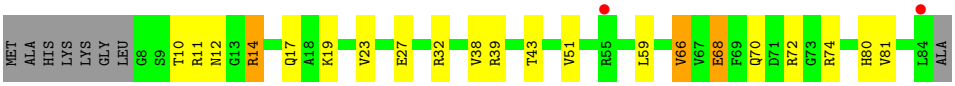


• Molecule 21: 50S ribosomal protein L25

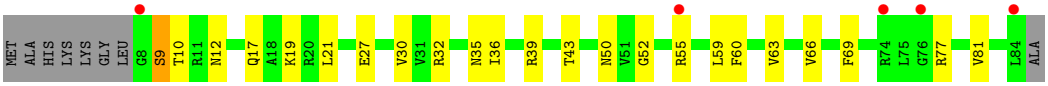
Chain 2Z:



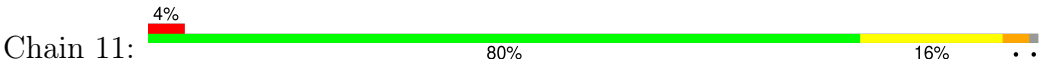
• Molecule 22: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28

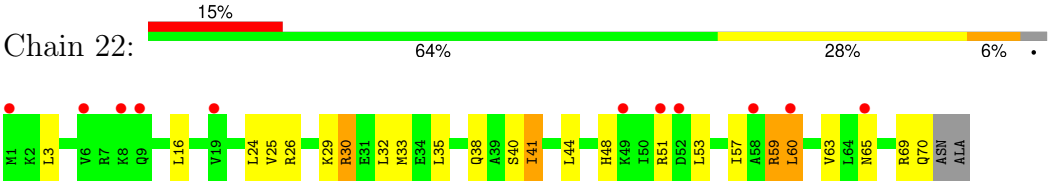


• Molecule 23: 50S ribosomal protein L28

• Molecule 24: 50S ribosomal protein L29

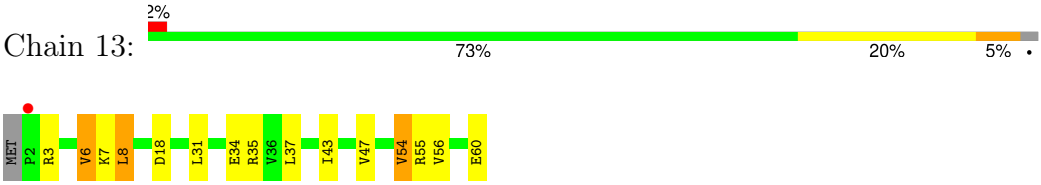
• Molecule 24: 50S ribosomal protein L29

Chain 22:



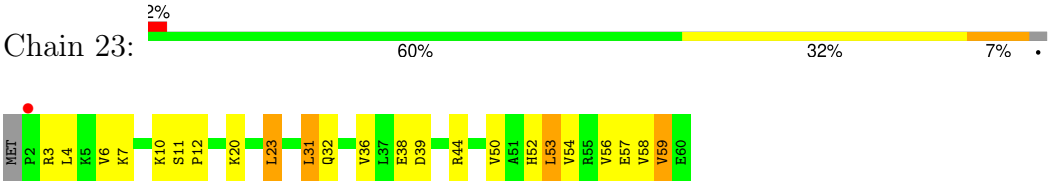
• Molecule 25: 50S ribosomal protein L30

Chain 13:



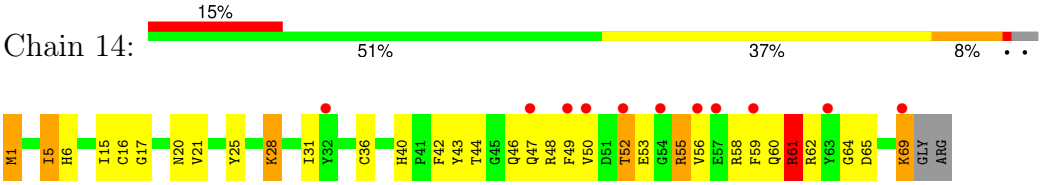
• Molecule 25: 50S ribosomal protein L30

Chain 23:



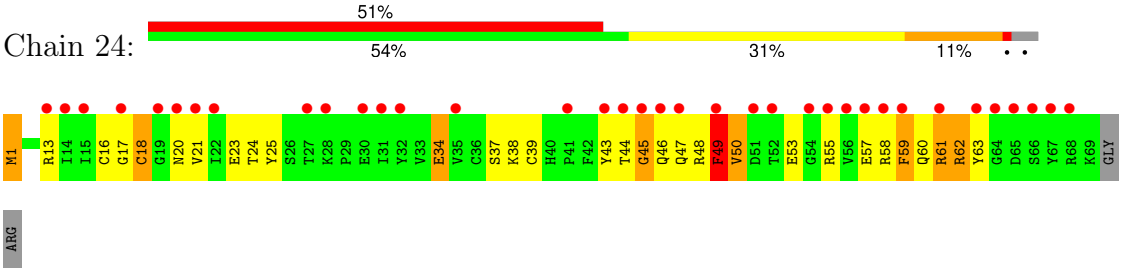
• Molecule 26: 50S ribosomal protein L31

Chain 14:



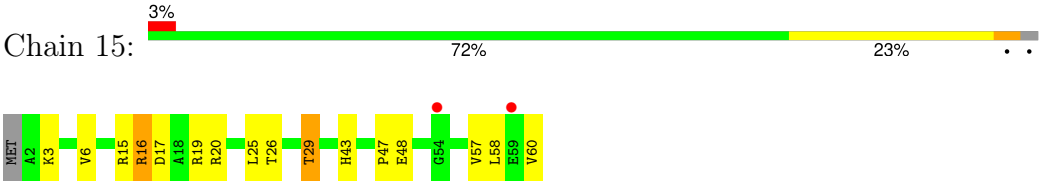
• Molecule 26: 50S ribosomal protein L31

Chain 24:



• Molecule 27: 50S ribosomal protein L32

Chain 15:

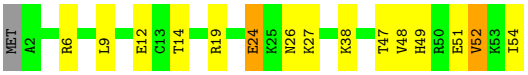


• Molecule 27: 50S ribosomal protein L32

Chain 25:

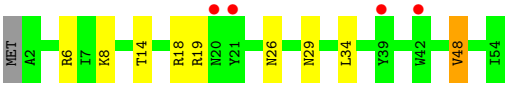
• Molecule 28: 50S ribosomal protein L33

Chain 16:



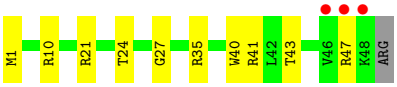
• Molecule 28: 50S ribosomal protein L33

Chain 26:



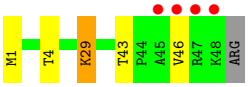
• Molecule 29: 50S ribosomal protein L34

Chain 17:



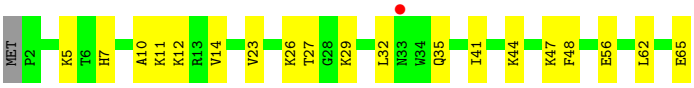
• Molecule 29: 50S ribosomal protein L34

Chain 27:



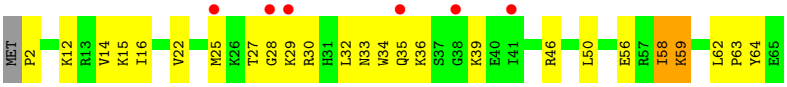
• Molecule 30: 50S ribosomal protein L35

Chain 18:



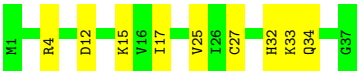
• Molecule 30: 50S ribosomal protein L35

Chain 28:



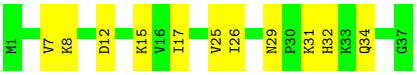
• Molecule 31: 50S ribosomal protein L36

Chain 19:



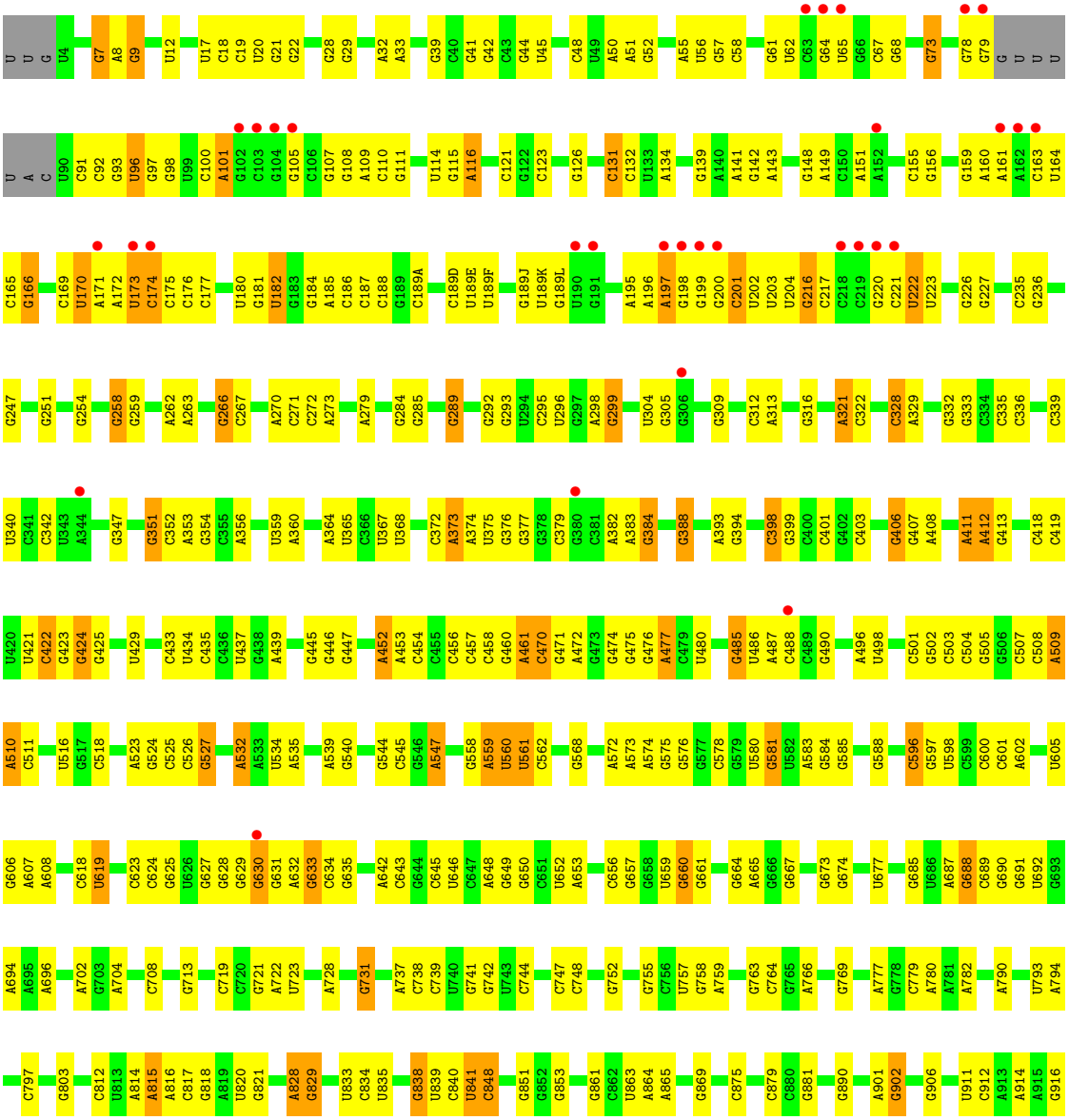
• Molecule 31: 50S ribosomal protein L36

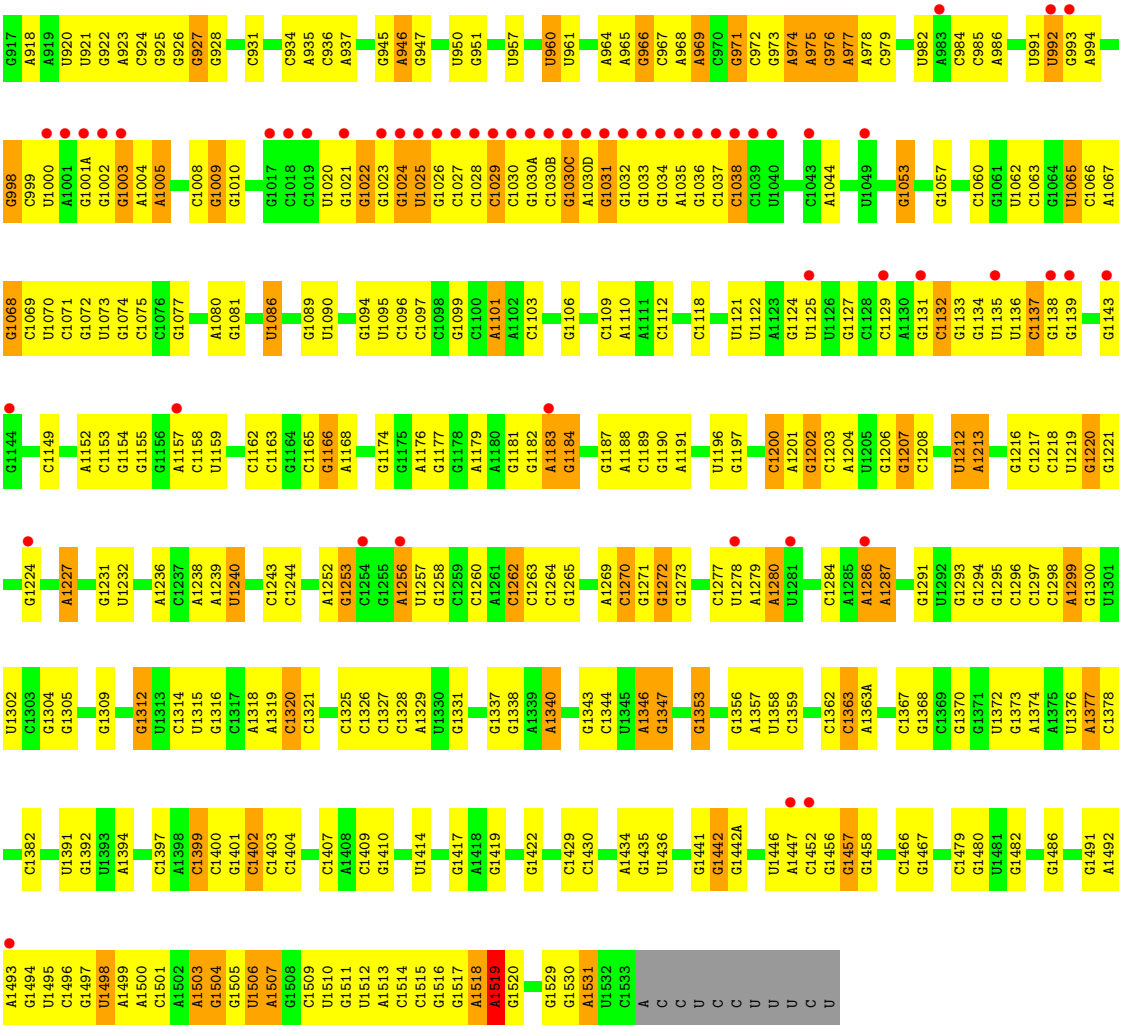
Chain 29:



• Molecule 32: 16S Ribosomal RNA

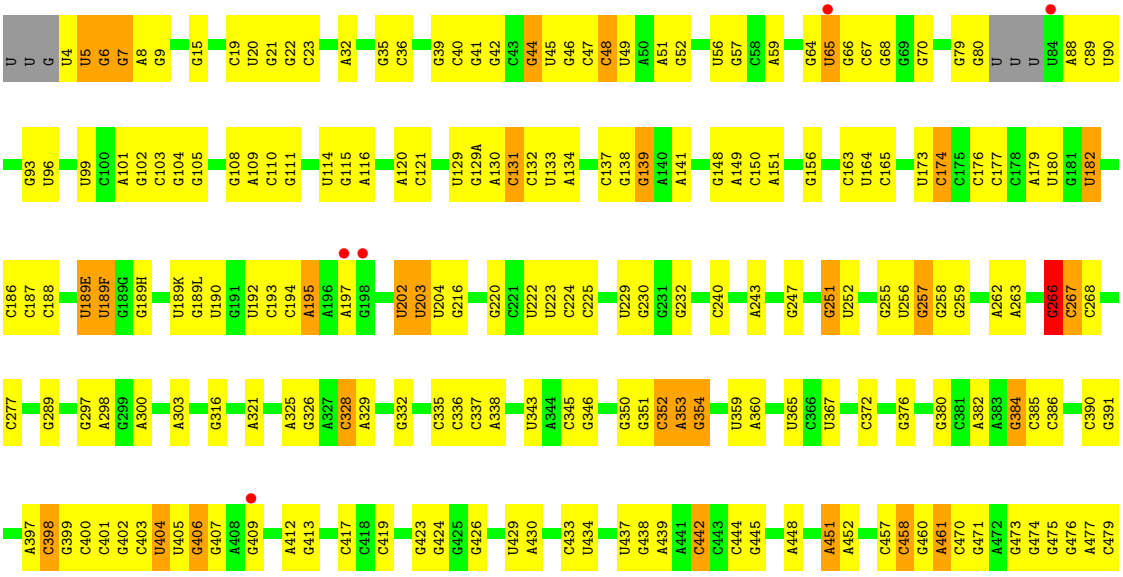
Chain 1a:

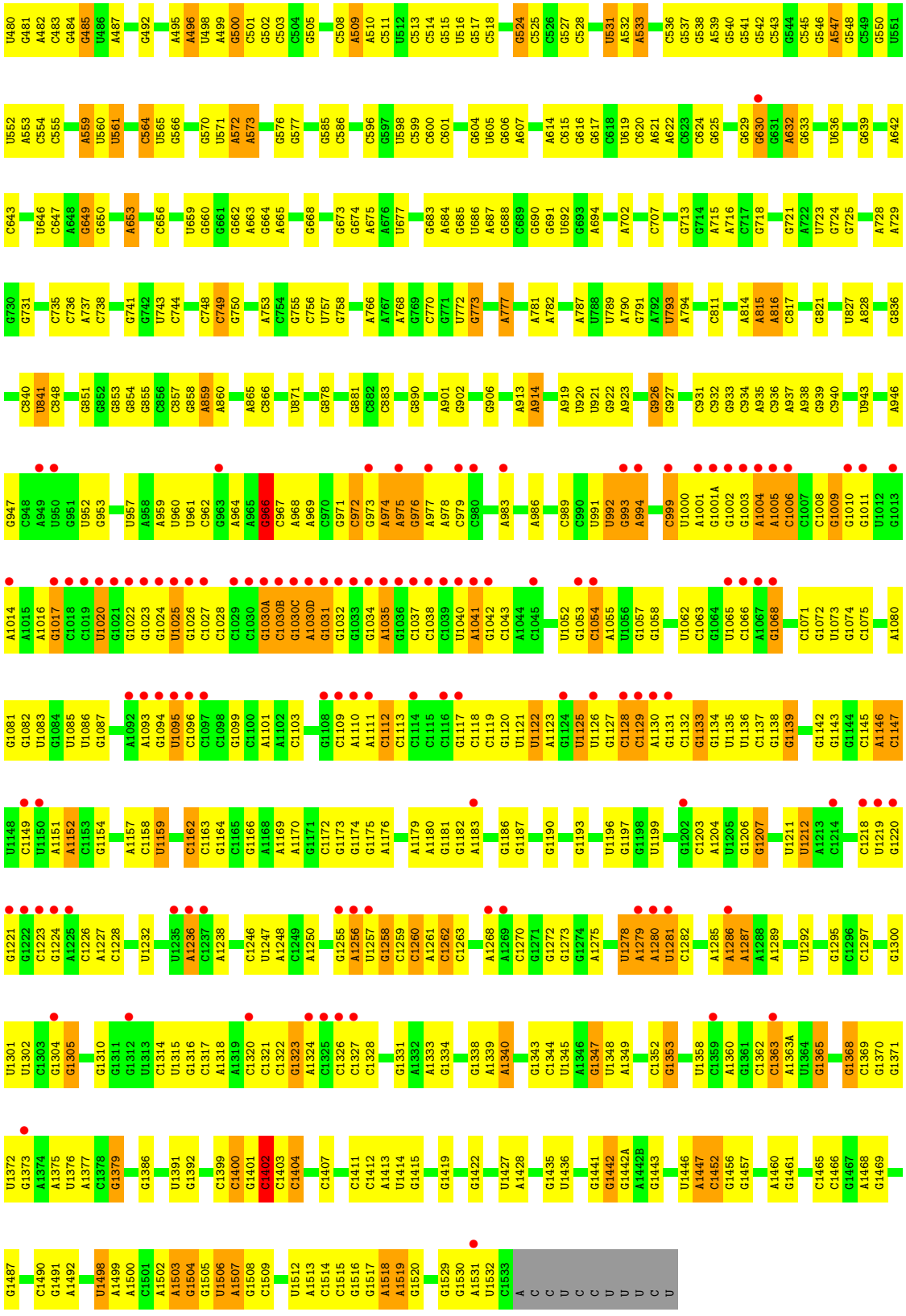




• Molecule 32: 16S Ribosomal RNA

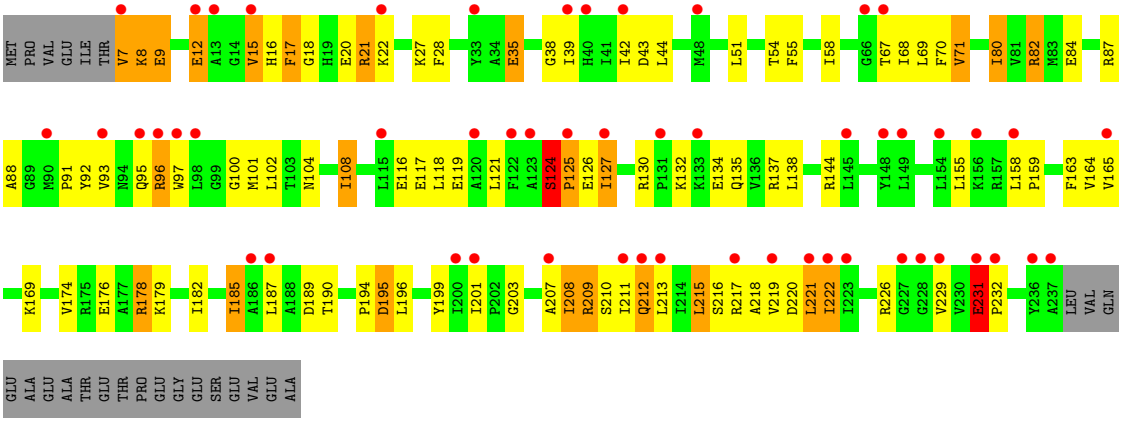
Chain 2a:





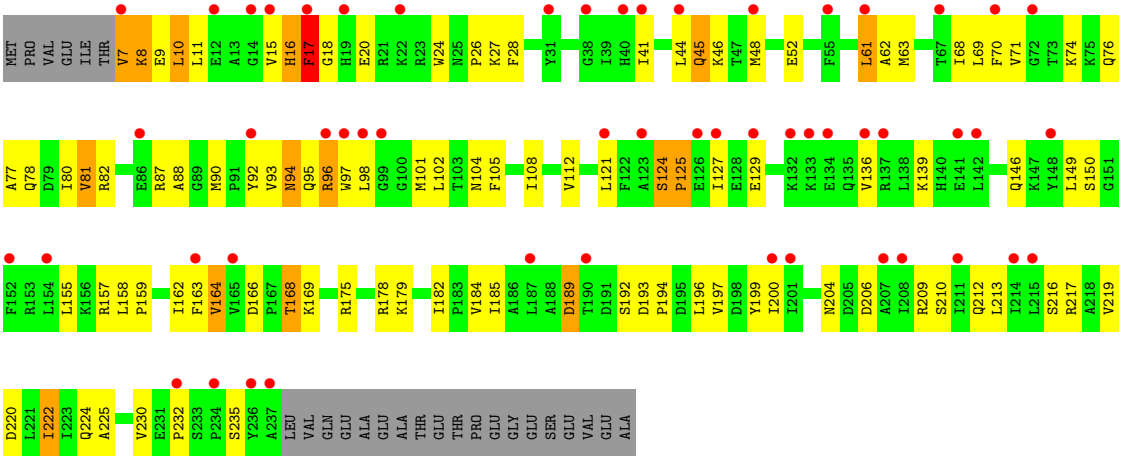
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



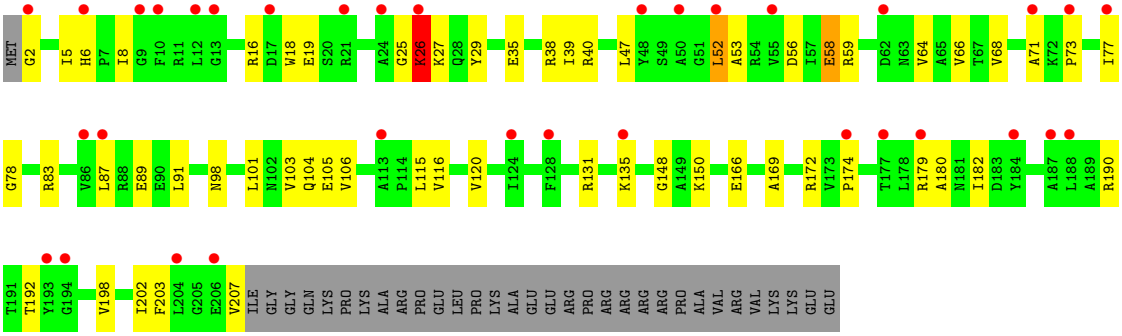
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



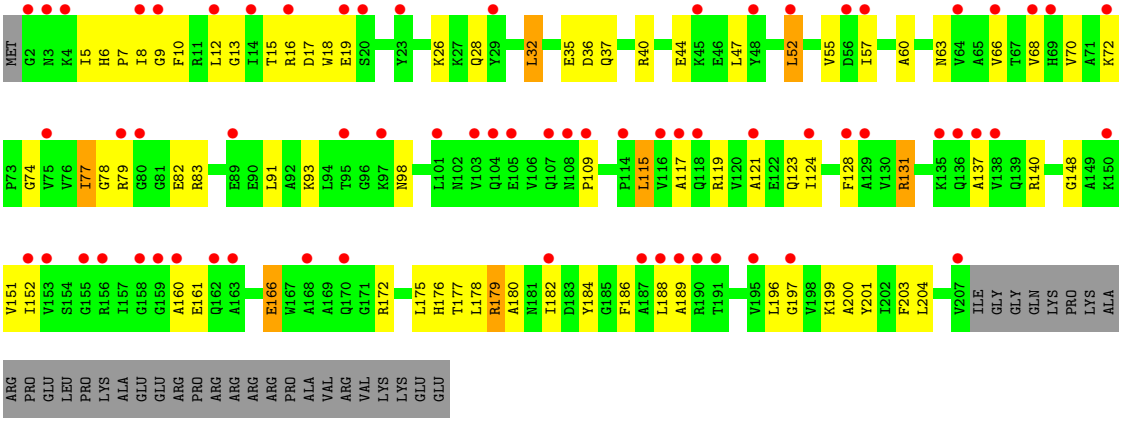
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



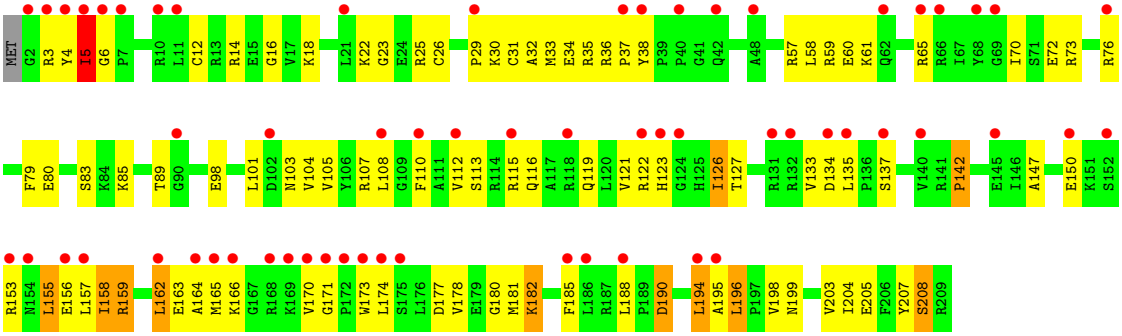
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



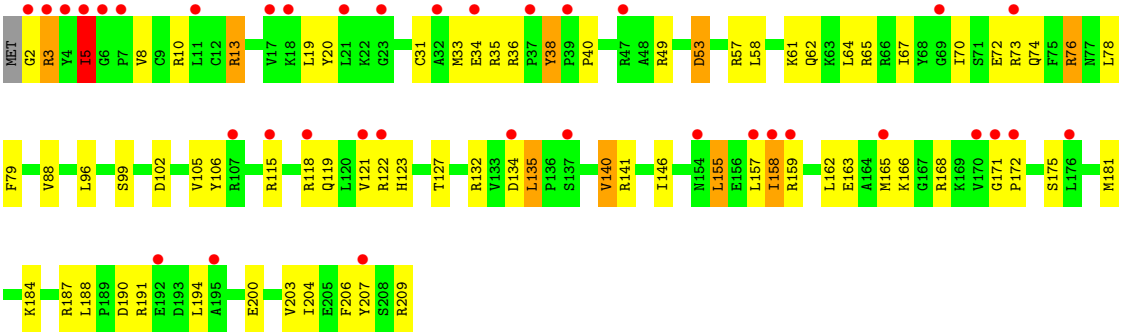
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



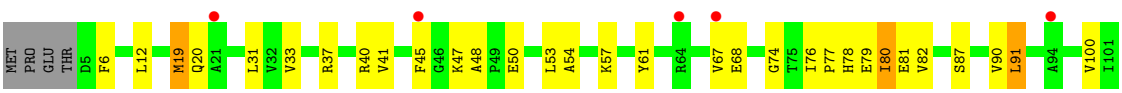
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



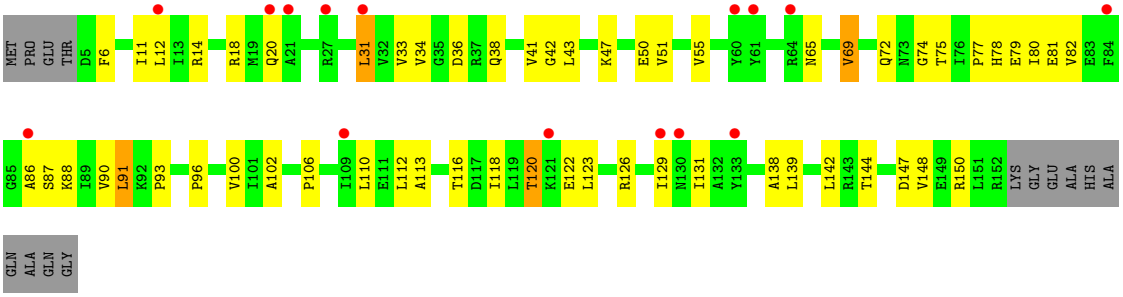
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



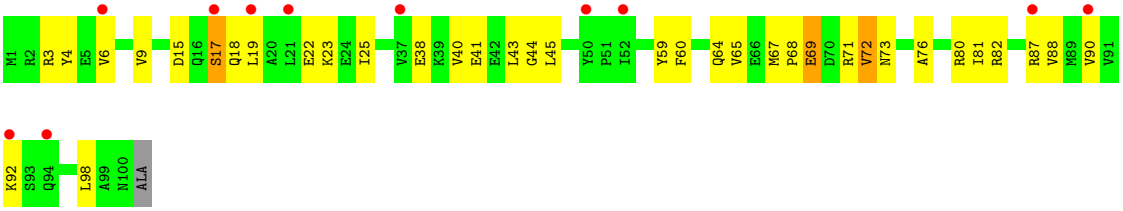
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



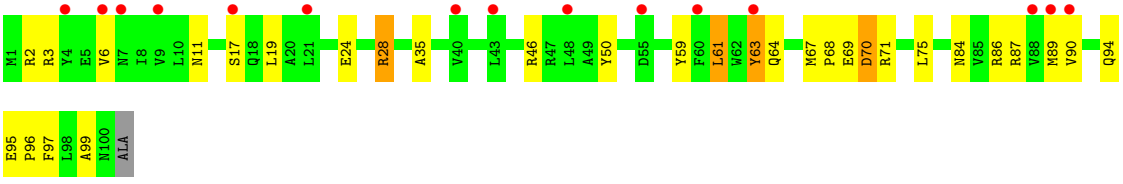
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



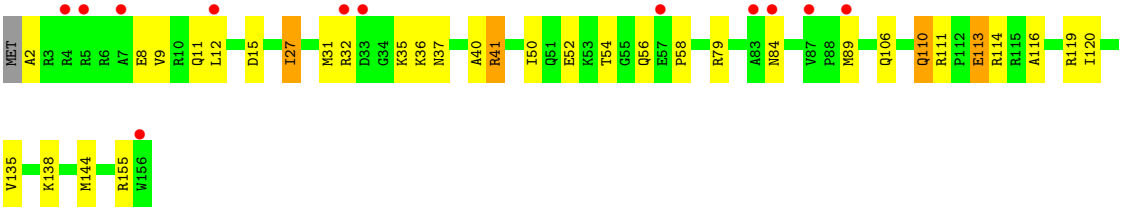
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



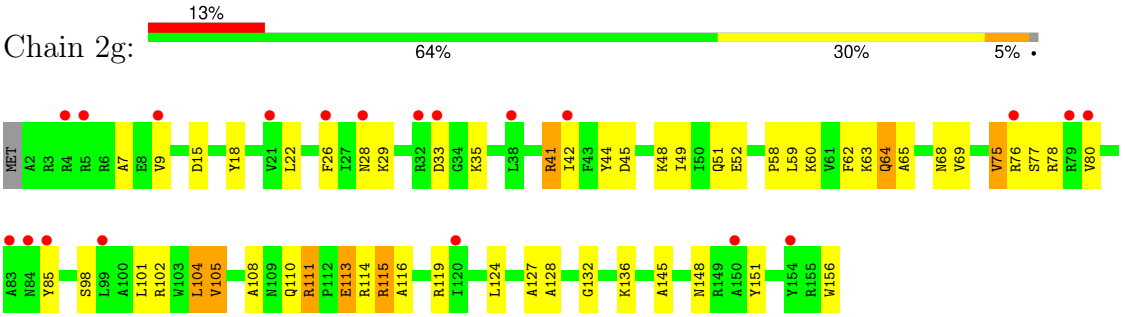
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



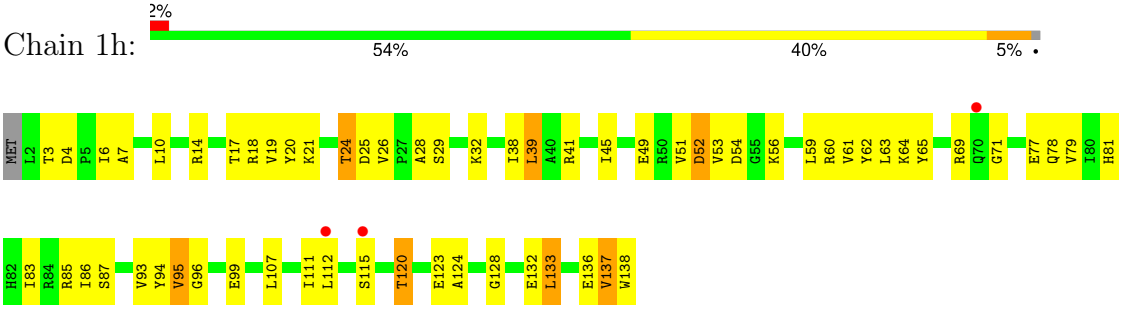
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



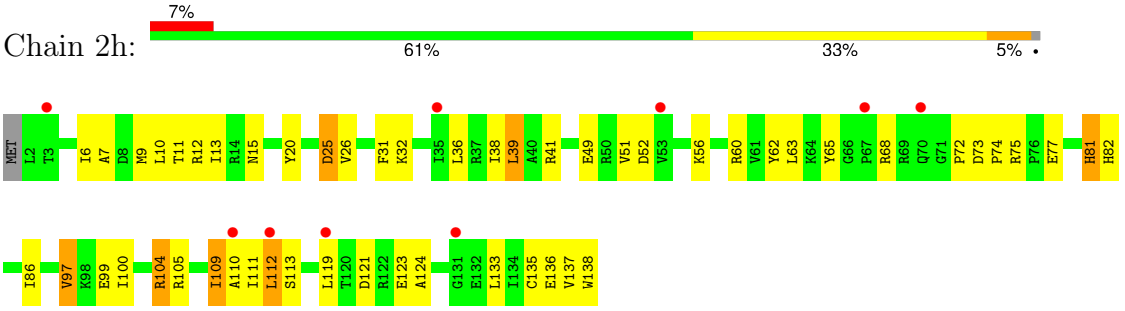
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



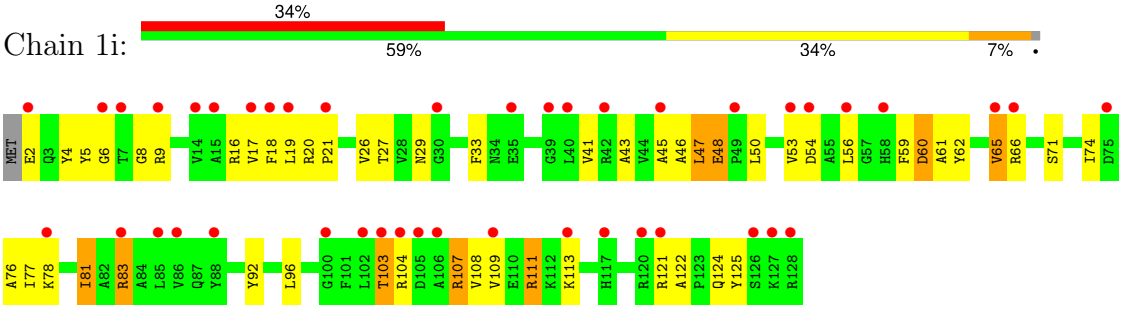
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



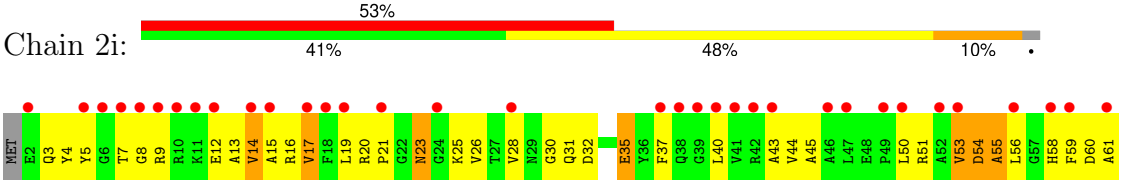
• Molecule 40: 30S ribosomal protein S9

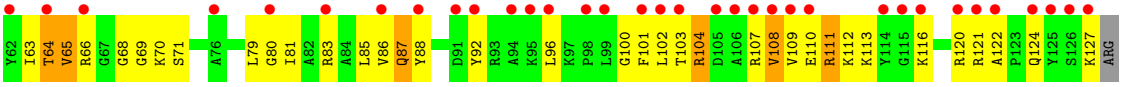
Chain 1i:



• Molecule 40: 30S ribosomal protein S9

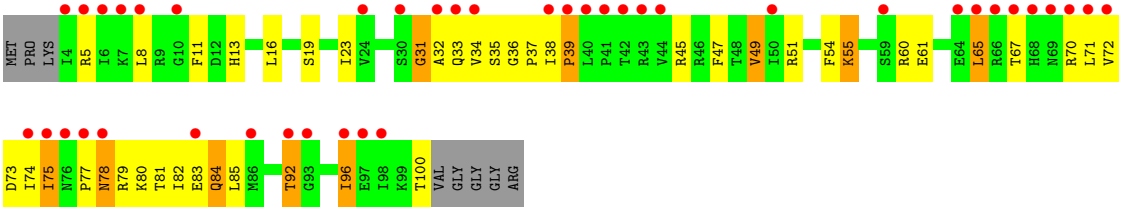
Chain 2i:





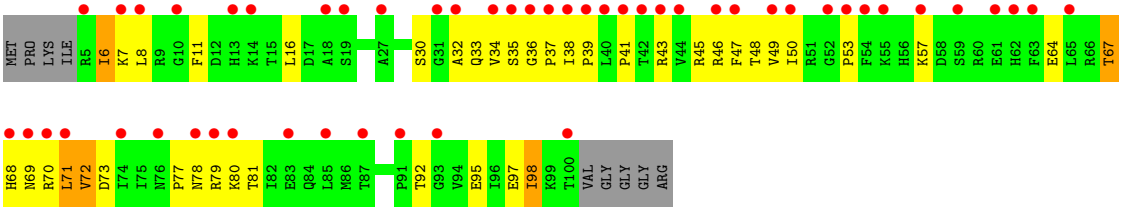
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



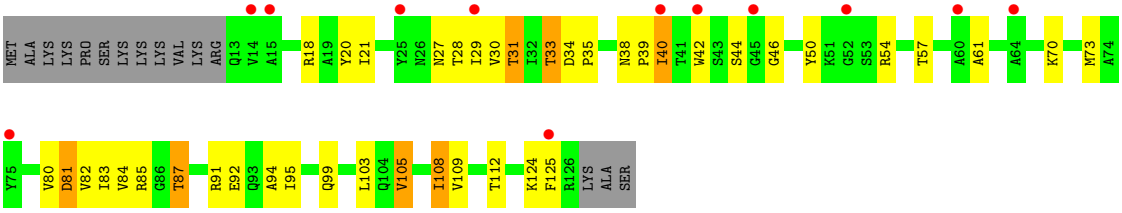
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



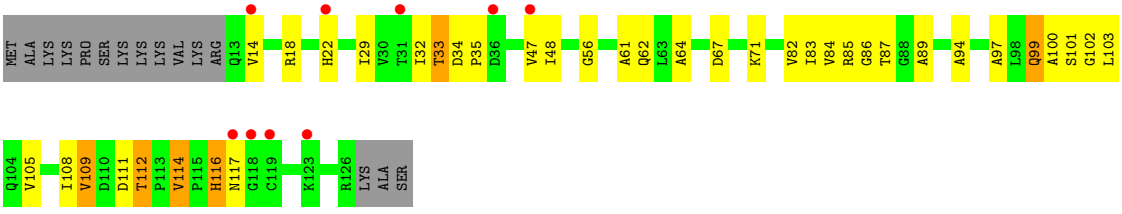
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



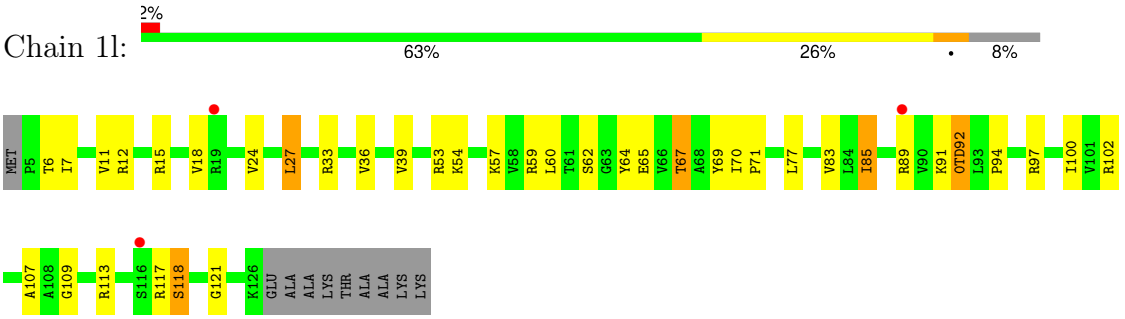
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



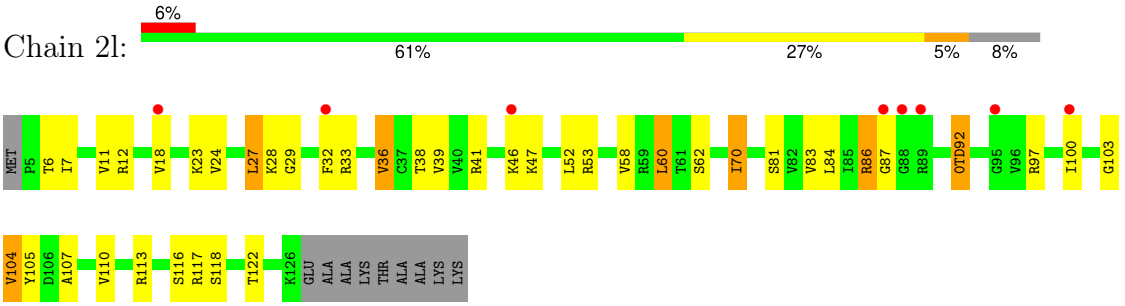
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



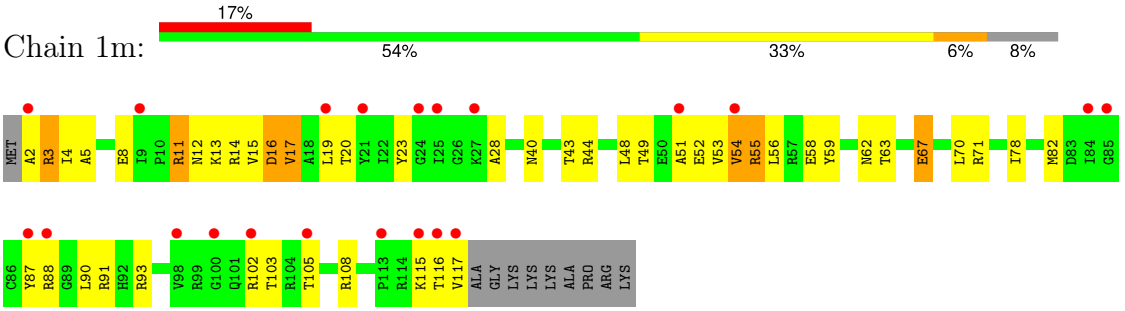
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



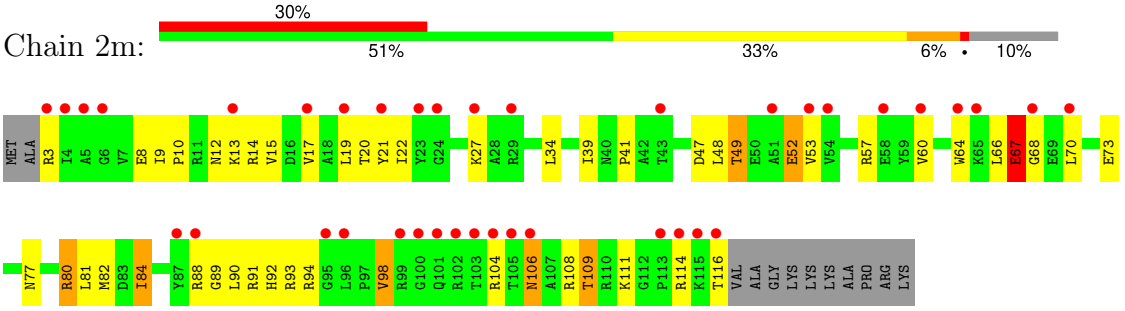
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



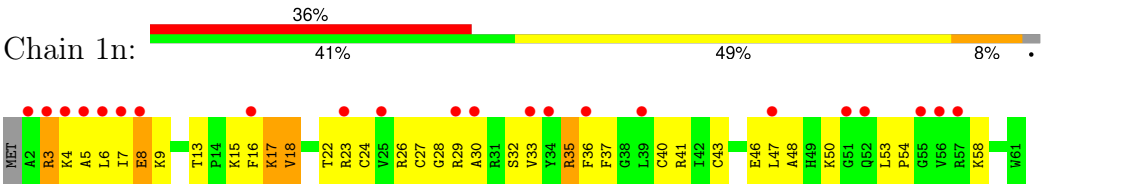
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



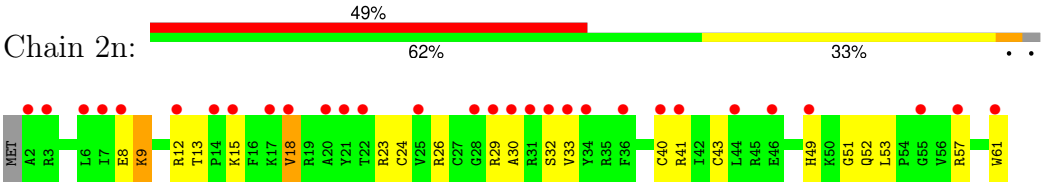
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



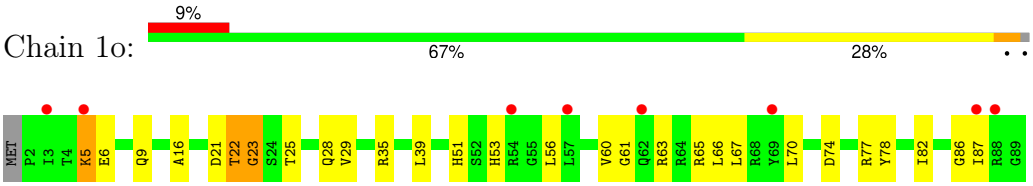
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



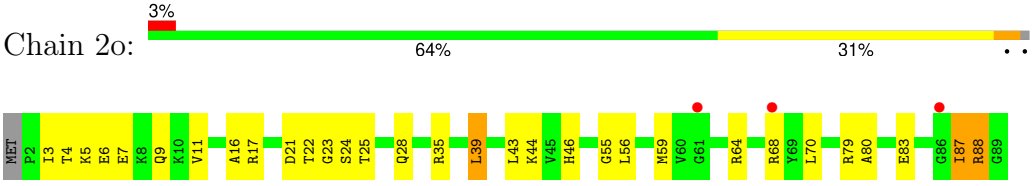
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



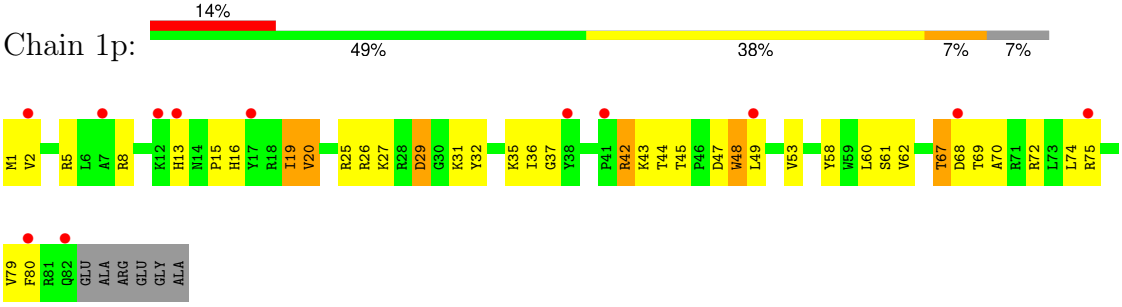
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



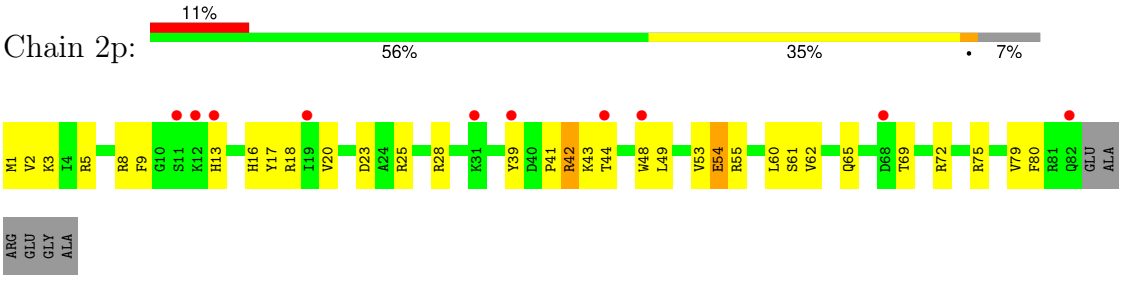
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



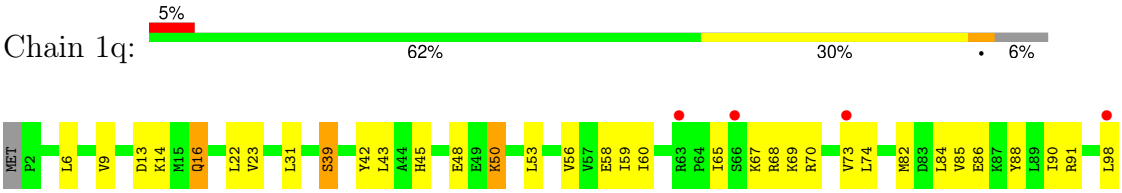
• Molecule 47: 30S ribosomal protein S16

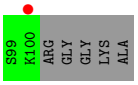
Chain 2p:



• Molecule 48: 30S ribosomal protein S17

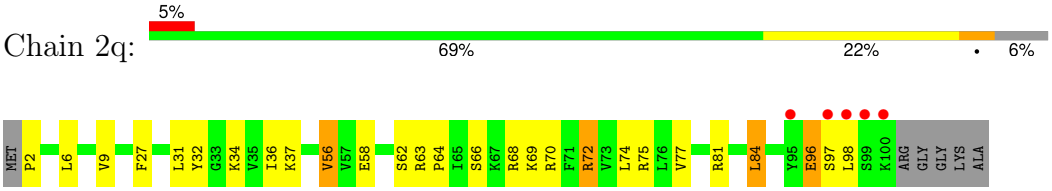
Chain 1q:





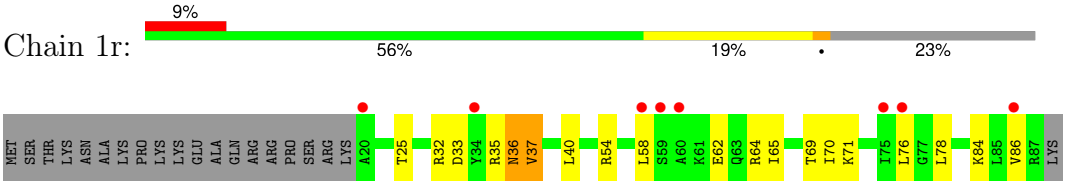
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



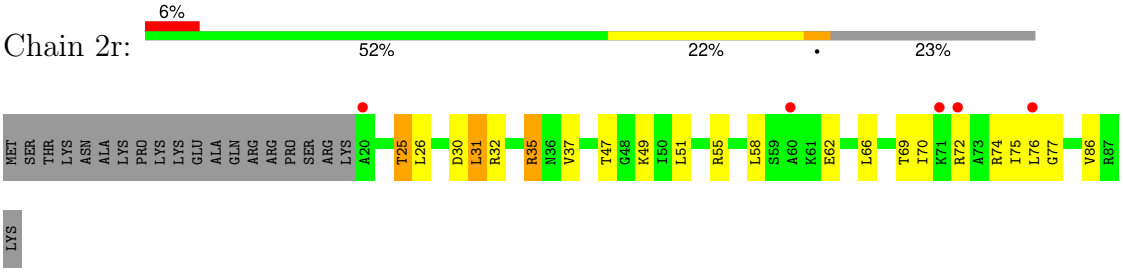
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



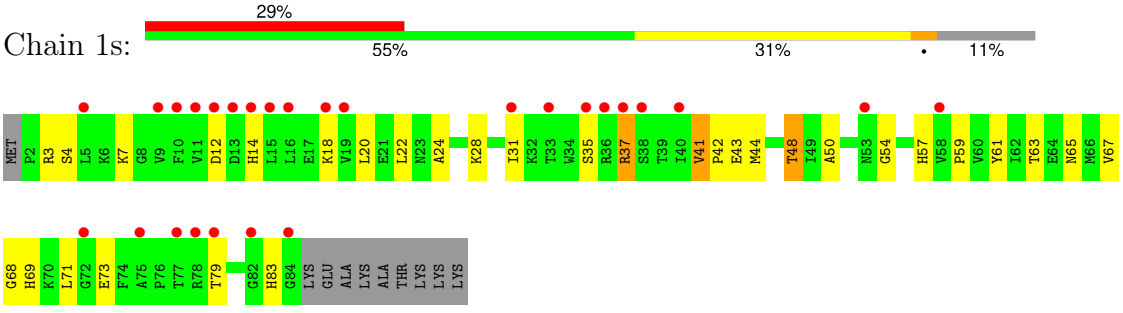
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



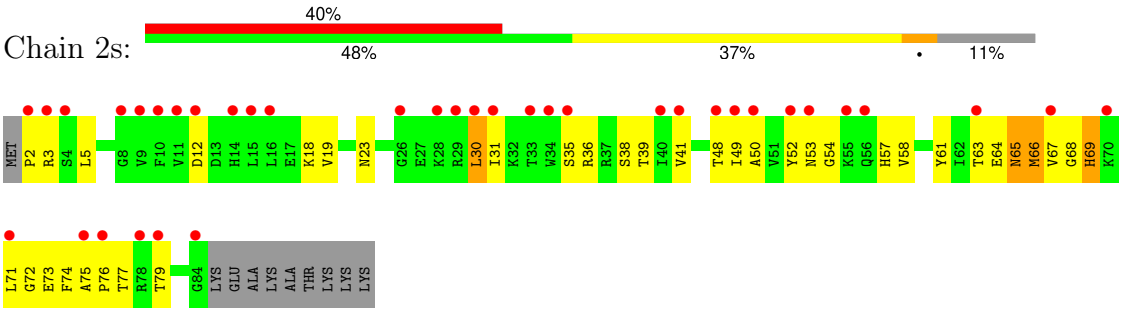
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



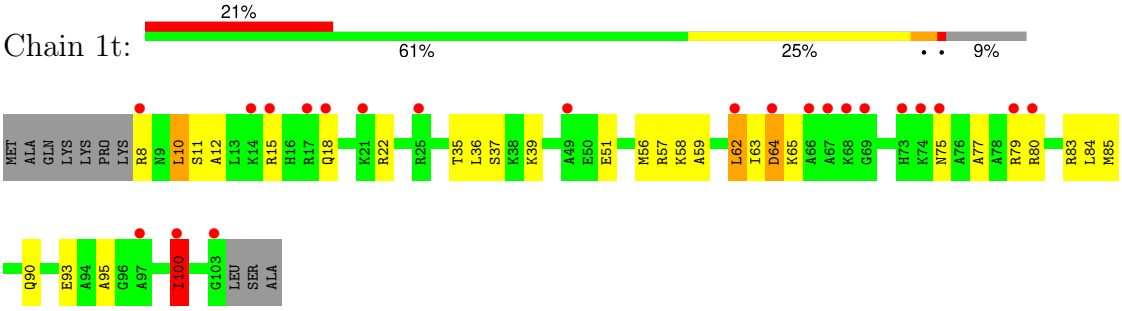
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



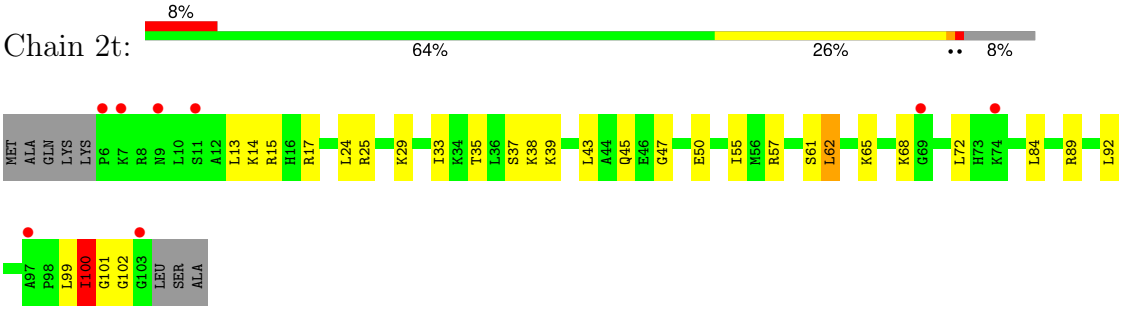
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



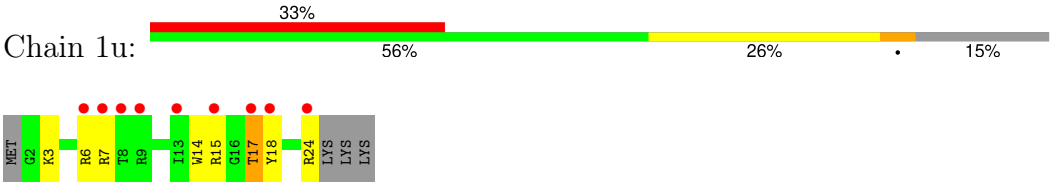
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



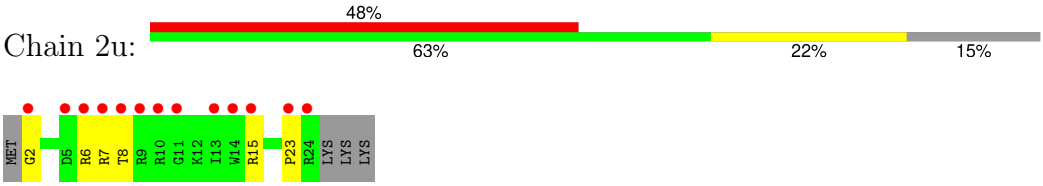
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



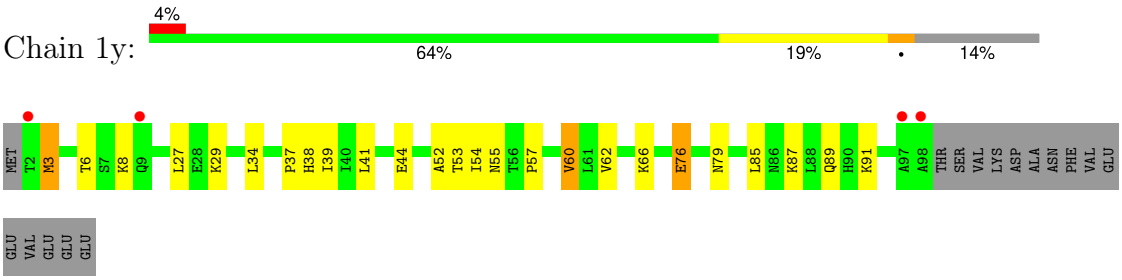
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



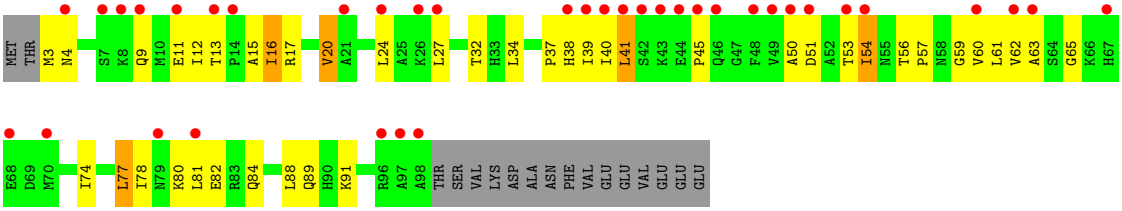
• Molecule 53: Ribosome-associated inhibitor A

Chain 1y:



• Molecule 53: Ribosome-associated inhibitor A

Chain 2y:


MET THR M3 N4 S7 K8 Q9 M10 E11 I12 T13 P14 A15 I16 R17 V20 A21 L24 A25 K26 L27 T32 H33 L34 P37 H38 I39 I40 L41 S42 K43 E44 P45 Q46 G47 F48 V49 A50 D51 A52 T53 I54 N55 T56 P57 N58 G59 V60 L61 V62 A63 S64 G65 K66 H67
E68 D69 M70 I74 L77 I78 N79 K80 L81 E82 R83 Q84 L88 Q89 H90 K91 R96 A97 A98 THR SER VAL LYS ASP ALA ASN PHE VAL GLU GLU VAL GLU GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.38Å 452.11Å 624.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	366.21 – 2.90 366.21 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (366.21-2.90) 99.5 (366.21-2.90)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.213 , 0.267 0.212 , 0.264	Depositor DCC
R_{free} test set	64774 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 337.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	297540	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, OMC, 2MA, 4OC, M2G, 5MC, ZN, 0TD, UR3, A1CRE, 5MU, MPD, SF4, MA6, OMU, PSU, 2MG, G7M, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.29	1/69031 (0.0%)	0.45	0/107754
1	2A	0.23	0/68903	0.40	1/107552 (0.0%)
2	1B	0.22	0/2876	0.40	0/4486
2	2B	0.20	0/2878	0.38	0/4490
3	1D	0.30	0/2181	0.51	0/2940
3	2D	0.24	0/2186	0.50	1/2944 (0.0%)
4	1E	0.28	0/1592	0.51	0/2149
4	2E	0.24	0/1592	0.49	0/2149
5	1F	0.28	0/1619	0.50	0/2193
5	2F	0.23	0/1615	0.47	2/2188 (0.1%)
6	1G	0.27	0/1451	0.45	0/1961
6	2G	0.21	0/1449	0.44	0/1957
7	1H	0.22	0/1356	0.47	0/1834
7	2H	0.21	0/1350	0.42	0/1826
8	1I	0.25	0/1109	0.48	0/1512
8	2I	0.20	0/1091	0.45	0/1490
9	1N	0.25	0/1148	0.45	0/1547
9	2N	0.22	0/1144	0.43	0/1543
10	1O	0.29	0/943	0.50	0/1269
10	2O	0.23	0/943	0.47	0/1269
11	1P	0.27	0/1152	0.50	0/1533
11	2P	0.22	0/1152	0.49	0/1533
12	1Q	0.26	0/1143	0.46	0/1527
12	2Q	0.25	0/1143	0.44	0/1527
13	1R	0.28	0/982	0.55	0/1312
13	2R	0.24	0/982	0.51	0/1312
14	1S	0.22	0/887	0.48	0/1180
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.27	0/1105	0.48	0/1477
15	2T	0.23	0/1097	0.46	0/1468
16	1U	0.30	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	2U	0.21	0/977	0.41	0/1301
17	1V	0.25	0/786	0.46	0/1053
17	2V	0.22	0/782	0.46	0/1049
18	1W	0.27	0/897	0.48	0/1205
18	2W	0.24	0/897	0.43	0/1205
19	1X	0.27	0/764	0.46	0/1025
19	2X	0.22	0/764	0.51	0/1025
20	1Y	0.26	0/823	0.52	0/1099
20	2Y	0.24	0/823	0.50	0/1100
21	1Z	0.22	0/1620	0.44	0/2200
21	2Z	0.24	0/1590	0.45	0/2162
22	10	0.29	0/616	0.56	0/821
22	20	0.22	0/616	0.45	0/821
23	11	0.26	0/761	0.47	0/1013
23	21	0.23	0/766	0.41	0/1018
24	12	0.24	0/590	0.45	0/781
24	22	0.21	0/594	0.39	0/785
25	13	0.26	0/474	0.49	0/635
25	23	0.20	0/469	0.42	0/630
26	14	0.28	0/559	0.58	0/754
26	24	0.29	0/549	0.68	2/741 (0.3%)
27	15	0.29	0/473	0.51	0/639
27	25	0.23	0/469	0.47	0/635
28	16	0.27	0/460	0.50	0/613
28	26	0.22	0/456	0.43	0/608
29	17	0.31	0/426	0.55	0/561
29	27	0.27	0/426	0.50	0/561
30	18	0.27	0/525	0.53	0/691
30	28	0.24	0/525	0.44	0/691
31	19	0.26	0/310	0.44	0/407
31	29	0.22	0/310	0.45	0/407
32	1a	0.21	0/35795	0.39	0/55864
32	2a	0.20	0/35890	0.38	1/56012 (0.0%)
33	1b	0.25	0/1876	0.56	1/2533 (0.0%)
33	2b	0.25	0/1860	0.50	0/2518
34	1c	0.21	0/1582	0.43	0/2137
34	2c	0.27	0/1566	0.48	0/2119
35	1d	0.21	0/1695	0.44	0/2274
35	2d	0.22	0/1698	0.45	0/2277
36	1e	0.23	0/1149	0.48	0/1548
36	2e	0.21	0/1149	0.46	0/1548
37	1f	0.20	0/827	0.42	0/1120
37	2f	0.23	0/829	0.46	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.21	0/1254	0.39	0/1683
38	2g	0.19	0/1248	0.40	0/1676
39	1h	0.20	0/1118	0.43	0/1506
39	2h	0.20	0/1108	0.44	0/1494
40	1i	0.21	0/1005	0.46	0/1351
40	2i	0.22	0/985	0.49	0/1329
41	1j	0.23	0/732	0.48	0/993
41	2j	0.22	0/723	0.50	0/984
42	1k	0.25	0/849	0.54	1/1150 (0.1%)
42	2k	0.21	0/848	0.49	1/1149 (0.1%)
43	1l	0.23	0/937	0.49	0/1260
43	2l	0.21	0/937	0.50	0/1260
44	1m	0.21	0/924	0.46	0/1242
44	2m	0.21	0/905	0.44	0/1217
45	1n	0.24	0/501	0.45	0/664
45	2n	0.25	0/501	0.47	0/664
46	1o	0.21	0/739	0.41	0/985
46	2o	0.21	0/739	0.48	1/985 (0.1%)
47	1p	0.23	0/697	0.51	0/939
47	2p	0.20	0/693	0.47	0/935
48	1q	0.21	0/836	0.45	0/1117
48	2q	0.24	0/836	0.45	0/1117
49	1r	0.37	0/560	0.48	0/746
49	2r	0.27	0/560	0.40	0/746
50	1s	0.19	0/663	0.43	0/895
50	2s	0.21	0/660	0.46	0/893
51	1t	0.21	0/734	0.47	0/969
51	2t	0.20	0/736	0.43	0/976
52	1u	0.28	0/203	0.48	0/266
52	2u	0.22	0/203	0.52	0/266
53	1y	0.20	0/776	0.34	0/1048
53	2y	0.25	0/761	0.45	0/1030
All	All	0.24	1/309941 (0.0%)	0.43	11/463239 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	2I	0	1
14	1S	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	1X	0	1
21	2Z	0	1
26	14	0	1
26	24	0	1
33	1b	0	2
43	2l	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	O3'-P	5.01	1.61	1.56

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	1b	222	ILE	N-CA-C	-10.39	102.53	112.29
42	1k	40	ILE	N-CA-C	-10.19	103.56	112.12
3	2D	41	GLY	N-CA-C	-7.33	105.12	115.30
32	2a	266	G	C2'-C3'-O3'	5.47	117.71	109.50
5	2F	21	ALA	CA-C-N	5.44	131.49	121.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	52	THR	Peptide
14	1S	58	LEU	Peptide
19	1X	93	GLU	Peptide
33	1b	220	ASP	Peptide
33	1b	231	GLU	Peptide

5.2 Too-close contacts (i)

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31203	704	0
1	2A	61758	0	31153	830	0
2	1B	2572	0	1305	31	0
2	2B	2573	0	1306	32	0
3	1D	2131	0	2207	47	0
3	2D	2136	0	2218	47	0
4	1E	1559	0	1618	42	0
4	2E	1559	0	1618	54	0
5	1F	1584	0	1625	36	0
5	2F	1580	0	1619	54	0
6	1G	1426	0	1445	48	0
6	2G	1424	0	1441	50	0
7	1H	1330	0	1407	31	0
7	2H	1324	0	1402	52	0
8	1I	1094	0	1127	26	0
8	2I	1076	0	1094	21	0
9	1N	1121	0	1195	27	0
9	2N	1117	0	1184	28	0
10	1O	933	0	996	23	0
10	2O	933	0	996	27	0
11	1P	1135	0	1212	30	0
11	2P	1135	0	1212	32	0
12	1Q	1122	0	1179	23	0
12	2Q	1122	0	1179	27	0
13	1R	968	0	1033	25	0
13	2R	968	0	1033	32	0
14	1S	877	0	938	19	0
14	2S	870	0	923	32	0
15	1T	1091	0	1151	26	0
15	2T	1083	0	1136	26	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	17	0
17	1V	775	0	841	14	0
17	2V	771	0	830	21	0
18	1W	886	0	940	14	0
18	2W	886	0	940	24	0
19	1X	750	0	814	18	0
19	2X	750	0	814	15	0
20	1Y	810	0	892	25	0
20	2Y	810	0	887	26	0
21	1Z	1587	0	1598	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	2Z	1557	0	1564	48	0
22	10	608	0	622	16	0
22	20	608	0	622	17	0
23	11	754	0	823	11	0
23	21	759	0	837	24	0
24	12	588	0	643	12	0
24	22	592	0	654	12	0
25	13	469	0	518	10	0
25	23	464	0	514	12	0
26	14	546	0	522	24	0
26	24	536	0	514	30	0
27	15	459	0	476	12	0
27	25	455	0	465	11	0
28	16	453	0	473	9	0
28	26	449	0	469	5	0
29	17	418	0	467	7	0
29	27	418	0	467	1	0
30	18	517	0	582	12	0
30	28	517	0	582	17	0
31	19	307	0	335	6	0
31	29	307	0	335	5	0
32	1a	32246	0	16294	512	0
32	2a	32331	0	16338	517	0
33	1b	1842	0	1862	66	0
33	2b	1825	0	1828	73	0
34	1c	1558	0	1557	37	0
34	2c	1542	0	1517	51	0
35	1d	1665	0	1687	68	0
35	2d	1668	0	1703	51	0
36	1e	1133	0	1190	33	0
36	2e	1133	0	1191	35	0
37	1f	814	0	808	22	0
37	2f	816	0	808	19	0
38	1g	1235	0	1249	19	0
38	2g	1229	0	1238	37	0
39	1h	1098	0	1143	35	0
39	2h	1088	0	1126	41	0
40	1i	986	0	990	34	0
40	2i	966	0	953	61	0
41	1j	719	0	672	30	0
41	2j	710	0	661	26	0
42	1k	834	0	838	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	2k	833	0	836	21	0
43	1l	932	0	981	23	0
43	2l	932	0	981	23	0
44	1m	914	0	954	29	0
44	2m	895	0	920	36	0
45	1n	492	0	529	27	0
45	2n	492	0	529	21	0
46	1o	728	0	760	20	0
46	2o	728	0	760	20	0
47	1p	681	0	697	28	0
47	2p	677	0	686	21	0
48	1q	823	0	891	20	0
48	2q	823	0	891	15	0
49	1r	555	0	618	9	0
49	2r	555	0	618	13	0
50	1s	648	0	658	23	0
50	2s	645	0	635	31	0
51	1t	732	0	809	23	0
51	2t	733	0	795	23	0
52	1u	199	0	208	6	0
52	2u	199	0	208	3	0
53	1y	764	0	786	19	0
53	2y	749	0	757	23	0
54	10	7	0	0	0	0
54	11	4	0	0	0	0
54	13	3	0	0	0	0
54	15	6	0	0	0	0
54	17	4	0	0	0	0
54	18	4	0	0	0	0
54	19	2	0	0	0	0
54	1A	1011	0	0	0	0
54	1B	30	0	0	0	0
54	1D	18	0	0	0	0
54	1E	9	0	0	0	0
54	1F	16	0	0	0	0
54	1G	4	0	0	0	0
54	1H	3	0	0	0	0
54	1N	2	0	0	0	0
54	1O	2	0	0	0	0
54	1P	6	0	0	0	0
54	1Q	7	0	0	0	0
54	1R	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1S	1	0	0	0	0
54	1T	5	0	0	0	0
54	1U	5	0	0	0	0
54	1V	6	0	0	0	0
54	1W	3	0	0	0	0
54	1Y	1	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	270	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	4	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	1	0	0	0	0
54	1n	2	0	0	0	0
54	1o	2	0	0	0	0
54	1p	1	0	0	0	0
54	1t	2	0	0	0	0
54	1y	5	0	0	0	0
54	20	2	0	0	0	0
54	21	1	0	0	0	0
54	23	1	0	0	0	0
54	25	3	0	0	0	0
54	27	1	0	0	0	0
54	28	2	0	0	0	0
54	2A	732	0	0	0	0
54	2B	20	0	0	0	0
54	2D	7	0	0	0	0
54	2E	8	0	0	0	0
54	2F	4	0	0	0	0
54	2G	3	0	0	0	0
54	2I	1	0	0	0	0
54	2N	1	0	0	0	0
54	2O	1	0	0	0	0
54	2P	3	0	0	0	0
54	2Q	4	0	0	0	0
54	2R	2	0	0	0	0
54	2T	3	0	0	0	0
54	2U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2V	1	0	0	0	0
54	2W	3	0	0	0	0
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	192	0	0	0	0
54	2e	2	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2k	1	0	0	0	0
54	2l	1	0	0	0	0
54	2o	1	0	0	0	0
54	2q	1	0	0	0	0
54	2r	1	0	0	0	0
54	2t	1	0	0	0	0
54	2y	1	0	0	0	0
55	1A	41	0	0	0	0
55	2A	41	0	0	0	0
56	18	8	0	12	1	0
56	1A	8	0	14	1	0
56	1a	16	0	27	2	0
56	2A	16	0	28	0	0
56	2B	8	0	14	1	0
57	1B	12	0	12	2	0
57	1F	12	0	12	2	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	1	0
59	2d	8	0	0	0	0
60	10	26	0	0	1	0
60	11	25	0	0	0	0
60	12	15	0	0	1	0
60	13	23	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	14	1	0	0	0	0
60	15	29	0	0	1	0
60	16	14	0	0	0	0
60	17	13	0	0	2	0
60	18	28	0	0	2	0
60	19	11	0	0	1	0
60	1A	3794	0	0	183	0
60	1B	98	0	0	11	0
60	1D	112	0	0	2	0
60	1E	73	0	0	4	0
60	1F	61	0	0	3	0
60	1G	20	0	0	1	0
60	1H	14	0	0	0	0
60	1I	8	0	0	0	0
60	1N	51	0	0	3	0
60	1O	20	0	0	3	0
60	1P	64	0	0	2	0
60	1Q	39	0	0	1	0
60	1R	30	0	0	3	0
60	1S	8	0	0	0	0
60	1T	39	0	0	2	0
60	1U	39	0	0	1	0
60	1V	38	0	0	0	0
60	1W	28	0	0	0	0
60	1X	26	0	0	2	0
60	1Y	15	0	0	2	0
60	1Z	11	0	0	2	0
60	1a	532	0	0	42	0
60	1b	1	0	0	0	0
60	1d	9	0	0	3	0
60	1e	6	0	0	0	0
60	1f	2	0	0	0	0
60	1g	1	0	0	0	0
60	1h	2	0	0	0	0
60	1i	1	0	0	0	0
60	1j	1	0	0	0	0
60	1l	5	0	0	0	0
60	1m	2	0	0	0	0
60	1o	2	0	0	0	0
60	1p	3	0	0	0	0
60	1q	1	0	0	0	0
60	1r	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1t	1	0	0	0	0
60	1u	1	0	0	0	0
60	1y	6	0	0	0	0
60	20	12	0	0	1	0
60	21	19	0	0	3	0
60	23	3	0	0	0	0
60	24	1	0	0	0	0
60	25	11	0	0	0	0
60	26	5	0	0	1	0
60	27	11	0	0	1	0
60	28	14	0	0	4	0
60	29	1	0	0	0	0
60	2A	2275	0	0	194	0
60	2B	60	0	0	7	0
60	2D	50	0	0	2	0
60	2E	29	0	0	2	0
60	2F	20	0	0	1	0
60	2G	6	0	0	1	0
60	2H	3	0	0	1	0
60	2I	3	0	0	1	0
60	2N	5	0	0	0	0
60	2O	15	0	0	1	0
60	2P	26	0	0	3	0
60	2Q	20	0	0	2	0
60	2R	17	0	0	2	0
60	2S	5	0	0	0	0
60	2T	13	0	0	0	0
60	2U	8	0	0	1	0
60	2V	7	0	0	0	0
60	2W	21	0	0	2	0
60	2X	7	0	0	0	0
60	2Y	3	0	0	0	0
60	2Z	13	0	0	2	0
60	2a	436	0	0	29	0
60	2d	5	0	0	0	0
60	2e	3	0	0	0	0
60	2f	2	0	0	0	0
60	2j	2	0	0	0	0
60	2l	4	0	0	1	0
60	2m	1	0	0	0	0
60	2n	1	0	0	0	0
60	2o	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2p	4	0	0	0	0
60	2q	1	0	0	0	0
60	2r	3	0	0	0	0
60	2t	1	0	0	0	0
60	2u	1	0	0	0	0
60	2y	8	0	0	1	0
All	All	297540	0	194512	4638	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 4638 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.34	1.25
32:2a:1003:G:H2'	32:2a:1004:A:H4'	1.40	1.02
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.26	0.97
32:2a:1256:A:H61	32:2a:1278:U:H1'	1.27	0.96
1:1A:1082:U:O4	1:1A:1086:A:N1	1.99	0.95

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
3	2D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
4	1E	202/206 (98%)	186 (92%)	15 (7%)	1 (0%)	24	54
4	2E	202/206 (98%)	187 (93%)	14 (7%)	1 (0%)	24	54
5	1F	201/210 (96%)	191 (95%)	8 (4%)	2 (1%)	12	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	2F	201/210 (96%)	190 (94%)	9 (4%)	2 (1%)	12 39
6	1G	179/182 (98%)	159 (89%)	16 (9%)	4 (2%)	5 20
6	2G	179/182 (98%)	158 (88%)	18 (10%)	3 (2%)	7 26
7	1H	172/180 (96%)	159 (92%)	11 (6%)	2 (1%)	10 34
7	2H	171/180 (95%)	151 (88%)	18 (10%)	2 (1%)	10 34
8	1I	145/148 (98%)	128 (88%)	15 (10%)	2 (1%)	9 30
8	2I	144/148 (97%)	124 (86%)	17 (12%)	3 (2%)	5 21
9	1N	138/140 (99%)	129 (94%)	9 (6%)	0	100 100
9	2N	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	18 48
10	1O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16 44
10	2O	120/122 (98%)	111 (92%)	9 (8%)	0	100 100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100 100
11	2P	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	9 30
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100 100
12	2Q	139/141 (99%)	129 (93%)	10 (7%)	0	100 100
13	1R	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	14 41
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100 100
14	1S	108/112 (96%)	99 (92%)	6 (6%)	3 (3%)	4 15
14	2S	108/112 (96%)	98 (91%)	7 (6%)	3 (3%)	4 15
15	1T	129/146 (88%)	120 (93%)	7 (5%)	2 (2%)	7 27
15	2T	129/146 (88%)	119 (92%)	9 (7%)	1 (1%)	16 44
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100 100
17	1V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12 39
17	2V	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6 22
18	1W	110/113 (97%)	110 (100%)	0	0	100 100
18	2W	110/113 (97%)	107 (97%)	2 (2%)	1 (1%)	14 41
19	1X	93/96 (97%)	93 (100%)	0	0	100 100
19	2X	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	11 36
20	1Y	105/110 (96%)	94 (90%)	11 (10%)	0	100 100
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	1Z	201/206 (98%)	187 (93%)	14 (7%)	0	100 100
21	2Z	199/206 (97%)	173 (87%)	25 (13%)	1 (0%)	24 54
22	10	75/85 (88%)	69 (92%)	6 (8%)	0	100 100
22	20	75/85 (88%)	67 (89%)	8 (11%)	0	100 100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11 36
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11 36
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100 100
25	13	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
25	23	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
26	14	67/71 (94%)	48 (72%)	13 (19%)	6 (9%)	0 1
26	24	67/71 (94%)	49 (73%)	13 (19%)	5 (8%)	1 2
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100 100
30	28	62/65 (95%)	57 (92%)	5 (8%)	0	100 100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
33	1b	229/256 (90%)	189 (82%)	30 (13%)	10 (4%)	2 8
33	2b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	2 10
34	1c	204/239 (85%)	175 (86%)	27 (13%)	2 (1%)	12 39
34	2c	204/239 (85%)	179 (88%)	22 (11%)	3 (2%)	8 28
35	1d	206/209 (99%)	180 (87%)	22 (11%)	4 (2%)	6 23
35	2d	206/209 (99%)	186 (90%)	17 (8%)	3 (2%)	8 28
36	1e	146/162 (90%)	133 (91%)	12 (8%)	1 (1%)	18 48
36	2e	146/162 (90%)	131 (90%)	13 (9%)	2 (1%)	9 30
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
37	2f	98/101 (97%)	89 (91%)	9 (9%)	0	100 100
38	1g	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	18 48
38	2g	153/156 (98%)	135 (88%)	17 (11%)	1 (1%)	18 48
39	1h	135/138 (98%)	124 (92%)	11 (8%)	0	100 100
39	2h	135/138 (98%)	123 (91%)	12 (9%)	0	100 100
40	1i	125/128 (98%)	102 (82%)	22 (18%)	1 (1%)	16 44
40	2i	124/128 (97%)	102 (82%)	18 (14%)	4 (3%)	3 13
41	1j	95/105 (90%)	78 (82%)	9 (10%)	8 (8%)	0 1
41	2j	94/105 (90%)	81 (86%)	12 (13%)	1 (1%)	11 36
42	1k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	14 41
42	2k	112/129 (87%)	102 (91%)	10 (9%)	0	100 100
43	1l	119/132 (90%)	107 (90%)	12 (10%)	0	100 100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100 100
44	1m	114/126 (90%)	100 (88%)	11 (10%)	3 (3%)	4 17
44	2m	112/126 (89%)	100 (89%)	11 (10%)	1 (1%)	14 41
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100 100
46	1o	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	10 34
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10 34
47	1p	80/88 (91%)	61 (76%)	18 (22%)	1 (1%)	9 32
47	2p	80/88 (91%)	73 (91%)	6 (8%)	1 (1%)	9 32
48	1q	97/105 (92%)	87 (90%)	10 (10%)	0	100 100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
49	1r	66/88 (75%)	58 (88%)	5 (8%)	3 (4%)	2 8
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
50	1s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	10 34
50	2s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	10 34
51	1t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	5 21
51	2t	96/106 (91%)	87 (91%)	7 (7%)	2 (2%)	5 21
52	1u	21/27 (78%)	20 (95%)	0	1 (5%)	2 7
52	2u	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	1y	95/113 (84%)	92 (97%)	3 (3%)	0	100 100
53	2y	94/113 (83%)	84 (89%)	9 (10%)	1 (1%)	11 36
All	All	11629/12354 (94%)	10577 (91%)	925 (8%)	127 (1%)	11 36

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
7	1H	126	PRO
8	1I	11	ASN
26	14	49	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	214/218 (98%)	198 (92%)	16 (8%)	12 37
3	2D	215/218 (99%)	196 (91%)	19 (9%)	9 29
4	1E	164/166 (99%)	141 (86%)	23 (14%)	3 11
4	2E	164/166 (99%)	142 (87%)	22 (13%)	4 12
5	1F	160/166 (96%)	139 (87%)	21 (13%)	4 13
5	2F	159/166 (96%)	133 (84%)	26 (16%)	2 8
6	1G	144/156 (92%)	123 (85%)	21 (15%)	3 10
6	2G	142/156 (91%)	117 (82%)	25 (18%)	2 6
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12 36
7	2H	143/148 (97%)	120 (84%)	23 (16%)	2 8
8	1I	111/124 (90%)	88 (79%)	23 (21%)	1 4
8	2I	108/124 (87%)	92 (85%)	16 (15%)	3 10
9	1N	119/119 (100%)	107 (90%)	12 (10%)	7 24
9	2N	118/119 (99%)	101 (86%)	17 (14%)	3 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	1O	100/100 (100%)	91 (91%)	9 (9%)	9 28
10	2O	100/100 (100%)	91 (91%)	9 (9%)	9 28
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8 26
11	2P	115/116 (99%)	101 (88%)	14 (12%)	5 16
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	7 24
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	7 24
13	1R	101/101 (100%)	86 (85%)	15 (15%)	3 10
13	2R	101/101 (100%)	89 (88%)	12 (12%)	5 16
14	1S	87/88 (99%)	76 (87%)	11 (13%)	4 14
14	2S	85/88 (97%)	71 (84%)	14 (16%)	2 8
15	1T	115/127 (91%)	106 (92%)	9 (8%)	11 35
15	2T	113/127 (89%)	101 (89%)	12 (11%)	6 22
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10 30
16	2U	93/94 (99%)	83 (89%)	10 (11%)	6 21
17	1V	81/82 (99%)	70 (86%)	11 (14%)	3 12
17	2V	80/82 (98%)	67 (84%)	13 (16%)	2 8
18	1W	90/92 (98%)	78 (87%)	12 (13%)	4 12
18	2W	90/92 (98%)	79 (88%)	11 (12%)	5 16
19	1X	77/78 (99%)	68 (88%)	9 (12%)	5 17
19	2X	77/78 (99%)	71 (92%)	6 (8%)	11 35
20	1Y	86/91 (94%)	77 (90%)	9 (10%)	6 22
20	2Y	86/91 (94%)	71 (83%)	15 (17%)	2 7
21	1Z	169/179 (94%)	145 (86%)	24 (14%)	3 11
21	2Z	165/179 (92%)	144 (87%)	21 (13%)	4 14
22	10	61/67 (91%)	55 (90%)	6 (10%)	7 25
22	20	61/67 (91%)	56 (92%)	5 (8%)	10 32
23	11	79/83 (95%)	72 (91%)	7 (9%)	9 28
23	21	81/83 (98%)	69 (85%)	12 (15%)	3 10
24	12	65/67 (97%)	60 (92%)	5 (8%)	12 35
24	22	66/67 (98%)	53 (80%)	13 (20%)	1 5
25	13	51/52 (98%)	47 (92%)	4 (8%)	11 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	23	50/52 (96%)	44 (88%)	6 (12%)	5 16
26	14	58/63 (92%)	51 (88%)	7 (12%)	5 16
26	24	54/63 (86%)	47 (87%)	7 (13%)	4 13
27	15	51/52 (98%)	44 (86%)	7 (14%)	3 12
27	25	50/52 (96%)	45 (90%)	5 (10%)	7 24
28	16	51/52 (98%)	46 (90%)	5 (10%)	7 25
28	26	50/52 (96%)	46 (92%)	4 (8%)	11 34
29	17	41/42 (98%)	38 (93%)	3 (7%)	13 38
29	27	41/42 (98%)	36 (88%)	5 (12%)	5 16
30	18	54/55 (98%)	50 (93%)	4 (7%)	13 38
30	28	54/55 (98%)	47 (87%)	7 (13%)	4 13
31	19	34/34 (100%)	32 (94%)	2 (6%)	18 48
31	29	34/34 (100%)	31 (91%)	3 (9%)	9 29
33	1b	191/220 (87%)	159 (83%)	32 (17%)	2 7
33	2b	187/220 (85%)	165 (88%)	22 (12%)	5 17
34	1c	144/188 (77%)	131 (91%)	13 (9%)	9 28
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7 24
35	1d	171/181 (94%)	151 (88%)	20 (12%)	5 17
35	2d	172/181 (95%)	147 (86%)	25 (14%)	3 10
36	1e	114/123 (93%)	100 (88%)	14 (12%)	4 15
36	2e	114/123 (93%)	104 (91%)	10 (9%)	9 29
37	1f	85/90 (94%)	76 (89%)	9 (11%)	6 22
37	2f	85/90 (94%)	75 (88%)	10 (12%)	5 17
38	1g	120/127 (94%)	109 (91%)	11 (9%)	8 27
38	2g	119/127 (94%)	108 (91%)	11 (9%)	8 27
39	1h	116/119 (98%)	99 (85%)	17 (15%)	3 10
39	2h	114/119 (96%)	101 (89%)	13 (11%)	5 18
40	1i	91/99 (92%)	75 (82%)	16 (18%)	2 6
40	2i	88/99 (89%)	71 (81%)	17 (19%)	1 5
41	1j	68/92 (74%)	62 (91%)	6 (9%)	9 29
41	2j	68/92 (74%)	55 (81%)	13 (19%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	1k	83/99 (84%)	71 (86%)	12 (14%)	3 10
42	2k	83/99 (84%)	72 (87%)	11 (13%)	4 12
43	1l	96/108 (89%)	86 (90%)	10 (10%)	7 23
43	2l	96/108 (89%)	81 (84%)	15 (16%)	2 9
44	1m	90/101 (89%)	77 (86%)	13 (14%)	3 11
44	2m	87/101 (86%)	69 (79%)	18 (21%)	1 4
45	1n	49/50 (98%)	41 (84%)	8 (16%)	2 8
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5 16
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16 44
46	2o	78/80 (98%)	70 (90%)	8 (10%)	7 23
47	1p	69/74 (93%)	58 (84%)	11 (16%)	2 8
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4 13
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13 38
48	2q	94/97 (97%)	84 (89%)	10 (11%)	6 22
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10 31
49	2r	59/77 (77%)	50 (85%)	9 (15%)	3 9
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7 23
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4 12
51	1t	71/82 (87%)	63 (89%)	8 (11%)	5 19
51	2t	70/82 (85%)	61 (87%)	9 (13%)	4 13
52	1u	18/22 (82%)	15 (83%)	3 (17%)	2 7
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19 50
53	1y	82/98 (84%)	77 (94%)	5 (6%)	17 46
53	2y	79/98 (81%)	66 (84%)	13 (16%)	2 8
All	All	9524/10260 (93%)	8360 (88%)	1164 (12%)	5 16

5 of 1164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	2b	164	VAL
51	2t	62	LEU
35	2d	38	TYR
33	2b	157	ARG
41	2j	69	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
38	2g	11	GLN
38	2g	148	ASN
50	2s	69	HIS
37	1f	7	ASN
36	1e	130	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	447 (15%)	26 (0%)
1	2A	2858/2915 (98%)	519 (18%)	33 (1%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	119/121 (98%)	21 (17%)	0
32	1a	1497/1521 (98%)	257 (17%)	0
32	2a	1501/1521 (98%)	283 (18%)	0
All	All	8959/9114 (98%)	1539 (17%)	59 (0%)

5 of 1539 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	8	A
1	1A	10	G
1	1A	12	U
1	1A	14	A
1	1A	34	C

5 of 59 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	196	A
1	2A	2601	C
1	2A	827	U
1	2A	2321	G
1	2A	1491	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	M2G	1a	966	32	24,27,28	1.28	3 (12%)	33,40,43	1.81	6 (18%)
43	0TD	1l	92	43	8,9,10	4.84	2 (25%)	6,11,13	6.10	2 (33%)
32	G7M	1a	527	54,32	23,26,27	1.54	4 (17%)	34,39,42	1.68	5 (14%)
1	OMU	2A	2552	54,1	19,22,23	1.21	3 (15%)	25,31,34	1.79	5 (20%)
32	UR3	2a	1498	32	19,22,23	0.94	1 (5%)	26,32,35	1.84	3 (11%)
1	5MU	1A	1939	1	19,22,23	1.37	4 (21%)	27,32,35	2.05	6 (22%)
32	5MC	1a	1407	32	19,22,23	1.72	3 (15%)	26,32,35	1.15	3 (11%)
32	5MC	2a	967	32	19,22,23	1.77	3 (15%)	26,32,35	1.12	2 (7%)
1	OMG	1A	2251	54,1	23,26,27	1.27	3 (13%)	32,38,41	2.03	5 (15%)
1	5MU	2A	1939	54,1	19,22,23	1.45	5 (26%)	27,32,35	2.19	6 (22%)
1	PSU	1A	2605	1	18,21,22	1.37	2 (11%)	21,30,33	1.93	4 (19%)
32	M2G	2a	966	32	24,27,28	1.28	4 (16%)	33,40,43	1.79	6 (18%)
32	2MG	2a	1207	32	23,26,27	1.28	4 (17%)	33,38,41	2.10	5 (15%)
1	PSU	1A	1911	1	18,21,22	1.37	3 (16%)	21,30,33	2.12	5 (23%)
1	2MA	2A	2503	54,1	22,25,26	1.48	5 (22%)	32,37,40	2.34	8 (25%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.99	5 (23%)
32	G7M	2a	527	54,32	23,26,27	1.52	3 (13%)	34,39,42	1.67	5 (14%)
1	5MC	1A	1942	1	19,22,23	1.50	3 (15%)	26,32,35	1.20	3 (11%)
32	5MC	1a	967	32	19,22,23	1.58	3 (15%)	26,32,35	1.11	3 (11%)
32	MA6	1a	1518	32	23,26,27	0.39	0	33,38,41	2.00	10 (30%)
1	5MU	1A	1915	1	19,22,23	1.46	5 (26%)	27,32,35	2.34	9 (33%)
1	OMC	1A	1920	1	19,22,23	0.83	0	25,31,34	0.96	1 (4%)
1	OMG	2A	2251	54,1	23,26,27	1.22	2 (8%)	32,38,41	2.04	6 (18%)
32	UR3	1a	1498	32	19,22,23	1.03	2 (10%)	26,32,35	1.70	5 (19%)
32	2MG	1a	1207	54,32	23,26,27	1.26	4 (17%)	33,38,41	2.32	8 (24%)
32	5MC	2a	1400	32	19,22,23	1.65	3 (15%)	26,32,35	1.20	4 (15%)
32	5MC	2a	1407	32	19,22,23	1.75	3 (15%)	26,32,35	1.25	3 (11%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.14	10 (30%)
1	PSU	1A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.02	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MU	2A	1915	1	19,22,23	1.48	4 (21%)	27,32,35	2.20	10 (37%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.96	1 (4%)
1	PSU	2A	2605	1	18,21,22	1.35	2 (11%)	21,30,33	1.98	4 (19%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.98	1 (4%)
1	PSU	2A	1917	1	18,21,22	1.41	3 (16%)	21,30,33	1.98	4 (19%)
1	5MC	2A	1942	1	19,22,23	1.65	3 (15%)	26,32,35	1.05	2 (7%)
1	OMU	1A	2552	54,1	19,22,23	1.26	3 (15%)	25,31,34	1.79	4 (16%)
32	PSU	1a	516	54,32	18,21,22	1.41	2 (11%)	21,30,33	1.92	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.31	2 (11%)	21,30,33	1.99	5 (23%)
32	5MC	2a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.21	3 (11%)
1	2MA	1A	2503	54,1	22,25,26	1.46	4 (18%)	32,37,40	2.29	6 (18%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.22	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.14	3 (11%)
32	MA6	1a	1519	32	23,26,27	0.43	0	33,38,41	1.94	9 (27%)
43	0TD	2l	92	43	8,9,10	4.34	1 (12%)	6,11,13	2.04	3 (50%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.03	9 (27%)
1	5MC	2A	1962	54,1	19,22,23	1.51	3 (15%)	26,32,35	1.14	2 (7%)
1	5MC	1A	1962	54,1	19,22,23	1.43	3 (15%)	26,32,35	1.19	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.77	0	25,32,35	0.92	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
32	G7M	1a	527	54,32	-	3/7/25/26	0/3/3/3
1	OMU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	54,1	-	1/9/27/28	0/3/3/3
1	5MU	2A	1939	54,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	54,1	-	3/7/25/26	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	54,32	-	2/7/25/26	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	OMG	2A	2251	54,1	-	2/9/27/28	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	54,32	-	0/9/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	1/11/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
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	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	54,1	-	0/9/27/28	0/2/2/2
32	PSU	1a	516	54,32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
1	2MA	1A	2503	54,1	-	2/7/25/26	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	5MC	2A	1962	54,1	-	2/7/25/26	0/2/2/2
1	5MC	1A	1962	54,1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	3/9/29/30	0/2/2/2

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.74	1.69	1.82
43	2l	92	0TD	CB-SB	-11.93	1.70	1.82
32	2a	967	5MC	C5-C4	6.63	1.49	1.44
32	2a	1407	5MC	C5-C4	6.38	1.49	1.44
32	1a	1407	5MC	C5-C4	6.31	1.48	1.44

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-14.60	76.11	102.36
1	1A	2503	2MA	C5-C4-N3	-8.40	118.33	127.18
1	2A	2503	2MA	C5-C4-N3	-8.31	118.42	127.18
32	2a	1498	UR3	C4-N3-C2	-7.53	118.52	124.58
32	1a	1207	2MG	C2-N3-C4	7.26	121.09	112.00

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6

There are no ring outliers.

27 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	966	M2G	2	0
43	1l	92	0TD	2	0
32	2a	1498	UR3	2	0
1	1A	1939	5MU	2	0
1	1A	2251	OMG	1	0
1	2A	1939	5MU	1	0
1	1A	2605	PSU	1	0
32	2a	966	M2G	1	0
32	2a	1207	2MG	1	0
1	2A	2503	2MA	1	0
1	1A	1942	5MC	1	0
32	1a	1518	MA6	2	0
1	1A	1915	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1920	OMC	2	0
1	2A	2251	OMG	1	0
32	1a	1498	UR3	1	0
32	1a	1207	2MG	1	0
32	2a	1400	5MC	2	0
32	2a	1519	MA6	1	0
1	2A	1915	5MU	1	0
1	2A	1920	OMC	1	0
32	2a	1402	4OC	2	0
1	2A	1917	PSU	1	0
32	1a	1519	MA6	3	0
43	2l	92	0TD	2	0
32	2a	1518	MA6	1	0
32	1a	1402	4OC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2505 ligands modelled in this entry, 2492 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	MPD	2A	3735	-	7,7,7	0.31	0	9,10,10	0.27	0
56	MPD	1a	3271	-	7,7,7	0.34	0	9,10,10	0.32	0
56	MPD	1a	3272	-	7,7,7	0.33	0	9,10,10	0.50	0
56	MPD	2B	221	-	7,7,7	0.32	0	9,10,10	0.30	0
59	SF4	1d	306	35	0,12,12	-	-	-		
55	A1CRE	1A	4012	-	43,45,45	2.53	11 (25%)	57,68,68	2.16	18 (31%)
57	ARG	1B	231	54	10,11,11	0.78	1 (10%)	9,13,13	1.04	1 (11%)
56	MPD	18	105	-	7,7,7	0.32	0	9,10,10	0.43	0
56	MPD	1A	4013	-	7,7,7	0.32	0	9,10,10	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
59	SF4	2d	501	35	0,12,12	-	-	-		
56	MPD	2A	3734	-	7,7,7	0.33	0	9,10,10	0.30	0
57	ARG	1F	317	-	10,11,11	0.80	1 (10%)	9,13,13	0.99	1 (11%)
55	A1CRE	2A	3733	-	43,45,45	2.50	13 (30%)	57,68,68	2.26	18 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	MPD	2A	3735	-	-	4/5/5/5	-
56	MPD	1a	3271	-	-	0/5/5/5	-
56	MPD	1a	3272	-	-	4/5/5/5	-
56	MPD	2B	221	-	-	1/5/5/5	-
59	SF4	1d	306	35	-	-	0/6/5/5
55	A1CRE	1A	4012	-	-	9/17/79/79	0/5/5/5
57	ARG	1B	231	54	-	1/11/11/11	-
56	MPD	18	105	-	-	4/5/5/5	-
56	MPD	1A	4013	-	-	2/5/5/5	-
59	SF4	2d	501	35	-	-	0/6/5/5
56	MPD	2A	3734	-	-	1/5/5/5	-
57	ARG	1F	317	-	-	5/11/11/11	-
55	A1CRE	2A	3733	-	-	4/17/79/79	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4012	A1CRE	CAT-CAQ	-9.09	1.36	1.51
55	1A	4012	A1CRE	CAA-CAQ	-8.58	1.40	1.53
55	2A	3733	A1CRE	CAA-CAQ	-8.27	1.41	1.53
55	2A	3733	A1CRE	CAT-CAQ	-7.73	1.38	1.51
55	1A	4012	A1CRE	CBI-CBJ	-4.91	1.39	1.50

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1A	4012	A1CRE	CAK-CAC-CAB	-7.75	107.96	116.28
55	2A	3733	A1CRE	CAK-CAC-CAB	-7.53	108.20	116.28
55	2A	3733	A1CRE	CAZ-CAB-CAC	-5.08	103.63	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1A	4012	A1CRE	CAF-CAG-CAB	-4.66	106.37	111.57
55	2A	3733	A1CRE	CAT-CAQ-CAA	4.41	113.22	108.53

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1A	4012	A1CRE	CAI-CAJ-CAN-CBA
55	1A	4012	A1CRE	CAK-CAJ-CAN-CBA
55	2A	3733	A1CRE	CAK-CAJ-CAN-CBA
55	2A	3733	A1CRE	CAJ-CAN-CBA-NBB
56	1a	3272	MPD	C2-C3-C4-O4

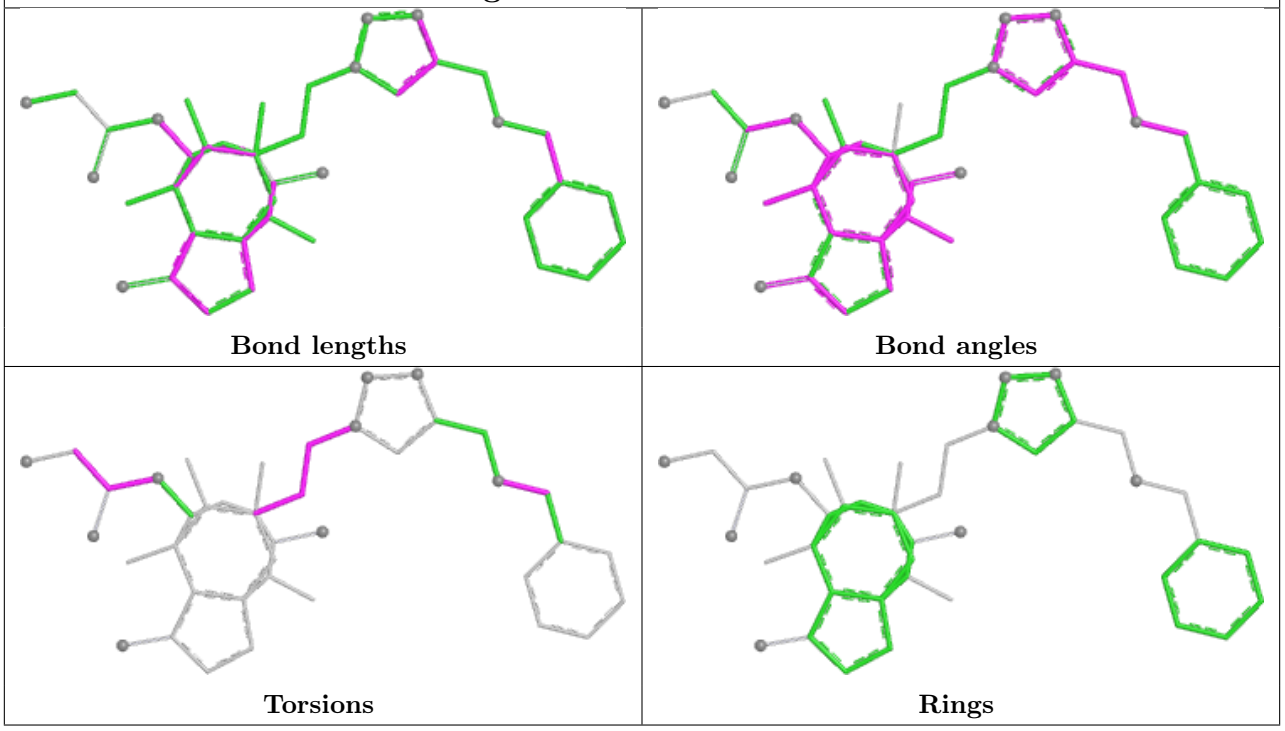
There are no ring outliers.

8 monomers are involved in 10 short contacts:

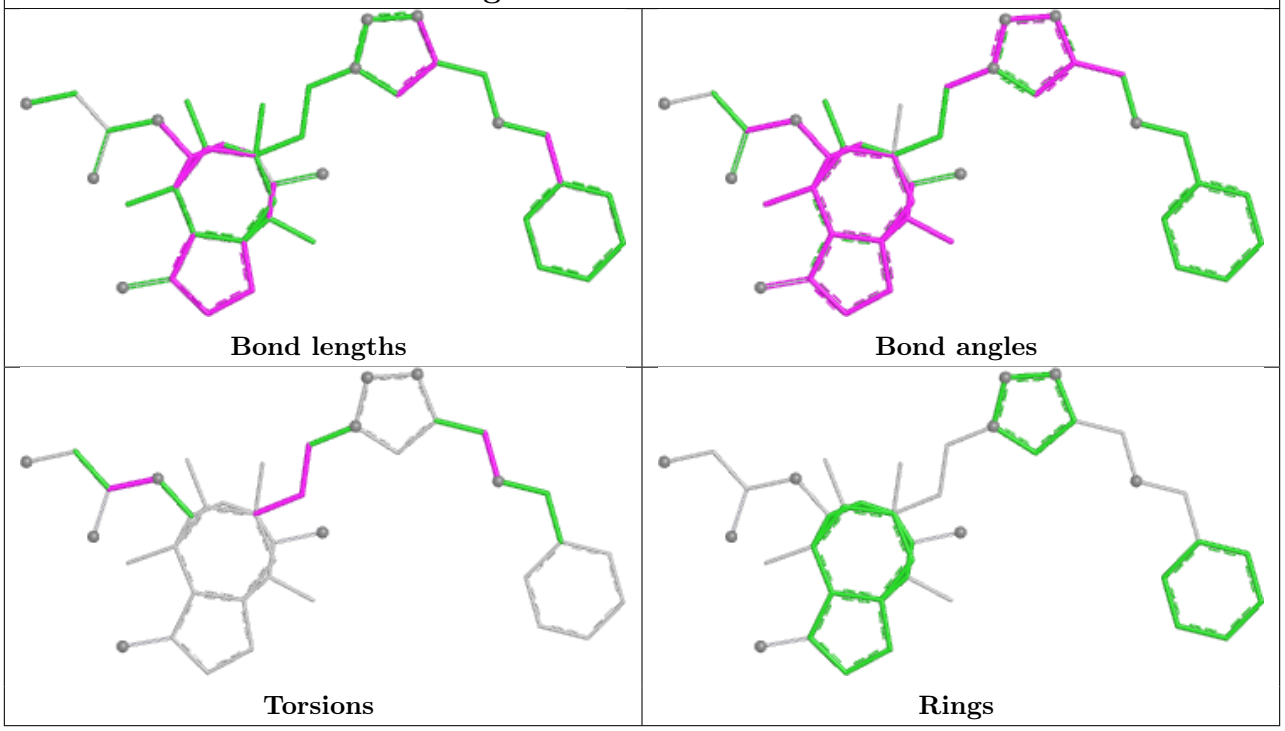
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	1a	3271	MPD	1	0
56	1a	3272	MPD	1	0
56	2B	221	MPD	1	0
59	1d	306	SF4	1	0
57	1B	231	ARG	2	0
56	18	105	MPD	1	0
56	1A	4013	MPD	1	0
57	1F	317	ARG	2	0

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

Ligand A1CRE 1A 4012



Ligand A1CRE 2A 3733



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.24	149 (5%) 33 26	14, 32, 95, 109	0
1	2A	2856/2915 (97%)	0.23	178 (6%) 26 21	28, 51, 97, 114	0
2	1B	120/121 (99%)	-0.09	1 (0%) 82 77	26, 49, 65, 83	0
2	2B	120/121 (99%)	0.97	11 (9%) 14 12	54, 76, 85, 91	0
3	1D	275/276 (99%)	-0.09	5 (1%) 67 59	18, 32, 47, 66	0
3	2D	275/276 (99%)	0.30	7 (2%) 58 48	27, 45, 60, 78	0
4	1E	204/206 (99%)	-0.07	1 (0%) 87 83	16, 36, 55, 79	0
4	2E	204/206 (99%)	0.46	5 (2%) 58 48	28, 51, 68, 78	0
5	1F	203/210 (96%)	-0.03	1 (0%) 87 83	15, 36, 65, 88	0
5	2F	203/210 (96%)	0.56	7 (3%) 48 39	33, 58, 75, 88	0
6	1G	181/182 (99%)	0.84	14 (7%) 19 16	42, 61, 79, 88	0
6	2G	181/182 (99%)	1.60	55 (30%) 1 1	68, 79, 90, 94	0
7	1H	174/180 (96%)	0.33	4 (2%) 61 52	33, 49, 62, 70	0
7	2H	173/180 (96%)	1.21	26 (15%) 5 4	62, 78, 87, 94	0
8	1I	147/148 (99%)	0.87	13 (8%) 15 13	39, 66, 76, 81	0
8	2I	146/148 (98%)	1.07	14 (9%) 13 11	47, 72, 84, 90	0
9	1N	140/140 (100%)	0.01	1 (0%) 84 79	22, 34, 58, 74	0
9	2N	140/140 (100%)	0.55	4 (2%) 53 45	39, 57, 73, 76	0
10	1O	122/122 (100%)	-0.04	1 (0%) 82 77	25, 34, 52, 58	0
10	2O	122/122 (100%)	0.54	7 (5%) 29 23	39, 50, 62, 71	0
11	1P	149/150 (99%)	0.08	5 (3%) 48 39	17, 40, 59, 72	0
11	2P	149/150 (99%)	0.51	3 (2%) 65 56	33, 61, 77, 83	0
12	1Q	141/141 (100%)	0.06	3 (2%) 63 54	22, 37, 51, 65	0
12	2Q	141/141 (100%)	0.73	8 (5%) 29 23	41, 56, 68, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.17	0 100 100	20, 32, 44, 53	0
13	2R	118/118 (100%)	0.21	1 (0%) 82 77	35, 47, 59, 70	0
14	1S	110/112 (98%)	0.34	1 (0%) 81 75	37, 50, 61, 70	0
14	2S	110/112 (98%)	1.29	15 (13%) 7 5	61, 70, 78, 84	0
15	1T	131/146 (89%)	0.16	4 (3%) 51 42	31, 41, 68, 80	0
15	2T	131/146 (89%)	0.39	5 (3%) 44 36	44, 53, 71, 78	0
16	1U	116/118 (98%)	-0.19	2 (1%) 69 61	18, 26, 47, 65	0
16	2U	116/118 (98%)	0.53	5 (4%) 40 31	33, 55, 70, 73	0
17	1V	101/101 (100%)	-0.14	1 (0%) 79 73	20, 38, 53, 65	0
17	2V	101/101 (100%)	0.77	4 (3%) 42 34	33, 63, 73, 83	0
18	1W	112/113 (99%)	-0.19	1 (0%) 81 75	18, 26, 47, 75	0
18	2W	112/113 (99%)	0.11	1 (0%) 81 75	30, 43, 59, 77	0
19	1X	95/96 (98%)	-0.07	1 (1%) 78 71	24, 34, 56, 71	0
19	2X	95/96 (98%)	0.62	3 (3%) 50 41	40, 53, 72, 80	0
20	1Y	107/110 (97%)	0.41	2 (1%) 66 58	31, 47, 64, 74	0
20	2Y	107/110 (97%)	1.29	22 (20%) 2 2	54, 67, 81, 90	0
21	1Z	203/206 (98%)	0.65	10 (4%) 35 27	34, 56, 75, 83	0
21	2Z	201/206 (97%)	1.26	34 (16%) 4 3	57, 73, 84, 90	0
22	10	77/85 (90%)	0.18	2 (2%) 57 48	24, 33, 50, 62	0
22	20	77/85 (90%)	0.84	5 (6%) 25 20	44, 55, 68, 75	0
23	11	97/98 (98%)	0.48	4 (4%) 41 33	23, 38, 63, 70	0
23	21	97/98 (98%)	0.55	4 (4%) 41 33	34, 50, 71, 75	0
24	12	70/72 (97%)	0.16	1 (1%) 73 65	29, 43, 54, 76	0
24	22	70/72 (97%)	1.13	11 (15%) 5 4	53, 65, 74, 75	0
25	13	59/60 (98%)	0.21	1 (1%) 69 61	23, 34, 57, 75	0
25	23	59/60 (98%)	0.55	1 (1%) 69 61	46, 55, 75, 80	0
26	14	69/71 (97%)	1.25	11 (15%) 5 4	61, 80, 91, 103	0
26	24	69/71 (97%)	2.10	36 (52%) 0 0	77, 88, 97, 102	0
27	15	59/60 (98%)	0.08	2 (3%) 48 39	17, 32, 63, 67	0
27	25	59/60 (98%)	0.52	1 (1%) 69 61	30, 51, 74, 80	0
28	16	53/54 (98%)	-0.06	0 100 100	28, 37, 50, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.56	4 (7%) 20 16	44, 54, 63, 71	0
29	17	48/49 (97%)	-0.23	3 (6%) 26 20	15, 22, 58, 64	0
29	27	48/49 (97%)	0.49	4 (8%) 17 14	29, 38, 63, 65	0
30	18	64/65 (98%)	-0.05	1 (1%) 70 62	21, 29, 37, 47	0
30	28	64/65 (98%)	0.66	6 (9%) 14 12	40, 47, 58, 63	0
31	19	37/37 (100%)	-0.24	0 100 100	29, 38, 54, 66	0
31	29	37/37 (100%)	0.72	0 100 100	51, 62, 72, 79	0
32	1a	1488/1521 (97%)	0.67	86 (5%) 29 22	29, 70, 96, 117	0
32	2a	1492/1521 (98%)	0.75	120 (8%) 18 15	39, 72, 96, 111	0
33	1b	231/256 (90%)	1.48	53 (22%) 2 2	64, 78, 89, 97	0
33	2b	231/256 (90%)	1.49	54 (23%) 2 2	69, 81, 90, 96	0
34	1c	206/239 (86%)	1.35	34 (16%) 4 3	62, 77, 85, 88	0
34	2c	206/239 (86%)	1.79	68 (33%) 1 1	68, 82, 88, 99	0
35	1d	208/209 (99%)	1.64	61 (29%) 1 1	55, 71, 80, 85	0
35	2d	208/209 (99%)	1.29	37 (17%) 4 3	57, 69, 79, 86	0
36	1e	148/162 (91%)	0.76	8 (5%) 31 24	41, 63, 72, 79	0
36	2e	148/162 (91%)	1.16	15 (10%) 12 10	52, 68, 79, 91	0
37	1f	100/101 (99%)	0.93	11 (11%) 10 9	55, 68, 75, 81	0
37	2f	100/101 (99%)	1.12	15 (15%) 5 4	54, 68, 78, 82	0
38	1g	155/156 (99%)	0.91	12 (7%) 19 16	62, 72, 81, 93	0
38	2g	155/156 (99%)	1.06	20 (12%) 7 6	65, 77, 84, 89	0
39	1h	137/138 (99%)	0.80	3 (2%) 62 53	52, 65, 72, 78	0
39	2h	137/138 (99%)	0.96	9 (6%) 24 19	60, 70, 76, 82	0
40	1i	127/128 (99%)	1.83	43 (33%) 1 1	67, 80, 88, 90	0
40	2i	126/128 (98%)	2.14	68 (53%) 0 0	68, 84, 89, 93	0
41	1j	97/105 (92%)	1.98	41 (42%) 0 0	66, 82, 89, 95	0
41	2j	96/105 (91%)	2.10	51 (53%) 0 0	74, 85, 92, 94	0
42	1k	114/129 (88%)	0.92	12 (10%) 11 10	39, 60, 74, 79	0
42	2k	114/129 (88%)	0.99	9 (7%) 18 15	57, 68, 78, 82	0
43	1l	121/132 (91%)	0.69	3 (2%) 58 48	46, 57, 68, 74	0
43	2l	121/132 (91%)	0.95	8 (6%) 24 19	51, 63, 71, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	1.34	21 (18%) 3 3	62, 76, 83, 86	0
44	2m	114/126 (90%)	1.66	38 (33%) 1 1	71, 82, 87, 89	0
45	1n	60/61 (98%)	1.72	22 (36%) 1 0	62, 75, 82, 85	0
45	2n	60/61 (98%)	2.32	30 (50%) 0 0	75, 83, 88, 90	0
46	1o	88/89 (98%)	0.80	8 (9%) 15 12	47, 63, 74, 80	0
46	2o	88/89 (98%)	0.66	3 (3%) 48 39	57, 68, 78, 82	0
47	1p	82/88 (93%)	1.22	12 (14%) 6 4	58, 71, 81, 87	0
47	2p	82/88 (93%)	1.06	10 (12%) 8 7	55, 64, 74, 79	0
48	1q	99/105 (94%)	0.82	5 (5%) 33 26	48, 63, 73, 78	0
48	2q	99/105 (94%)	0.77	5 (5%) 33 26	51, 63, 74, 78	0
49	1r	68/88 (77%)	1.14	8 (11%) 9 7	54, 66, 78, 82	0
49	2r	68/88 (77%)	0.93	5 (7%) 20 17	59, 68, 79, 81	0
50	1s	83/93 (89%)	1.73	27 (32%) 1 1	69, 79, 86, 90	0
50	2s	83/93 (89%)	2.11	37 (44%) 0 0	72, 86, 93, 97	0
51	1t	96/106 (90%)	1.23	22 (22%) 2 2	57, 70, 77, 83	0
51	2t	98/106 (92%)	0.81	8 (8%) 17 14	56, 65, 76, 83	0
52	1u	23/27 (85%)	1.85	9 (39%) 1 0	66, 72, 78, 81	0
52	2u	23/27 (85%)	2.11	13 (56%) 0 0	72, 81, 85, 88	0
53	1y	97/113 (85%)	0.79	4 (4%) 41 33	50, 64, 74, 78	0
53	2y	96/113 (84%)	1.88	37 (38%) 1 0	68, 81, 88, 92	0
All	All	20766/21468 (96%)	0.57	1897 (9%) 15 12	14, 60, 89, 117	0

The worst 5 of 1897 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	11	2	SER	12.1
1	2A	2119	A	8.9
1	1A	1087	G	8.6
45	2n	2	ALA	8.4
1	1A	1091	G	8.4

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	5MU	2A	1915	21/22	0.79	0.14	78,83,92,101	0
32	2MG	2a	1207	24/25	0.81	0.16	82,87,93,96	0
1	5MU	1A	1915	21/22	0.84	0.14	66,78,92,99	0
32	2MG	1a	1207	24/25	0.86	0.14	74,80,84,89	0
32	5MC	2a	967	21/22	0.87	0.13	73,77,87,91	0
32	PSU	2a	516	20/21	0.88	0.11	76,81,88,98	0
1	PSU	2A	1917	20/21	0.89	0.11	70,73,87,91	0
1	PSU	2A	1911	20/21	0.90	0.12	61,68,75,78	0
43	0TD	1l	92	10/11	0.90	0.15	53,59,63,75	0
32	M2G	2a	966	25/26	0.91	0.12	69,74,83,92	0
32	M2G	1a	966	25/26	0.91	0.13	54,61,70,76	0
32	G7M	2a	527	24/25	0.91	0.13	60,65,68,71	0
43	0TD	2l	92	10/11	0.91	0.13	65,68,73,79	0
32	5MC	1a	967	21/22	0.92	0.12	58,63,75,81	0
32	PSU	1a	516	20/21	0.92	0.11	60,70,76,82	0
32	5MC	2a	1400	21/22	0.92	0.14	57,71,76,79	0
1	PSU	1A	1917	20/21	0.92	0.10	57,68,77,78	0
32	4OC	2a	1402	22/23	0.93	0.12	55,62,64,73	0
1	PSU	1A	1911	20/21	0.93	0.11	43,62,65,66	0
32	5MC	1a	1400	21/22	0.94	0.12	37,55,59,61	0
32	5MC	2a	1407	21/22	0.94	0.10	55,63,67,67	0
32	UR3	2a	1498	21/22	0.94	0.12	49,56,61,68	0
32	5MC	1a	1407	21/22	0.94	0.10	45,53,59,61	0
32	UR3	1a	1498	21/22	0.95	0.12	39,46,51,60	0
32	MA6	1a	1519	24/25	0.95	0.11	37,44,53,56	0
32	4OC	1a	1402	22/23	0.95	0.12	45,52,60,64	0
1	OMC	2A	1920	21/22	0.95	0.11	59,62,66,70	0
32	MA6	2a	1518	24/25	0.95	0.10	56,63,66,69	0
32	MA6	2a	1519	24/25	0.95	0.12	53,60,66,70	0
1	5MC	2A	1942	21/22	0.95	0.11	43,50,54,55	0
32	5MC	2a	1404	21/22	0.96	0.10	44,56,60,66	0
32	G7M	1a	527	24/25	0.96	0.09	47,55,61,65	0
1	OMG	2A	2251	24/25	0.96	0.08	32,37,43,50	0
1	2MA	2A	2503	23/24	0.96	0.09	27,30,38,40	0
1	5MC	1A	1942	21/22	0.96	0.11	22,33,37,37	0
32	MA6	1a	1518	24/25	0.96	0.10	39,44,49,57	0
1	5MU	2A	1939	21/22	0.97	0.09	33,39,44,46	0
1	OMG	1A	2251	24/25	0.97	0.08	15,22,25,27	0
1	5MC	2A	1962	21/22	0.97	0.07	40,42,49,59	0
1	5MU	1A	1939	21/22	0.97	0.08	19,24,28,30	0
32	5MC	1a	1404	21/22	0.97	0.09	41,44,48,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OMC	1A	1920	21/22	0.97	0.09	39,54,61,62	0
1	PSU	1A	2605	20/21	0.98	0.07	23,24,30,30	0
1	5MC	1A	1962	21/22	0.98	0.07	30,34,37,44	0
1	2MA	1A	2503	23/24	0.98	0.06	13,18,21,22	0
1	OMU	2A	2552	21/22	0.98	0.07	30,36,42,44	0
1	PSU	2A	2605	20/21	0.98	0.07	32,37,41,45	0
1	OMU	1A	2552	21/22	0.98	0.07	21,23,29,35	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3119	1/1	0.43	0.20	85,85,85,85	0
54	MG	2A	3118	1/1	0.51	0.33	80,80,80,80	0
54	MG	1a	3233	1/1	0.53	0.26	78,78,78,78	0
54	MG	2A	3452	1/1	0.54	0.32	78,78,78,78	0
54	MG	1T	203	1/1	0.56	0.15	77,77,77,77	0
54	MG	2a	3151	1/1	0.56	0.20	74,74,74,74	0
54	MG	2A	3409	1/1	0.57	0.19	77,77,77,77	0
54	MG	1A	3902	1/1	0.58	0.21	35,35,35,35	0
54	MG	1Z	301	1/1	0.59	0.23	63,63,63,63	0
54	MG	1t	202	1/1	0.60	0.17	80,80,80,80	0
54	MG	2A	3199	1/1	0.62	0.20	58,58,58,58	0
54	MG	2a	3066	1/1	0.64	0.12	74,74,74,74	0
54	MG	2A	3518	1/1	0.65	0.20	75,75,75,75	0
54	MG	2A	3593	1/1	0.66	0.26	88,88,88,88	0
54	MG	1y	201	1/1	0.66	0.26	76,76,76,76	0
54	MG	1B	202	1/1	0.66	0.20	55,55,55,55	0
54	MG	2a	3126	1/1	0.67	0.19	76,76,76,76	0
54	MG	2A	3704	1/1	0.68	0.18	73,73,73,73	0
54	MG	2A	3453	1/1	0.68	0.27	67,67,67,67	0
54	MG	1A	3853	1/1	0.68	0.18	79,79,79,79	0
54	MG	2A	3112	1/1	0.68	0.21	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3161	1/1	0.69	0.24	69,69,69,69	0
54	MG	1a	3089	1/1	0.70	0.33	71,71,71,71	0
54	MG	2A	3462	1/1	0.70	0.20	65,65,65,65	0
54	MG	2A	3510	1/1	0.70	0.19	81,81,81,81	0
54	MG	1B	227	1/1	0.71	0.18	64,64,64,64	0
54	MG	1A	3283	1/1	0.71	0.17	78,78,78,78	0
54	MG	2A	3732	1/1	0.71	0.22	76,76,76,76	0
54	MG	2a	3063	1/1	0.71	0.17	80,80,80,80	0
54	MG	1a	3190	1/1	0.71	0.22	69,69,69,69	0
54	MG	1A	3939	1/1	0.71	0.14	70,70,70,70	0
54	MG	1A	3221	1/1	0.71	0.17	70,70,70,70	0
54	MG	2A	3229	1/1	0.72	0.19	68,68,68,68	0
54	MG	2A	3523	1/1	0.72	0.22	59,59,59,59	0
54	MG	2A	3277	1/1	0.72	0.23	78,78,78,78	0
54	MG	1A	3198	1/1	0.72	0.20	58,58,58,58	0
54	MG	2A	3078	1/1	0.72	0.12	74,74,74,74	0
54	MG	2a	3004	1/1	0.72	0.22	69,69,69,69	0
54	MG	2a	3047	1/1	0.72	0.16	75,75,75,75	0
54	MG	1a	3065	1/1	0.72	0.28	74,74,74,74	0
54	MG	2A	3460	1/1	0.72	0.19	65,65,65,65	0
54	MG	1G	202	1/1	0.72	0.17	54,54,54,54	0
54	MG	1A	3767	1/1	0.72	0.27	74,74,74,74	0
54	MG	2A	3496	1/1	0.73	0.16	58,58,58,58	0
54	MG	2A	3345	1/1	0.73	0.16	57,57,57,57	0
54	MG	1A	4005	1/1	0.73	0.12	49,49,49,49	0
54	MG	1A	3769	1/1	0.73	0.20	59,59,59,59	0
54	MG	2a	3033	1/1	0.73	0.16	69,69,69,69	0
54	MG	1a	3098	1/1	0.74	0.17	57,57,57,57	0
54	MG	2A	3706	1/1	0.74	0.48	55,55,55,55	0
54	MG	1B	228	1/1	0.74	0.13	57,57,57,57	0
54	MG	1A	3996	1/1	0.74	0.52	43,43,43,43	0
54	MG	1A	3671	1/1	0.74	0.18	58,58,58,58	0
54	MG	1A	3558	1/1	0.75	0.20	68,68,68,68	0
54	MG	2A	3157	1/1	0.75	0.12	58,58,58,58	0
54	MG	1d	302	1/1	0.75	0.24	68,68,68,68	0
54	MG	2a	3024	1/1	0.75	0.23	70,70,70,70	0
54	MG	1e	201	1/1	0.75	0.27	53,53,53,53	0
54	MG	1a	3097	1/1	0.75	0.35	72,72,72,72	0
54	MG	2A	3316	1/1	0.75	0.14	56,56,56,56	0
54	MG	1a	3164	1/1	0.75	0.19	53,53,53,53	0
54	MG	1a	3076	1/1	0.75	0.23	80,80,80,80	0
54	MG	1a	3198	1/1	0.75	0.14	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3068	1/1	0.76	0.34	67,67,67,67	0
54	MG	1f	202	1/1	0.76	0.22	73,73,73,73	0
54	MG	2a	3034	1/1	0.76	0.14	69,69,69,69	0
54	MG	1a	3197	1/1	0.76	0.14	78,78,78,78	0
54	MG	1A	3677	1/1	0.76	0.15	71,71,71,71	0
54	MG	1A	3664	1/1	0.76	0.17	69,69,69,69	0
54	MG	2A	3110	1/1	0.76	0.16	88,88,88,88	0
54	MG	1A	3176	1/1	0.76	0.17	52,52,52,52	0
54	MG	2a	3107	1/1	0.77	0.15	66,66,66,66	0
54	MG	1A	3946	1/1	0.77	0.30	84,84,84,84	0
54	MG	1a	3013	1/1	0.77	0.17	74,74,74,74	0
54	MG	2A	3724	1/1	0.78	0.17	60,60,60,60	0
54	MG	1A	3856	1/1	0.78	0.46	35,35,35,35	0
54	MG	2A	3475	1/1	0.78	0.11	71,71,71,71	0
54	MG	1A	3275	1/1	0.78	0.24	52,52,52,52	0
54	MG	1a	3085	1/1	0.78	0.18	67,67,67,67	0
54	MG	1f	201	1/1	0.78	0.15	55,55,55,55	0
54	MG	2A	3450	1/1	0.78	0.14	53,53,53,53	0
54	MG	2A	3533	1/1	0.78	0.18	63,63,63,63	0
54	MG	1A	3920	1/1	0.78	0.11	49,49,49,49	0
54	MG	2A	3673	1/1	0.78	0.16	64,64,64,64	0
54	MG	1a	3213	1/1	0.78	0.12	57,57,57,57	0
54	MG	1a	3215	1/1	0.78	0.25	65,65,65,65	0
54	MG	2a	3171	1/1	0.78	0.14	68,68,68,68	0
54	MG	2A	3164	1/1	0.79	0.14	69,69,69,69	0
54	MG	2A	3612	1/1	0.79	0.14	40,40,40,40	0
54	MG	2A	3653	1/1	0.79	0.21	95,95,95,95	0
54	MG	2A	3084	1/1	0.79	0.19	68,68,68,68	0
54	MG	2A	3702	1/1	0.79	0.16	54,54,54,54	0
54	MG	1a	3152	1/1	0.79	0.25	55,55,55,55	0
54	MG	2a	3068	1/1	0.79	0.23	69,69,69,69	0
54	MG	1d	305	1/1	0.79	0.13	78,78,78,78	0
54	MG	2a	3125	1/1	0.79	0.17	52,52,52,52	0
54	MG	1A	3871	1/1	0.79	0.17	51,51,51,51	0
54	MG	1A	3439	1/1	0.79	0.15	61,61,61,61	0
54	MG	2A	3570	1/1	0.79	0.20	73,73,73,73	0
56	MPD	1a	3271	8/8	0.79	0.28	68,72,77,78	0
54	MG	2A	3077	1/1	0.80	0.28	60,60,60,60	0
54	MG	1A	3189	1/1	0.80	0.13	57,57,57,57	0
54	MG	2A	3708	1/1	0.80	0.15	59,59,59,59	0
54	MG	1A	3507	1/1	0.80	0.13	42,42,42,42	0
54	MG	1a	3049	1/1	0.80	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3058	1/1	0.80	0.19	69,69,69,69	0
54	MG	1a	3251	1/1	0.80	0.15	55,55,55,55	0
54	MG	2A	3481	1/1	0.80	0.13	60,60,60,60	0
54	MG	1a	3263	1/1	0.80	0.17	63,63,63,63	0
54	MG	2a	3046	1/1	0.80	0.25	76,76,76,76	0
54	MG	1a	3146	1/1	0.80	0.15	50,50,50,50	0
54	MG	2A	3195	1/1	0.80	0.18	67,67,67,67	0
54	MG	1A	3805	1/1	0.80	0.14	57,57,57,57	0
54	MG	1A	3813	1/1	0.80	0.19	34,34,34,34	0
54	MG	2a	3074	1/1	0.80	0.14	58,58,58,58	0
54	MG	2a	3093	1/1	0.80	0.26	70,70,70,70	0
54	MG	1A	3272	1/1	0.80	0.27	48,48,48,48	0
54	MG	2a	3124	1/1	0.80	0.21	58,58,58,58	0
54	MG	2A	3289	1/1	0.80	0.13	55,55,55,55	0
54	MG	1a	3177	1/1	0.80	0.11	77,77,77,77	0
54	MG	1a	3081	1/1	0.80	0.18	90,90,90,90	0
54	MG	2a	3152	1/1	0.80	0.27	98,98,98,98	0
54	MG	1A	3689	1/1	0.80	0.11	49,49,49,49	0
54	MG	2A	3443	1/1	0.80	0.29	78,78,78,78	0
54	MG	1A	3188	1/1	0.81	0.30	35,35,35,35	0
54	MG	18	104	1/1	0.81	0.16	54,54,54,54	0
54	MG	1B	207	1/1	0.81	0.14	54,54,54,54	0
54	MG	2G	201	1/1	0.81	0.14	81,81,81,81	0
54	MG	1a	3027	1/1	0.81	0.14	67,67,67,67	0
54	MG	2A	3201	1/1	0.81	0.21	61,61,61,61	0
54	MG	2A	3502	1/1	0.81	0.16	26,26,26,26	0
54	MG	1a	3048	1/1	0.81	0.12	60,60,60,60	0
54	MG	2A	3023	1/1	0.81	0.24	76,76,76,76	0
54	MG	1A	3949	1/1	0.81	0.22	73,73,73,73	0
54	MG	2a	3057	1/1	0.81	0.16	67,67,67,67	0
54	MG	1A	3979	1/1	0.81	0.10	83,83,83,83	0
54	MG	2A	3568	1/1	0.81	0.13	77,77,77,77	0
54	MG	1A	3772	1/1	0.81	0.14	49,49,49,49	0
54	MG	2A	3577	1/1	0.81	0.16	51,51,51,51	0
54	MG	2A	3092	1/1	0.81	0.36	71,71,71,71	0
54	MG	2A	3606	1/1	0.81	0.15	42,42,42,42	0
54	MG	2A	3432	1/1	0.81	0.11	57,57,57,57	0
54	MG	2A	3435	1/1	0.81	0.22	62,62,62,62	0
54	MG	1A	3817	1/1	0.81	0.11	27,27,27,27	0
54	MG	2A	3689	1/1	0.81	0.24	65,65,65,65	0
54	MG	1T	205	1/1	0.81	0.16	48,48,48,48	0
54	MG	1a	3166	1/1	0.81	0.17	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3181	1/1	0.81	0.17	58,58,58,58	0
54	MG	2a	3183	1/1	0.81	0.15	69,69,69,69	0
54	MG	2A	3121	1/1	0.81	0.13	42,42,42,42	0
56	MPD	1a	3272	8/8	0.81	0.23	59,70,79,81	0
54	MG	1a	3257	1/1	0.82	0.15	54,54,54,54	0
54	MG	2A	3355	1/1	0.82	0.17	63,63,63,63	0
54	MG	2A	3369	1/1	0.82	0.28	70,70,70,70	0
54	MG	1A	3257	1/1	0.82	0.10	42,42,42,42	0
54	MG	2A	3173	1/1	0.82	0.17	52,52,52,52	0
54	MG	1A	3367	1/1	0.82	0.20	43,43,43,43	0
54	MG	2a	3103	1/1	0.82	0.18	75,75,75,75	0
54	MG	2a	3105	1/1	0.82	0.11	61,61,61,61	0
54	MG	1A	3076	1/1	0.82	0.29	46,46,46,46	0
54	MG	2B	207	1/1	0.82	0.17	81,81,81,81	0
54	MG	2B	216	1/1	0.82	0.14	77,77,77,77	0
54	MG	2E	304	1/1	0.82	0.12	55,55,55,55	0
54	MG	18	102	1/1	0.82	0.47	42,42,42,42	0
54	MG	1B	208	1/1	0.82	0.12	44,44,44,44	0
54	MG	1A	3027	1/1	0.82	0.26	56,56,56,56	0
54	MG	2a	3177	1/1	0.82	0.12	60,60,60,60	0
54	MG	2A	3280	1/1	0.82	0.11	53,53,53,53	0
54	MG	1A	3683	1/1	0.82	0.25	43,43,43,43	0
54	MG	2A	3293	1/1	0.82	0.12	28,28,28,28	0
54	MG	1A	3811	1/1	0.82	0.22	48,48,48,48	0
54	MG	2A	3730	1/1	0.83	0.16	58,58,58,58	0
54	MG	2A	3136	1/1	0.83	0.23	58,58,58,58	0
54	MG	1a	3017	1/1	0.83	0.21	59,59,59,59	0
54	MG	1A	3271	1/1	0.83	0.33	47,47,47,47	0
54	MG	1a	3042	1/1	0.83	0.16	69,69,69,69	0
54	MG	1a	3269	1/1	0.83	0.09	55,55,55,55	0
54	MG	1A	3969	1/1	0.83	0.14	54,54,54,54	0
54	MG	1A	3655	1/1	0.83	0.16	53,53,53,53	0
54	MG	1A	3987	1/1	0.83	0.15	32,32,32,32	0
54	MG	2A	3239	1/1	0.83	0.18	62,62,62,62	0
54	MG	2a	3035	1/1	0.83	0.16	85,85,85,85	0
54	MG	2A	3514	1/1	0.83	0.18	77,77,77,77	0
54	MG	2A	3516	1/1	0.83	0.13	57,57,57,57	0
54	MG	2A	3248	1/1	0.83	0.15	63,63,63,63	0
54	MG	1a	3059	1/1	0.83	0.18	65,65,65,65	0
54	MG	1a	3172	1/1	0.83	0.19	72,72,72,72	0
54	MG	1a	3173	1/1	0.83	0.15	62,62,62,62	0
54	MG	1A	3438	1/1	0.83	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3086	1/1	0.83	0.12	50,50,50,50	0
54	MG	1A	4000	1/1	0.83	0.11	52,52,52,52	0
54	MG	1A	3089	1/1	0.83	0.17	61,61,61,61	0
54	MG	13	103	1/1	0.83	0.24	43,43,43,43	0
54	MG	2A	3368	1/1	0.83	0.18	64,64,64,64	0
54	MG	2A	3616	1/1	0.83	0.14	66,66,66,66	0
54	MG	1A	3845	1/1	0.83	0.14	31,31,31,31	0
54	MG	2A	3398	1/1	0.83	0.24	59,59,59,59	0
54	MG	2A	3680	1/1	0.83	0.17	78,78,78,78	0
54	MG	1B	206	1/1	0.83	0.28	56,56,56,56	0
54	MG	2A	3425	1/1	0.83	0.20	65,65,65,65	0
54	MG	1a	3227	1/1	0.83	0.12	79,79,79,79	0
54	MG	1a	3229	1/1	0.83	0.23	69,69,69,69	0
54	MG	1A	3365	1/1	0.83	0.14	38,38,38,38	0
54	MG	2A	3720	1/1	0.83	0.09	76,76,76,76	0
54	MG	1a	3250	1/1	0.83	0.19	72,72,72,72	0
56	MPD	2B	221	8/8	0.83	0.29	58,69,74,76	0
57	ARG	1F	317	12/12	0.83	0.17	44,58,74,78	0
54	MG	2B	212	1/1	0.84	0.12	49,49,49,49	0
54	MG	1A	3506	1/1	0.84	0.21	36,36,36,36	0
54	MG	1A	3259	1/1	0.84	0.22	42,42,42,42	0
54	MG	1a	3158	1/1	0.84	0.19	73,73,73,73	0
54	MG	2A	3233	1/1	0.84	0.16	53,53,53,53	0
54	MG	2a	3021	1/1	0.84	0.17	50,50,50,50	0
54	MG	1A	3678	1/1	0.84	0.15	52,52,52,52	0
54	MG	1a	3031	1/1	0.84	0.14	57,57,57,57	0
54	MG	2A	3251	1/1	0.84	0.16	45,45,45,45	0
54	MG	1A	3516	1/1	0.84	0.64	32,32,32,32	0
54	MG	1i	3100	1/1	0.84	0.15	69,69,69,69	0
54	MG	1B	217	1/1	0.84	0.25	64,64,64,64	0
54	MG	2a	3053	1/1	0.84	0.21	62,62,62,62	0
54	MG	1B	225	1/1	0.84	0.15	50,50,50,50	0
54	MG	2a	3059	1/1	0.84	0.14	69,69,69,69	0
54	MG	2a	3061	1/1	0.84	0.15	75,75,75,75	0
54	MG	2A	3562	1/1	0.84	0.15	50,50,50,50	0
54	MG	1A	3963	1/1	0.84	0.10	55,55,55,55	0
54	MG	2A	3051	1/1	0.84	0.13	43,43,43,43	0
54	MG	1a	3182	1/1	0.84	0.16	66,66,66,66	0
54	MG	1A	3383	1/1	0.84	0.11	24,24,24,24	0
54	MG	1E	302	1/1	0.84	0.89	43,43,43,43	0
54	MG	2A	3376	1/1	0.84	0.15	52,52,52,52	0
54	MG	2a	3104	1/1	0.84	0.18	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1F	312	1/1	0.84	0.23	34,34,34,34	0
54	MG	1A	3972	1/1	0.84	0.42	54,54,54,54	0
54	MG	2A	3414	1/1	0.84	0.17	64,64,64,64	0
54	MG	1A	3729	1/1	0.84	0.20	56,56,56,56	0
54	MG	1A	3981	1/1	0.84	0.14	57,57,57,57	0
54	MG	2A	3433	1/1	0.84	0.18	59,59,59,59	0
54	MG	1A	3740	1/1	0.84	0.14	51,51,51,51	0
54	MG	2a	3161	1/1	0.84	0.14	66,66,66,66	0
54	MG	1A	3285	1/1	0.84	0.16	62,62,62,62	0
54	MG	1A	3199	1/1	0.84	0.15	46,46,46,46	0
54	MG	1a	3103	1/1	0.84	0.16	51,51,51,51	0
54	MG	1A	3770	1/1	0.84	0.27	62,62,62,62	0
54	MG	2j	201	1/1	0.84	0.10	75,75,75,75	0
54	MG	2t	201	1/1	0.84	0.16	56,56,56,56	0
54	MG	2y	201	1/1	0.84	0.20	93,93,93,93	0
54	MG	2A	3456	1/1	0.84	0.32	70,70,70,70	0
54	MG	2A	3457	1/1	0.84	0.20	62,62,62,62	0
56	MPD	2A	3734	8/8	0.84	0.26	36,44,51,51	0
54	MG	2B	201	1/1	0.84	0.15	73,73,73,73	0
54	MG	1a	3133	1/1	0.84	0.16	54,54,54,54	0
54	MG	2A	3241	1/1	0.85	0.21	59,59,59,59	0
54	MG	1a	3080	1/1	0.85	0.21	67,67,67,67	0
54	MG	1O	202	1/1	0.85	0.09	52,52,52,52	0
54	MG	2A	3266	1/1	0.85	0.18	68,68,68,68	0
54	MG	2A	3275	1/1	0.85	0.14	53,53,53,53	0
54	MG	1T	202	1/1	0.85	0.14	42,42,42,42	0
54	MG	1A	3411	1/1	0.85	0.12	65,65,65,65	0
54	MG	1a	3267	1/1	0.85	0.12	50,50,50,50	0
54	MG	2A	3290	1/1	0.85	0.15	45,45,45,45	0
54	MG	1A	3989	1/1	0.85	0.25	43,43,43,43	0
54	MG	1b	301	1/1	0.85	0.17	62,62,62,62	0
54	MG	1A	3418	1/1	0.85	0.14	25,25,25,25	0
54	MG	2B	206	1/1	0.85	0.19	57,57,57,57	0
54	MG	1d	304	1/1	0.85	0.11	91,91,91,91	0
54	MG	2B	208	1/1	0.85	0.15	72,72,72,72	0
54	MG	1A	3426	1/1	0.85	0.25	55,55,55,55	0
54	MG	2B	213	1/1	0.85	0.18	61,61,61,61	0
54	MG	1a	3117	1/1	0.85	0.11	56,56,56,56	0
54	MG	15	106	1/1	0.85	0.11	55,55,55,55	0
54	MG	18	101	1/1	0.85	0.44	40,40,40,40	0
54	MG	2I	201	1/1	0.85	0.15	79,79,79,79	0
54	MG	2a	3002	1/1	0.85	0.28	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1g	202	1/1	0.85	0.09	53,53,53,53	0
54	MG	2a	3005	1/1	0.85	0.17	69,69,69,69	0
54	MG	2a	3011	1/1	0.85	0.09	54,54,54,54	0
54	MG	1g	203	1/1	0.85	0.23	68,68,68,68	0
54	MG	1A	4003	1/1	0.85	0.17	58,58,58,58	0
54	MG	1t	201	1/1	0.85	0.17	61,61,61,61	0
54	MG	1A	3877	1/1	0.85	0.12	55,55,55,55	0
54	MG	1a	3006	1/1	0.85	0.13	66,66,66,66	0
54	MG	2A	3006	1/1	0.85	0.18	62,62,62,62	0
54	MG	1A	3168	1/1	0.85	0.12	51,51,51,51	0
54	MG	2A	3042	1/1	0.85	0.27	55,55,55,55	0
54	MG	1A	3791	1/1	0.85	0.48	31,31,31,31	0
54	MG	2A	3071	1/1	0.85	0.15	59,59,59,59	0
54	MG	1A	3933	1/1	0.85	0.14	20,20,20,20	0
54	MG	2a	3062	1/1	0.85	0.24	68,68,68,68	0
54	MG	1a	3028	1/1	0.85	0.19	50,50,50,50	0
54	MG	1A	3797	1/1	0.85	0.17	59,59,59,59	0
54	MG	1a	3176	1/1	0.85	0.13	73,73,73,73	0
54	MG	1A	3700	1/1	0.85	0.35	34,34,34,34	0
54	MG	2a	3076	1/1	0.85	0.15	52,52,52,52	0
54	MG	1a	3043	1/1	0.85	0.15	48,48,48,48	0
54	MG	1A	3727	1/1	0.85	0.09	69,69,69,69	0
54	MG	1a	3196	1/1	0.85	0.13	57,57,57,57	0
54	MG	2A	3123	1/1	0.85	0.18	54,54,54,54	0
54	MG	2A	3515	1/1	0.85	0.36	69,69,69,69	0
54	MG	1A	3237	1/1	0.85	0.82	28,28,28,28	0
54	MG	2a	3116	1/1	0.85	0.17	62,62,62,62	0
54	MG	1A	3393	1/1	0.85	0.13	23,23,23,23	0
54	MG	1D	318	1/1	0.85	0.15	49,49,49,49	0
54	MG	1a	3061	1/1	0.85	0.21	65,65,65,65	0
54	MG	2A	3537	1/1	0.85	0.11	61,61,61,61	0
54	MG	2A	3544	1/1	0.85	0.23	83,83,83,83	0
54	MG	2a	3156	1/1	0.85	0.13	58,58,58,58	0
54	MG	2a	3158	1/1	0.85	0.11	80,80,80,80	0
54	MG	2a	3159	1/1	0.85	0.13	65,65,65,65	0
54	MG	2A	3183	1/1	0.85	0.17	64,64,64,64	0
54	MG	2A	3185	1/1	0.85	0.12	45,45,45,45	0
54	MG	2a	3175	1/1	0.85	0.16	74,74,74,74	0
54	MG	1A	3838	1/1	0.85	0.18	64,64,64,64	0
54	MG	2A	3573	1/1	0.85	0.11	54,54,54,54	0
54	MG	1a	3228	1/1	0.85	0.12	67,67,67,67	0
54	MG	1A	3764	1/1	0.85	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
54	MG	2q	201	1/1	0.85	0.10	52,52,52,52	0
54	MG	2A	3604	1/1	0.85	0.11	38,38,38,38	0
54	MG	2A	3220	1/1	0.85	0.12	50,50,50,50	0
54	MG	2A	3610	1/1	0.85	0.24	92,92,92,92	0
54	MG	1A	3848	1/1	0.85	0.13	38,38,38,38	0
54	MG	1a	3239	1/1	0.85	0.09	56,56,56,56	0
56	MPD	2A	3735	8/8	0.85	0.22	58,65,69,71	0
54	MG	2A	3641	1/1	0.85	0.14	83,83,83,83	0
54	MG	1a	3248	1/1	0.85	0.19	73,73,73,73	0
54	MG	2P	203	1/1	0.86	0.15	61,61,61,61	0
54	MG	1a	3093	1/1	0.86	0.26	55,55,55,55	0
54	MG	2A	3511	1/1	0.86	0.16	46,46,46,46	0
54	MG	1a	3094	1/1	0.86	0.15	65,65,65,65	0
54	MG	2a	3006	1/1	0.86	0.12	64,64,64,64	0
54	MG	1A	3192	1/1	0.86	0.32	34,34,34,34	0
54	MG	2a	3017	1/1	0.86	0.21	68,68,68,68	0
54	MG	1y	205	1/1	0.86	0.12	66,66,66,66	0
54	MG	1a	3217	1/1	0.86	0.15	69,69,69,69	0
54	MG	2A	3017	1/1	0.86	0.42	53,53,53,53	0
54	MG	2A	3531	1/1	0.86	0.11	52,52,52,52	0
54	MG	1a	3226	1/1	0.86	0.10	63,63,63,63	0
54	MG	2A	3031	1/1	0.86	0.11	53,53,53,53	0
54	MG	1E	305	1/1	0.86	0.21	50,50,50,50	0
54	MG	2a	3051	1/1	0.86	0.25	54,54,54,54	0
54	MG	1A	3936	1/1	0.86	0.17	43,43,43,43	0
54	MG	1a	3104	1/1	0.86	0.25	57,57,57,57	0
54	MG	2A	3296	1/1	0.86	0.25	62,62,62,62	0
54	MG	1A	3300	1/1	0.86	0.14	70,70,70,70	0
54	MG	2A	3341	1/1	0.86	0.25	66,66,66,66	0
54	MG	1A	3941	1/1	0.86	0.12	67,67,67,67	0
54	MG	1a	3126	1/1	0.86	0.15	72,72,72,72	0
54	MG	2A	3605	1/1	0.86	0.11	65,65,65,65	0
54	MG	2a	3071	1/1	0.86	0.14	59,59,59,59	0
54	MG	1T	201	1/1	0.86	0.15	59,59,59,59	0
54	MG	2A	3099	1/1	0.86	0.28	59,59,59,59	0
54	MG	1A	3597	1/1	0.86	0.28	31,31,31,31	0
54	MG	2A	3382	1/1	0.86	0.15	59,59,59,59	0
54	MG	2a	3098	1/1	0.86	0.28	54,54,54,54	0
54	MG	2A	3619	1/1	0.86	0.12	52,52,52,52	0
54	MG	1A	3603	1/1	0.86	0.21	58,58,58,58	0
54	MG	2A	3642	1/1	0.86	0.24	60,60,60,60	0
54	MG	2A	3648	1/1	0.86	0.18	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3778	1/1	0.86	0.19	59,59,59,59	0
54	MG	2A	3412	1/1	0.86	0.23	63,63,63,63	0
54	MG	2A	3676	1/1	0.86	0.13	66,66,66,66	0
54	MG	1A	3628	1/1	0.86	0.15	58,58,58,58	0
54	MG	2a	3137	1/1	0.86	0.14	70,70,70,70	0
54	MG	2a	3149	1/1	0.86	0.19	64,64,64,64	0
54	MG	11	103	1/1	0.86	0.12	53,53,53,53	0
54	MG	2A	3431	1/1	0.86	0.13	53,53,53,53	0
54	MG	1A	3864	1/1	0.86	0.10	22,22,22,22	0
54	MG	1d	301	1/1	0.86	0.21	49,49,49,49	0
54	MG	1B	221	1/1	0.86	0.14	53,53,53,53	0
54	MG	1a	3073	1/1	0.86	0.21	47,47,47,47	0
54	MG	2A	3448	1/1	0.86	0.11	56,56,56,56	0
54	MG	2A	3449	1/1	0.86	0.13	71,71,71,71	0
54	MG	1a	3175	1/1	0.86	0.18	61,61,61,61	0
54	MG	1A	3629	1/1	0.86	0.16	48,48,48,48	0
54	MG	2B	203	1/1	0.86	0.23	79,79,79,79	0
54	MG	2a	3190	1/1	0.86	0.10	45,45,45,45	0
54	MG	2A	3190	1/1	0.86	0.22	56,56,56,56	0
54	MG	1A	3409	1/1	0.86	0.13	23,23,23,23	0
54	MG	1A	3267	1/1	0.86	0.08	52,52,52,52	0
54	MG	1B	230	1/1	0.86	0.14	61,61,61,61	0
54	MG	2A	3205	1/1	0.86	0.12	49,49,49,49	0
54	MG	2B	214	1/1	0.86	0.17	93,93,93,93	0
54	MG	2A	3216	1/1	0.86	0.17	59,59,59,59	0
54	MG	1a	3088	1/1	0.86	0.21	59,59,59,59	0
54	MG	1A	3025	1/1	0.86	0.56	46,46,46,46	0
54	MG	1p	101	1/1	0.86	0.10	50,50,50,50	0
54	MG	2A	3152	1/1	0.87	0.20	56,56,56,56	0
54	MG	1a	3019	1/1	0.87	0.10	44,44,44,44	0
54	MG	2A	3163	1/1	0.87	0.32	64,64,64,64	0
54	MG	1a	3022	1/1	0.87	0.14	53,53,53,53	0
54	MG	1a	3121	1/1	0.87	0.24	60,60,60,60	0
54	MG	2A	3175	1/1	0.87	0.12	69,69,69,69	0
54	MG	1A	3149	1/1	0.87	0.27	54,54,54,54	0
54	MG	2G	202	1/1	0.87	0.15	81,81,81,81	0
54	MG	1A	3156	1/1	0.87	0.36	37,37,37,37	0
54	MG	1a	3142	1/1	0.87	0.17	52,52,52,52	0
54	MG	23	101	1/1	0.87	0.27	54,54,54,54	0
54	MG	2A	3194	1/1	0.87	0.14	52,52,52,52	0
54	MG	1D	314	1/1	0.87	0.12	28,28,28,28	0
54	MG	2A	3489	1/1	0.87	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3494	1/1	0.87	0.14	72,72,72,72	0
54	MG	1a	3150	1/1	0.87	0.15	58,58,58,58	0
54	MG	2A	3497	1/1	0.87	0.37	48,48,48,48	0
54	MG	2A	3499	1/1	0.87	0.12	55,55,55,55	0
54	MG	1a	3038	1/1	0.87	0.17	59,59,59,59	0
54	MG	2a	3029	1/1	0.87	0.30	78,78,78,78	0
54	MG	2A	3504	1/1	0.87	0.14	57,57,57,57	0
54	MG	2A	3506	1/1	0.87	0.25	61,61,61,61	0
54	MG	1a	3040	1/1	0.87	0.19	61,61,61,61	0
54	MG	2A	3211	1/1	0.87	0.28	62,62,62,62	0
54	MG	2A	3512	1/1	0.87	0.14	68,68,68,68	0
54	MG	1A	3965	1/1	0.87	0.15	39,39,39,39	0
54	MG	1a	3163	1/1	0.87	0.13	70,70,70,70	0
54	MG	1A	3517	1/1	0.87	0.17	51,51,51,51	0
54	MG	1A	3555	1/1	0.87	0.29	34,34,34,34	0
54	MG	1A	3974	1/1	0.87	0.14	25,25,25,25	0
54	MG	1A	3055	1/1	0.87	0.09	41,41,41,41	0
54	MG	1A	3709	1/1	0.87	0.17	50,50,50,50	0
54	MG	2A	3249	1/1	0.87	0.10	64,64,64,64	0
54	MG	2A	3539	1/1	0.87	0.24	72,72,72,72	0
54	MG	2a	3069	1/1	0.87	0.24	58,58,58,58	0
54	MG	1A	3711	1/1	0.87	0.15	54,54,54,54	0
54	MG	2A	3262	1/1	0.87	0.20	70,70,70,70	0
54	MG	1a	3064	1/1	0.87	0.28	79,79,79,79	0
54	MG	1A	3712	1/1	0.87	0.12	30,30,30,30	0
54	MG	2a	3087	1/1	0.87	0.11	49,49,49,49	0
54	MG	2a	3092	1/1	0.87	0.10	57,57,57,57	0
54	MG	1a	3186	1/1	0.87	0.14	72,72,72,72	0
54	MG	1a	3067	1/1	0.87	0.16	61,61,61,61	0
54	MG	2A	3281	1/1	0.87	0.25	53,53,53,53	0
54	MG	1A	3282	1/1	0.87	0.20	63,63,63,63	0
54	MG	2A	3025	1/1	0.87	0.17	44,44,44,44	0
54	MG	1a	3072	1/1	0.87	0.25	54,54,54,54	0
54	MG	2a	3108	1/1	0.87	0.12	69,69,69,69	0
54	MG	2A	3036	1/1	0.87	0.14	71,71,71,71	0
54	MG	2a	3122	1/1	0.87	0.13	62,62,62,62	0
54	MG	1A	3057	1/1	0.87	0.12	53,53,53,53	0
54	MG	2A	3615	1/1	0.87	0.17	68,68,68,68	0
54	MG	2A	3326	1/1	0.87	0.11	39,39,39,39	0
54	MG	2A	3327	1/1	0.87	0.14	53,53,53,53	0
54	MG	1a	3212	1/1	0.87	0.21	64,64,64,64	0
54	MG	2A	3053	1/1	0.87	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3056	1/1	0.87	0.16	53,53,53,53	0
54	MG	1A	3100	1/1	0.87	0.15	49,49,49,49	0
54	MG	2A	3655	1/1	0.87	0.10	31,31,31,31	0
54	MG	2A	3662	1/1	0.87	0.16	73,73,73,73	0
54	MG	1A	3120	1/1	0.87	0.37	40,40,40,40	0
54	MG	2a	3167	1/1	0.87	0.12	48,48,48,48	0
54	MG	1A	3647	1/1	0.87	0.18	55,55,55,55	0
54	MG	1A	3908	1/1	0.87	0.11	38,38,38,38	0
54	MG	1A	3650	1/1	0.87	0.32	62,62,62,62	0
54	MG	2A	3696	1/1	0.87	0.14	68,68,68,68	0
54	MG	2A	3404	1/1	0.87	0.16	56,56,56,56	0
54	MG	2a	3189	1/1	0.87	0.12	58,58,58,58	0
54	MG	1A	3651	1/1	0.87	0.15	57,57,57,57	0
54	MG	2A	3410	1/1	0.87	0.15	58,58,58,58	0
54	MG	1A	3652	1/1	0.87	0.11	50,50,50,50	0
54	MG	2A	3413	1/1	0.87	0.13	50,50,50,50	0
54	MG	1a	3005	1/1	0.87	0.16	50,50,50,50	0
54	MG	1A	3266	1/1	0.87	0.15	53,53,53,53	0
54	MG	1A	3458	1/1	0.87	0.12	35,35,35,35	0
54	MG	1A	3139	1/1	0.87	0.20	34,34,34,34	0
54	MG	1a	3018	1/1	0.87	0.09	61,61,61,61	0
54	MG	2A	3137	1/1	0.87	0.21	45,45,45,45	0
54	MG	2A	3147	1/1	0.87	0.43	52,52,52,52	0
54	MG	2A	3509	1/1	0.88	0.14	50,50,50,50	0
54	MG	1a	3079	1/1	0.88	0.16	52,52,52,52	0
54	MG	28	102	1/1	0.88	0.14	54,54,54,54	0
54	MG	2A	3022	1/1	0.88	0.18	63,63,63,63	0
54	MG	2A	3261	1/1	0.88	0.14	58,58,58,58	0
54	MG	1A	3621	1/1	0.88	0.13	28,28,28,28	0
54	MG	2A	3024	1/1	0.88	0.15	52,52,52,52	0
54	MG	1A	3742	1/1	0.88	0.13	54,54,54,54	0
54	MG	2a	3014	1/1	0.88	0.16	61,61,61,61	0
54	MG	1A	3744	1/1	0.88	0.19	47,47,47,47	0
54	MG	1A	3827	1/1	0.88	0.13	59,59,59,59	0
54	MG	2A	3529	1/1	0.88	0.17	33,33,33,33	0
54	MG	1A	3750	1/1	0.88	0.12	57,57,57,57	0
54	MG	1a	3091	1/1	0.88	0.14	45,45,45,45	0
54	MG	1A	3954	1/1	0.88	0.13	43,43,43,43	0
54	MG	2A	3055	1/1	0.88	0.15	55,55,55,55	0
54	MG	2A	3541	1/1	0.88	0.37	51,51,51,51	0
54	MG	1a	3219	1/1	0.88	0.32	67,67,67,67	0
54	MG	2A	3549	1/1	0.88	0.15	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3308	1/1	0.88	0.10	40,40,40,40	0
54	MG	1A	3962	1/1	0.88	0.15	48,48,48,48	0
54	MG	1A	3841	1/1	0.88	0.13	63,63,63,63	0
54	MG	1D	307	1/1	0.88	0.17	50,50,50,50	0
54	MG	1A	3761	1/1	0.88	0.12	13,13,13,13	0
54	MG	1a	3021	1/1	0.88	0.20	68,68,68,68	0
54	MG	2A	3598	1/1	0.88	0.13	38,38,38,38	0
54	MG	1a	3235	1/1	0.88	0.14	69,69,69,69	0
54	MG	2A	3101	1/1	0.88	0.14	49,49,49,49	0
54	MG	1a	3108	1/1	0.88	0.17	58,58,58,58	0
54	MG	2A	3371	1/1	0.88	0.12	38,38,38,38	0
54	MG	2A	3111	1/1	0.88	0.13	65,65,65,65	0
54	MG	1a	3240	1/1	0.88	0.09	64,64,64,64	0
54	MG	1a	3241	1/1	0.88	0.16	67,67,67,67	0
54	MG	2A	3618	1/1	0.88	0.14	92,92,92,92	0
54	MG	1D	315	1/1	0.88	0.28	31,31,31,31	0
54	MG	2a	3094	1/1	0.88	0.13	68,68,68,68	0
54	MG	2A	3620	1/1	0.88	0.20	53,53,53,53	0
54	MG	2A	3622	1/1	0.88	0.32	64,64,64,64	0
54	MG	2A	3632	1/1	0.88	0.23	71,71,71,71	0
54	MG	1A	3310	1/1	0.88	0.20	42,42,42,42	0
54	MG	2A	3134	1/1	0.88	0.12	55,55,55,55	0
54	MG	1A	3397	1/1	0.88	0.21	58,58,58,58	0
54	MG	1A	3538	1/1	0.88	0.09	59,59,59,59	0
54	MG	2A	3140	1/1	0.88	0.12	54,54,54,54	0
54	MG	1A	3468	1/1	0.88	0.10	26,26,26,26	0
54	MG	1a	3138	1/1	0.88	0.10	56,56,56,56	0
54	MG	1A	3482	1/1	0.88	0.11	29,29,29,29	0
54	MG	2a	3131	1/1	0.88	0.17	68,68,68,68	0
54	MG	1N	201	1/1	0.88	0.18	49,49,49,49	0
54	MG	1a	3149	1/1	0.88	0.11	67,67,67,67	0
54	MG	1A	3562	1/1	0.88	0.12	64,64,64,64	0
54	MG	2A	3174	1/1	0.88	0.26	61,61,61,61	0
54	MG	1a	3045	1/1	0.88	0.09	65,65,65,65	0
54	MG	1a	3156	1/1	0.88	0.23	66,66,66,66	0
54	MG	1R	206	1/1	0.88	0.12	50,50,50,50	0
54	MG	1A	3899	1/1	0.88	0.40	37,37,37,37	0
54	MG	1A	3569	1/1	0.88	0.30	35,35,35,35	0
54	MG	1A	3402	1/1	0.88	0.11	36,36,36,36	0
54	MG	1T	204	1/1	0.88	0.10	56,56,56,56	0
54	MG	1A	3096	1/1	0.88	0.32	43,43,43,43	0
54	MG	2A	3465	1/1	0.88	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1n	101	1/1	0.88	0.11	63,63,63,63	0
54	MG	2a	3185	1/1	0.88	0.12	86,86,86,86	0
54	MG	2a	3187	1/1	0.88	0.11	65,65,65,65	0
54	MG	1V	204	1/1	0.88	0.11	40,40,40,40	0
54	MG	1A	3922	1/1	0.88	0.20	42,42,42,42	0
54	MG	2A	3490	1/1	0.88	0.13	43,43,43,43	0
54	MG	10	103	1/1	0.88	0.11	35,35,35,35	0
54	MG	1A	3927	1/1	0.88	0.16	47,47,47,47	0
54	MG	1A	3806	1/1	0.88	0.12	21,21,21,21	0
54	MG	2D	307	1/1	0.88	0.12	35,35,35,35	0
54	MG	2A	3235	1/1	0.88	0.09	44,44,44,44	0
54	MG	2A	3002	1/1	0.88	0.15	54,54,54,54	0
54	MG	15	104	1/1	0.88	0.16	46,46,46,46	0
54	MG	2G	203	1/1	0.88	0.11	63,63,63,63	0
54	MG	2A	3010	1/1	0.88	0.17	64,64,64,64	0
54	MG	2A	3426	1/1	0.89	0.11	46,46,46,46	0
54	MG	2A	3115	1/1	0.89	0.18	59,59,59,59	0
54	MG	1A	3579	1/1	0.89	0.12	21,21,21,21	0
54	MG	1A	3725	1/1	0.89	0.11	39,39,39,39	0
54	MG	1a	3236	1/1	0.89	0.17	64,64,64,64	0
54	MG	2A	3440	1/1	0.89	0.10	46,46,46,46	0
54	MG	2A	3126	1/1	0.89	0.10	59,59,59,59	0
54	MG	2A	3447	1/1	0.89	0.10	38,38,38,38	0
54	MG	1A	3580	1/1	0.89	0.12	35,35,35,35	0
54	MG	1a	3101	1/1	0.89	0.13	67,67,67,67	0
54	MG	1B	209	1/1	0.89	0.19	52,52,52,52	0
54	MG	1a	3246	1/1	0.89	0.09	54,54,54,54	0
54	MG	1a	3010	1/1	0.89	0.15	58,58,58,58	0
54	MG	2E	301	1/1	0.89	0.13	47,47,47,47	0
54	MG	1a	3107	1/1	0.89	0.19	54,54,54,54	0
54	MG	1A	3132	1/1	0.89	0.09	35,35,35,35	0
54	MG	2A	3459	1/1	0.89	0.11	28,28,28,28	0
54	MG	1a	3252	1/1	0.89	0.13	62,62,62,62	0
54	MG	1B	218	1/1	0.89	0.12	57,57,57,57	0
54	MG	1A	3448	1/1	0.89	0.28	64,64,64,64	0
54	MG	2W	203	1/1	0.89	0.11	61,61,61,61	0
54	MG	2A	3474	1/1	0.89	0.10	46,46,46,46	0
54	MG	25	102	1/1	0.89	0.13	64,64,64,64	0
54	MG	1a	3120	1/1	0.89	0.09	69,69,69,69	0
54	MG	1A	3604	1/1	0.89	0.16	52,52,52,52	0
54	MG	2A	3486	1/1	0.89	0.26	64,64,64,64	0
54	MG	2A	3488	1/1	0.89	0.16	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3181	1/1	0.89	0.18	50,50,50,50	0
54	MG	2a	3009	1/1	0.89	0.17	56,56,56,56	0
54	MG	2A	3182	1/1	0.89	0.18	43,43,43,43	0
54	MG	2a	3012	1/1	0.89	0.13	68,68,68,68	0
54	MG	2A	3492	1/1	0.89	0.12	70,70,70,70	0
54	MG	1a	3125	1/1	0.89	0.10	62,62,62,62	0
54	MG	2A	3495	1/1	0.89	0.09	53,53,53,53	0
54	MG	1A	3208	1/1	0.89	0.45	38,38,38,38	0
54	MG	1A	3274	1/1	0.89	0.35	56,56,56,56	0
54	MG	2a	3030	1/1	0.89	0.22	53,53,53,53	0
54	MG	1a	3024	1/1	0.89	0.10	45,45,45,45	0
54	MG	1A	3138	1/1	0.89	0.07	22,22,22,22	0
54	MG	2A	3196	1/1	0.89	0.15	58,58,58,58	0
54	MG	2a	3037	1/1	0.89	0.09	61,61,61,61	0
54	MG	2a	3040	1/1	0.89	0.15	67,67,67,67	0
54	MG	1A	3631	1/1	0.89	0.29	33,33,33,33	0
54	MG	1A	3504	1/1	0.89	0.09	37,37,37,37	0
54	MG	1A	3279	1/1	0.89	0.27	58,58,58,58	0
54	MG	1g	201	1/1	0.89	0.12	52,52,52,52	0
54	MG	1A	3184	1/1	0.89	0.21	30,30,30,30	0
54	MG	1A	3115	1/1	0.89	0.14	50,50,50,50	0
54	MG	1h	201	1/1	0.89	0.09	46,46,46,46	0
54	MG	1a	3157	1/1	0.89	0.08	57,57,57,57	0
54	MG	1A	3142	1/1	0.89	0.15	55,55,55,55	0
54	MG	1A	3782	1/1	0.89	0.22	57,57,57,57	0
54	MG	1F	315	1/1	0.89	0.15	45,45,45,45	0
54	MG	2A	3245	1/1	0.89	0.15	55,55,55,55	0
54	MG	1A	3656	1/1	0.89	0.14	35,35,35,35	0
54	MG	1a	3054	1/1	0.89	0.29	50,50,50,50	0
54	MG	1a	3169	1/1	0.89	0.12	62,62,62,62	0
54	MG	2a	3077	1/1	0.89	0.13	54,54,54,54	0
54	MG	2a	3079	1/1	0.89	0.25	54,54,54,54	0
54	MG	2A	3260	1/1	0.89	0.33	59,59,59,59	0
54	MG	1a	3055	1/1	0.89	0.18	64,64,64,64	0
54	MG	1A	3661	1/1	0.89	0.11	53,53,53,53	0
54	MG	2A	3558	1/1	0.89	0.14	39,39,39,39	0
54	MG	2A	3263	1/1	0.89	0.13	50,50,50,50	0
54	MG	2A	3566	1/1	0.89	0.12	57,57,57,57	0
54	MG	1A	3532	1/1	0.89	0.13	31,31,31,31	0
54	MG	1A	3536	1/1	0.89	0.12	29,29,29,29	0
54	MG	1A	3807	1/1	0.89	0.33	40,40,40,40	0
54	MG	1a	3180	1/1	0.89	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3417	1/1	0.89	0.13	31,31,31,31	0
54	MG	2a	3113	1/1	0.89	0.15	61,61,61,61	0
54	MG	2A	3288	1/1	0.89	0.15	56,56,56,56	0
54	MG	2A	3600	1/1	0.89	0.12	36,36,36,36	0
54	MG	1A	3543	1/1	0.89	0.18	43,43,43,43	0
54	MG	1a	3188	1/1	0.89	0.12	64,64,64,64	0
54	MG	2A	3291	1/1	0.89	0.11	40,40,40,40	0
54	MG	1A	3980	1/1	0.89	0.13	56,56,56,56	0
54	MG	1a	3195	1/1	0.89	0.11	69,69,69,69	0
54	MG	2a	3148	1/1	0.89	0.16	79,79,79,79	0
54	MG	2A	3043	1/1	0.89	0.15	56,56,56,56	0
54	MG	2A	3044	1/1	0.89	0.13	58,58,58,58	0
54	MG	2A	3045	1/1	0.89	0.14	49,49,49,49	0
54	MG	1A	3110	1/1	0.89	0.21	35,35,35,35	0
54	MG	1A	3131	1/1	0.89	0.11	61,61,61,61	0
54	MG	2A	3054	1/1	0.89	0.30	65,65,65,65	0
54	MG	2A	3631	1/1	0.89	0.15	75,75,75,75	0
54	MG	1a	3074	1/1	0.89	0.11	52,52,52,52	0
54	MG	1a	3206	1/1	0.89	0.11	83,83,83,83	0
54	MG	1A	3696	1/1	0.89	0.49	27,27,27,27	0
54	MG	1A	3991	1/1	0.89	0.19	33,33,33,33	0
54	MG	10	105	1/1	0.89	0.12	35,35,35,35	0
54	MG	2A	3378	1/1	0.89	0.14	65,65,65,65	0
54	MG	2A	3083	1/1	0.89	0.18	49,49,49,49	0
54	MG	2A	3383	1/1	0.89	0.14	51,51,51,51	0
54	MG	1a	3216	1/1	0.89	0.20	73,73,73,73	0
54	MG	10	107	1/1	0.89	0.13	58,58,58,58	0
54	MG	2A	3687	1/1	0.89	0.22	63,63,63,63	0
54	MG	2A	3407	1/1	0.89	0.11	46,46,46,46	0
54	MG	1A	3697	1/1	0.89	0.22	56,56,56,56	0
54	MG	2A	3698	1/1	0.89	0.17	60,60,60,60	0
56	MPD	1A	4013	8/8	0.89	0.25	42,54,56,59	0
54	MG	1A	3699	1/1	0.89	0.21	78,78,78,78	0
54	MG	2A	3108	1/1	0.89	0.23	40,40,40,40	0
54	MG	1A	3437	1/1	0.89	0.24	57,57,57,57	0
54	MG	1A	3353	1/1	0.89	0.10	44,44,44,44	0
54	MG	2A	3716	1/1	0.89	0.21	53,53,53,53	0
54	MG	1A	3577	1/1	0.89	0.08	58,58,58,58	0
54	MG	1A	3748	1/1	0.90	0.10	40,40,40,40	0
54	MG	1A	3865	1/1	0.90	0.13	82,82,82,82	0
54	MG	2a	3013	1/1	0.90	0.30	49,49,49,49	0
54	MG	1A	3302	1/1	0.90	0.10	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3016	1/1	0.90	0.12	44,44,44,44	0
54	MG	1A	3127	1/1	0.90	0.14	44,44,44,44	0
54	MG	2a	3019	1/1	0.90	0.18	46,46,46,46	0
54	MG	2a	3020	1/1	0.90	0.09	47,47,47,47	0
54	MG	2A	3187	1/1	0.90	0.12	43,43,43,43	0
54	MG	1A	3890	1/1	0.90	0.11	29,29,29,29	0
54	MG	2A	3607	1/1	0.90	0.12	64,64,64,64	0
54	MG	2A	3191	1/1	0.90	0.15	49,49,49,49	0
54	MG	1A	3574	1/1	0.90	0.12	21,21,21,21	0
54	MG	1A	3488	1/1	0.90	0.09	60,60,60,60	0
54	MG	1A	3903	1/1	0.90	0.24	50,50,50,50	0
54	MG	1a	3008	1/1	0.90	0.28	66,66,66,66	0
54	MG	1A	3311	1/1	0.90	0.33	38,38,38,38	0
54	MG	1a	3012	1/1	0.90	0.09	24,24,24,24	0
54	MG	1a	3222	1/1	0.90	0.13	72,72,72,72	0
54	MG	1a	3224	1/1	0.90	0.13	53,53,53,53	0
54	MG	2a	3052	1/1	0.90	0.19	55,55,55,55	0
54	MG	1A	3910	1/1	0.90	0.24	45,45,45,45	0
54	MG	1A	3505	1/1	0.90	0.09	36,36,36,36	0
54	MG	1A	3584	1/1	0.90	0.10	40,40,40,40	0
54	MG	2A	3645	1/1	0.90	0.09	47,47,47,47	0
54	MG	1A	3351	1/1	0.90	0.11	52,52,52,52	0
54	MG	2A	3651	1/1	0.90	0.09	45,45,45,45	0
54	MG	1A	3244	1/1	0.90	0.17	45,45,45,45	0
54	MG	1A	3788	1/1	0.90	0.11	38,38,38,38	0
54	MG	1A	3062	1/1	0.90	0.08	30,30,30,30	0
54	MG	1A	3698	1/1	0.90	0.26	45,45,45,45	0
54	MG	2A	3059	1/1	0.90	0.11	54,54,54,54	0
54	MG	2A	3068	1/1	0.90	0.14	43,43,43,43	0
54	MG	1A	3802	1/1	0.90	0.18	32,32,32,32	0
54	MG	1A	3284	1/1	0.90	0.14	49,49,49,49	0
54	MG	1a	3037	1/1	0.90	0.28	55,55,55,55	0
54	MG	1F	304	1/1	0.90	0.45	42,42,42,42	0
54	MG	1a	3039	1/1	0.90	0.15	76,76,76,76	0
54	MG	1A	3531	1/1	0.90	0.11	32,32,32,32	0
54	MG	2A	3276	1/1	0.90	0.16	57,57,57,57	0
54	MG	1A	3705	1/1	0.90	0.14	22,22,22,22	0
54	MG	2A	3711	1/1	0.90	0.12	60,60,60,60	0
54	MG	1G	201	1/1	0.90	0.13	69,69,69,69	0
54	MG	1A	3809	1/1	0.90	0.09	19,19,19,19	0
54	MG	1a	3264	1/1	0.90	0.16	77,77,77,77	0
54	MG	2A	3726	1/1	0.90	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3728	1/1	0.90	0.10	45,45,45,45	0
54	MG	1A	3708	1/1	0.90	0.12	28,28,28,28	0
54	MG	2a	3117	1/1	0.90	0.14	62,62,62,62	0
54	MG	2a	3120	1/1	0.90	0.12	57,57,57,57	0
54	MG	1A	3007	1/1	0.90	0.09	38,38,38,38	0
54	MG	1P	201	1/1	0.90	0.47	27,27,27,27	0
54	MG	2B	202	1/1	0.90	0.18	59,59,59,59	0
54	MG	1a	3162	1/1	0.90	0.18	64,64,64,64	0
54	MG	2B	205	1/1	0.90	0.12	49,49,49,49	0
54	MG	1P	204	1/1	0.90	0.37	35,35,35,35	0
54	MG	2A	3306	1/1	0.90	0.13	48,48,48,48	0
54	MG	1A	3296	1/1	0.90	0.18	52,52,52,52	0
54	MG	2B	210	1/1	0.90	0.13	61,61,61,61	0
54	MG	2A	3309	1/1	0.90	0.11	52,52,52,52	0
54	MG	2a	3153	1/1	0.90	0.11	88,88,88,88	0
54	MG	1A	3824	1/1	0.90	0.12	53,53,53,53	0
54	MG	2A	3131	1/1	0.90	0.12	54,54,54,54	0
54	MG	1a	3168	1/1	0.90	0.14	56,56,56,56	0
54	MG	2B	218	1/1	0.90	0.14	83,83,83,83	0
54	MG	2A	3334	1/1	0.90	0.09	40,40,40,40	0
54	MG	2A	3135	1/1	0.90	0.10	61,61,61,61	0
54	MG	1A	3632	1/1	0.90	0.15	44,44,44,44	0
54	MG	2A	3354	1/1	0.90	0.14	53,53,53,53	0
54	MG	1A	3830	1/1	0.90	0.08	30,30,30,30	0
54	MG	2A	3367	1/1	0.90	0.13	27,27,27,27	0
54	MG	1A	3222	1/1	0.90	0.14	44,44,44,44	0
54	MG	2A	3146	1/1	0.90	0.11	54,54,54,54	0
54	MG	2Q	204	1/1	0.90	0.17	69,69,69,69	0
54	MG	2T	203	1/1	0.90	0.12	58,58,58,58	0
54	MG	2U	201	1/1	0.90	0.38	67,67,67,67	0
54	MG	2k	201	1/1	0.90	0.12	64,64,64,64	0
54	MG	1A	3986	1/1	0.90	0.11	45,45,45,45	0
54	MG	1A	3648	1/1	0.90	0.15	27,27,27,27	0
54	MG	1A	3453	1/1	0.90	0.11	57,57,57,57	0
54	MG	1A	3549	1/1	0.90	0.25	52,52,52,52	0
54	MG	1A	3456	1/1	0.90	0.08	41,41,41,41	0
54	MG	2a	3003	1/1	0.90	0.17	57,57,57,57	0
54	MG	2A	3165	1/1	0.90	0.10	80,80,80,80	0
54	MG	1A	3400	1/1	0.90	0.19	52,52,52,52	0
54	MG	1A	3862	1/1	0.90	0.11	48,48,48,48	0
54	MG	13	102	1/1	0.90	0.13	61,61,61,61	0
58	ZN	24	501	1/1	0.90	0.12	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3129	1/1	0.91	0.24	62,62,62,62	0
54	MG	1A	3760	1/1	0.91	0.10	43,43,43,43	0
54	MG	1a	3220	1/1	0.91	0.09	72,72,72,72	0
54	MG	2B	211	1/1	0.91	0.13	58,58,58,58	0
54	MG	2A	3439	1/1	0.91	0.09	56,56,56,56	0
54	MG	1H	4102	1/1	0.91	0.09	60,60,60,60	0
54	MG	1A	3513	1/1	0.91	0.16	66,66,66,66	0
54	MG	1a	3069	1/1	0.91	0.12	55,55,55,55	0
54	MG	1A	3413	1/1	0.91	0.09	53,53,53,53	0
54	MG	2D	304	1/1	0.91	0.24	42,42,42,42	0
54	MG	1A	3935	1/1	0.91	0.27	35,35,35,35	0
54	MG	1A	3636	1/1	0.91	0.14	69,69,69,69	0
54	MG	2A	3149	1/1	0.91	0.11	41,41,41,41	0
54	MG	2F	301	1/1	0.91	0.16	38,38,38,38	0
54	MG	1a	3230	1/1	0.91	0.10	69,69,69,69	0
54	MG	1P	206	1/1	0.91	0.11	74,74,74,74	0
54	MG	1a	3234	1/1	0.91	0.08	67,67,67,67	0
54	MG	1A	3319	1/1	0.91	0.11	48,48,48,48	0
54	MG	1A	3527	1/1	0.91	0.11	43,43,43,43	0
54	MG	2Q	202	1/1	0.91	0.22	47,47,47,47	0
54	MG	1A	3942	1/1	0.91	0.08	46,46,46,46	0
54	MG	1A	3528	1/1	0.91	0.10	42,42,42,42	0
54	MG	1A	3777	1/1	0.91	0.11	47,47,47,47	0
54	MG	1A	3065	1/1	0.91	0.09	48,48,48,48	0
54	MG	1A	3425	1/1	0.91	0.12	46,46,46,46	0
54	MG	1a	3092	1/1	0.91	0.16	46,46,46,46	0
54	MG	1A	3039	1/1	0.91	0.14	53,53,53,53	0
54	MG	1A	3429	1/1	0.91	0.22	55,55,55,55	0
54	MG	2A	3188	1/1	0.91	0.14	61,61,61,61	0
54	MG	1A	3360	1/1	0.91	0.10	41,41,41,41	0
54	MG	1A	3800	1/1	0.91	0.15	64,64,64,64	0
54	MG	1A	3548	1/1	0.91	0.11	37,37,37,37	0
54	MG	1A	3364	1/1	0.91	0.16	45,45,45,45	0
54	MG	1a	3268	1/1	0.91	0.14	60,60,60,60	0
54	MG	2A	3498	1/1	0.91	0.09	55,55,55,55	0
54	MG	1A	3672	1/1	0.91	0.11	69,69,69,69	0
54	MG	1A	3002	1/1	0.91	0.11	46,46,46,46	0
54	MG	1A	3141	1/1	0.91	0.45	27,27,27,27	0
54	MG	1a	3111	1/1	0.91	0.15	68,68,68,68	0
54	MG	1a	3114	1/1	0.91	0.16	68,68,68,68	0
54	MG	2A	3219	1/1	0.91	0.09	44,44,44,44	0
54	MG	1A	3681	1/1	0.91	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3223	1/1	0.91	0.16	45,45,45,45	0
54	MG	2A	3225	1/1	0.91	0.31	40,40,40,40	0
54	MG	1A	3373	1/1	0.91	0.08	37,37,37,37	0
54	MG	2A	3230	1/1	0.91	0.14	61,61,61,61	0
54	MG	1A	3564	1/1	0.91	0.11	19,19,19,19	0
54	MG	19	102	1/1	0.91	0.10	54,54,54,54	0
54	MG	2a	3036	1/1	0.91	0.15	42,42,42,42	0
54	MG	1a	3001	1/1	0.91	0.15	68,68,68,68	0
54	MG	1A	3567	1/1	0.91	0.07	35,35,35,35	0
54	MG	2a	3045	1/1	0.91	0.09	50,50,50,50	0
54	MG	2A	3532	1/1	0.91	0.17	79,79,79,79	0
54	MG	1a	3132	1/1	0.91	0.09	72,72,72,72	0
54	MG	1A	3381	1/1	0.91	0.12	34,34,34,34	0
54	MG	1a	3135	1/1	0.91	0.13	54,54,54,54	0
54	MG	2A	3250	1/1	0.91	0.17	35,35,35,35	0
54	MG	1a	3007	1/1	0.91	0.10	58,58,58,58	0
54	MG	2a	3058	1/1	0.91	0.14	61,61,61,61	0
54	MG	2A	3252	1/1	0.91	0.10	40,40,40,40	0
54	MG	2A	3553	1/1	0.91	0.10	56,56,56,56	0
54	MG	1a	3140	1/1	0.91	0.16	72,72,72,72	0
54	MG	1a	3141	1/1	0.91	0.15	58,58,58,58	0
54	MG	2a	3065	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3270	1/1	0.91	0.12	52,52,52,52	0
54	MG	1a	3144	1/1	0.91	0.23	61,61,61,61	0
54	MG	2A	3569	1/1	0.91	0.09	34,34,34,34	0
54	MG	1A	3293	1/1	0.91	0.13	57,57,57,57	0
54	MG	1a	3148	1/1	0.91	0.15	64,64,64,64	0
54	MG	2a	3075	1/1	0.91	0.10	59,59,59,59	0
54	MG	1A	3476	1/1	0.91	0.10	21,21,21,21	0
54	MG	1A	3842	1/1	0.91	0.12	30,30,30,30	0
54	MG	1a	3014	1/1	0.91	0.11	55,55,55,55	0
54	MG	1A	3701	1/1	0.91	0.16	44,44,44,44	0
54	MG	2A	3284	1/1	0.91	0.09	37,37,37,37	0
54	MG	1A	3847	1/1	0.91	0.08	31,31,31,31	0
54	MG	1A	3033	1/1	0.91	0.41	43,43,43,43	0
54	MG	1a	3159	1/1	0.91	0.12	50,50,50,50	0
54	MG	1A	3038	1/1	0.91	0.11	44,44,44,44	0
54	MG	1A	3592	1/1	0.91	0.13	47,47,47,47	0
54	MG	2A	3614	1/1	0.91	0.09	46,46,46,46	0
54	MG	1a	3023	1/1	0.91	0.12	50,50,50,50	0
54	MG	1B	220	1/1	0.91	0.10	43,43,43,43	0
54	MG	2A	3617	1/1	0.91	0.19	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3499	1/1	0.91	0.11	38,38,38,38	0
54	MG	1A	3601	1/1	0.91	0.16	56,56,56,56	0
54	MG	1A	3719	1/1	0.91	0.31	48,48,48,48	0
54	MG	2A	3322	1/1	0.91	0.14	56,56,56,56	0
54	MG	2A	3052	1/1	0.91	0.11	60,60,60,60	0
54	MG	1a	3034	1/1	0.91	0.31	69,69,69,69	0
54	MG	2A	3636	1/1	0.91	0.12	66,66,66,66	0
54	MG	2A	3330	1/1	0.91	0.15	63,63,63,63	0
54	MG	1a	3035	1/1	0.91	0.10	37,37,37,37	0
54	MG	1a	3036	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3154	1/1	0.91	0.26	55,55,55,55	0
54	MG	2A	3350	1/1	0.91	0.13	60,60,60,60	0
54	MG	1A	3872	1/1	0.91	0.18	43,43,43,43	0
54	MG	1A	3403	1/1	0.91	0.17	39,39,39,39	0
54	MG	2A	3356	1/1	0.91	0.14	49,49,49,49	0
54	MG	1A	3887	1/1	0.91	0.10	14,14,14,14	0
54	MG	1a	3183	1/1	0.91	0.12	90,90,90,90	0
54	MG	2A	3678	1/1	0.91	0.12	58,58,58,58	0
54	MG	1A	3609	1/1	0.91	0.10	16,16,16,16	0
54	MG	1D	316	1/1	0.91	0.13	59,59,59,59	0
54	MG	1A	3613	1/1	0.91	0.17	52,52,52,52	0
54	MG	2a	3172	1/1	0.91	0.14	52,52,52,52	0
54	MG	1a	3192	1/1	0.91	0.16	72,72,72,72	0
54	MG	1A	3620	1/1	0.91	0.20	68,68,68,68	0
54	MG	1A	3250	1/1	0.91	0.28	46,46,46,46	0
54	MG	2A	3396	1/1	0.91	0.20	63,63,63,63	0
54	MG	2A	3397	1/1	0.91	0.11	58,58,58,58	0
54	MG	1E	307	1/1	0.91	0.07	43,43,43,43	0
54	MG	2A	3109	1/1	0.91	0.10	57,57,57,57	0
54	MG	2A	3406	1/1	0.91	0.09	67,67,67,67	0
54	MG	2a	3191	1/1	0.91	0.11	72,72,72,72	0
54	MG	1A	3278	1/1	0.91	0.13	35,35,35,35	0
54	MG	1a	3057	1/1	0.91	0.12	36,36,36,36	0
54	MG	1F	307	1/1	0.91	0.18	25,25,25,25	0
54	MG	2A	3727	1/1	0.91	0.15	52,52,52,52	0
54	MG	2A	3411	1/1	0.91	0.11	37,37,37,37	0
54	MG	2A	3113	1/1	0.91	0.08	35,35,35,35	0
54	MG	2A	3731	1/1	0.91	0.08	43,43,43,43	0
54	MG	1A	3511	1/1	0.91	0.12	45,45,45,45	0
54	MG	1A	3912	1/1	0.91	0.13	54,54,54,54	0
54	MG	2A	3418	1/1	0.91	0.11	56,56,56,56	0
54	MG	1a	3063	1/1	0.91	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3756	1/1	0.91	0.23	43,43,43,43	0
54	MG	1a	3218	1/1	0.91	0.08	62,62,62,62	0
54	MG	1A	3035	1/1	0.92	0.10	36,36,36,36	0
54	MG	1A	3851	1/1	0.92	0.07	33,33,33,33	0
54	MG	1a	3062	1/1	0.92	0.17	64,64,64,64	0
54	MG	1h	202	1/1	0.92	0.11	49,49,49,49	0
54	MG	1A	3160	1/1	0.92	0.16	43,43,43,43	0
54	MG	2A	3445	1/1	0.92	0.08	73,73,73,73	0
54	MG	2A	3446	1/1	0.92	0.10	56,56,56,56	0
54	MG	2A	3193	1/1	0.92	0.12	60,60,60,60	0
54	MG	1A	3572	1/1	0.92	0.10	43,43,43,43	0
54	MG	1n	102	1/1	0.92	0.16	58,58,58,58	0
54	MG	1A	3166	1/1	0.92	0.14	44,44,44,44	0
54	MG	2A	3197	1/1	0.92	0.09	48,48,48,48	0
54	MG	1a	3066	1/1	0.92	0.05	45,45,45,45	0
54	MG	1A	3037	1/1	0.92	0.09	39,39,39,39	0
54	MG	2A	3202	1/1	0.92	0.06	33,33,33,33	0
54	MG	2A	3204	1/1	0.92	0.09	50,50,50,50	0
54	MG	1Y	201	1/1	0.92	0.17	76,76,76,76	0
54	MG	1A	3376	1/1	0.92	0.12	36,36,36,36	0
54	MG	2A	3463	1/1	0.92	0.12	56,56,56,56	0
54	MG	2A	3213	1/1	0.92	0.06	44,44,44,44	0
54	MG	2A	3471	1/1	0.92	0.10	37,37,37,37	0
54	MG	1a	3178	1/1	0.92	0.12	84,84,84,84	0
54	MG	2A	3005	1/1	0.92	0.17	50,50,50,50	0
54	MG	1a	3071	1/1	0.92	0.15	52,52,52,52	0
54	MG	2A	3483	1/1	0.92	0.14	58,58,58,58	0
54	MG	1a	3181	1/1	0.92	0.11	70,70,70,70	0
54	MG	2P	201	1/1	0.92	0.28	57,57,57,57	0
54	MG	2A	3014	1/1	0.92	0.09	42,42,42,42	0
54	MG	1A	3172	1/1	0.92	0.07	30,30,30,30	0
54	MG	1A	4002	1/1	0.92	0.07	57,57,57,57	0
54	MG	2A	3231	1/1	0.92	0.17	59,59,59,59	0
54	MG	1a	3185	1/1	0.92	0.17	64,64,64,64	0
54	MG	2W	202	1/1	0.92	0.26	53,53,53,53	0
54	MG	2A	3234	1/1	0.92	0.17	58,58,58,58	0
54	MG	21	101	1/1	0.92	0.15	46,46,46,46	0
54	MG	1A	3210	1/1	0.92	0.08	27,27,27,27	0
54	MG	1A	4004	1/1	0.92	0.15	43,43,43,43	0
54	MG	27	101	1/1	0.92	0.11	42,42,42,42	0
54	MG	2A	3240	1/1	0.92	0.13	47,47,47,47	0
54	MG	1A	3585	1/1	0.92	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3243	1/1	0.92	0.23	44,44,44,44	0
54	MG	2A	3244	1/1	0.92	0.11	45,45,45,45	0
54	MG	1A	4006	1/1	0.92	0.17	54,54,54,54	0
54	MG	1A	4007	1/1	0.92	0.11	41,41,41,41	0
54	MG	2a	3008	1/1	0.92	0.09	73,73,73,73	0
54	MG	1a	3083	1/1	0.92	0.18	47,47,47,47	0
54	MG	1A	3884	1/1	0.92	0.10	26,26,26,26	0
54	MG	1a	3087	1/1	0.92	0.12	54,54,54,54	0
54	MG	2A	3048	1/1	0.92	0.12	50,50,50,50	0
54	MG	2A	3255	1/1	0.92	0.20	52,52,52,52	0
54	MG	1a	3204	1/1	0.92	0.13	72,72,72,72	0
54	MG	2A	3517	1/1	0.92	0.10	50,50,50,50	0
54	MG	1A	3682	1/1	0.92	0.10	48,48,48,48	0
54	MG	2A	3521	1/1	0.92	0.09	57,57,57,57	0
54	MG	2A	3522	1/1	0.92	0.09	53,53,53,53	0
54	MG	2a	3023	1/1	0.92	0.23	67,67,67,67	0
54	MG	1a	3210	1/1	0.92	0.09	93,93,93,93	0
54	MG	2a	3026	1/1	0.92	0.12	52,52,52,52	0
54	MG	1A	3775	1/1	0.92	0.14	58,58,58,58	0
54	MG	1A	3892	1/1	0.92	0.08	15,15,15,15	0
54	MG	2a	3032	1/1	0.92	0.08	42,42,42,42	0
54	MG	2A	3271	1/1	0.92	0.12	22,22,22,22	0
54	MG	2A	3273	1/1	0.92	0.22	44,44,44,44	0
54	MG	2A	3536	1/1	0.92	0.14	63,63,63,63	0
54	MG	1a	3214	1/1	0.92	0.26	63,63,63,63	0
54	MG	1A	3893	1/1	0.92	0.09	35,35,35,35	0
54	MG	2A	3061	1/1	0.92	0.31	53,53,53,53	0
54	MG	2A	3063	1/1	0.92	0.09	56,56,56,56	0
54	MG	1A	3898	1/1	0.92	0.63	34,34,34,34	0
54	MG	2A	3070	1/1	0.92	0.27	53,53,53,53	0
54	MG	2a	3048	1/1	0.92	0.09	50,50,50,50	0
54	MG	2a	3049	1/1	0.92	0.10	47,47,47,47	0
54	MG	2A	3554	1/1	0.92	0.11	35,35,35,35	0
54	MG	1A	3173	1/1	0.92	0.14	45,45,45,45	0
54	MG	2A	3561	1/1	0.92	0.10	51,51,51,51	0
54	MG	1A	3901	1/1	0.92	0.20	42,42,42,42	0
54	MG	2A	3564	1/1	0.92	0.14	70,70,70,70	0
54	MG	1A	3440	1/1	0.92	0.10	30,30,30,30	0
54	MG	2A	3567	1/1	0.92	0.09	53,53,53,53	0
54	MG	1A	3693	1/1	0.92	0.16	35,35,35,35	0
54	MG	1A	3521	1/1	0.92	0.10	48,48,48,48	0
54	MG	1A	3790	1/1	0.92	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3299	1/1	0.92	0.12	46,46,46,46	0
54	MG	2A	3093	1/1	0.92	0.16	54,54,54,54	0
54	MG	2A	3579	1/1	0.92	0.09	40,40,40,40	0
54	MG	2A	3582	1/1	0.92	0.09	50,50,50,50	0
54	MG	2a	3072	1/1	0.92	0.09	58,58,58,58	0
54	MG	2a	3073	1/1	0.92	0.10	63,63,63,63	0
54	MG	2A	3095	1/1	0.92	0.07	35,35,35,35	0
54	MG	2A	3595	1/1	0.92	0.10	49,49,49,49	0
54	MG	1a	3225	1/1	0.92	0.10	39,39,39,39	0
54	MG	1A	3522	1/1	0.92	0.21	30,30,30,30	0
54	MG	2A	3603	1/1	0.92	0.08	27,27,27,27	0
54	MG	2a	3084	1/1	0.92	0.24	61,61,61,61	0
54	MG	2A	3318	1/1	0.92	0.09	38,38,38,38	0
54	MG	1A	3447	1/1	0.92	0.13	46,46,46,46	0
54	MG	2A	3323	1/1	0.92	0.08	47,47,47,47	0
54	MG	1D	309	1/1	0.92	0.13	42,42,42,42	0
54	MG	1A	3056	1/1	0.92	0.21	39,39,39,39	0
54	MG	2A	3329	1/1	0.92	0.14	25,25,25,25	0
54	MG	2a	3102	1/1	0.92	0.12	61,61,61,61	0
54	MG	1A	3315	1/1	0.92	0.09	32,32,32,32	0
54	MG	1A	3455	1/1	0.92	0.08	41,41,41,41	0
54	MG	1A	3702	1/1	0.92	0.08	22,22,22,22	0
54	MG	1A	3535	1/1	0.92	0.16	38,38,38,38	0
54	MG	1E	304	1/1	0.92	0.10	17,17,17,17	0
54	MG	2A	3352	1/1	0.92	0.15	52,52,52,52	0
54	MG	2A	3120	1/1	0.92	0.24	45,45,45,45	0
54	MG	1A	3625	1/1	0.92	0.12	47,47,47,47	0
54	MG	2A	3629	1/1	0.92	0.09	52,52,52,52	0
54	MG	1a	3130	1/1	0.92	0.11	52,52,52,52	0
54	MG	2a	3123	1/1	0.92	0.09	54,54,54,54	0
54	MG	2A	3359	1/1	0.92	0.14	44,44,44,44	0
54	MG	1a	3131	1/1	0.92	0.07	63,63,63,63	0
54	MG	1A	3004	1/1	0.92	0.08	48,48,48,48	0
54	MG	2a	3128	1/1	0.92	0.08	56,56,56,56	0
54	MG	1A	3349	1/1	0.92	0.11	27,27,27,27	0
54	MG	1A	3815	1/1	0.92	0.13	43,43,43,43	0
54	MG	2a	3147	1/1	0.92	0.09	73,73,73,73	0
54	MG	2A	3646	1/1	0.92	0.09	49,49,49,49	0
54	MG	2A	3647	1/1	0.92	0.20	76,76,76,76	0
54	MG	2A	3372	1/1	0.92	0.11	30,30,30,30	0
54	MG	2A	3650	1/1	0.92	0.14	63,63,63,63	0
54	MG	1a	3136	1/1	0.92	0.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1F	309	1/1	0.92	0.08	30,30,30,30	0
54	MG	2a	3157	1/1	0.92	0.10	86,86,86,86	0
54	MG	1A	3405	1/1	0.92	0.15	49,49,49,49	0
54	MG	2A	3659	1/1	0.92	0.11	32,32,32,32	0
54	MG	1F	314	1/1	0.92	0.31	53,53,53,53	0
54	MG	2a	3165	1/1	0.92	0.09	74,74,74,74	0
54	MG	2A	3386	1/1	0.92	0.09	49,49,49,49	0
54	MG	2A	3675	1/1	0.92	0.08	46,46,46,46	0
54	MG	2A	3143	1/1	0.92	0.13	39,39,39,39	0
54	MG	1A	3470	1/1	0.92	0.08	17,17,17,17	0
54	MG	1A	3185	1/1	0.92	0.35	32,32,32,32	0
54	MG	2a	3179	1/1	0.92	0.09	61,61,61,61	0
54	MG	2A	3683	1/1	0.92	0.11	36,36,36,36	0
54	MG	1A	3478	1/1	0.92	0.10	18,18,18,18	0
54	MG	1G	204	1/1	0.92	0.10	46,46,46,46	0
54	MG	2A	3690	1/1	0.92	0.12	59,59,59,59	0
54	MG	2A	3695	1/1	0.92	0.10	48,48,48,48	0
54	MG	2A	3153	1/1	0.92	0.15	33,33,33,33	0
54	MG	2A	3408	1/1	0.92	0.14	51,51,51,51	0
54	MG	2a	3192	1/1	0.92	0.09	62,62,62,62	0
54	MG	1a	3270	1/1	0.92	0.09	53,53,53,53	0
54	MG	1A	3964	1/1	0.92	0.09	46,46,46,46	0
54	MG	2A	3705	1/1	0.92	0.15	42,42,42,42	0
54	MG	1H	4103	1/1	0.92	0.11	61,61,61,61	0
54	MG	1a	3047	1/1	0.92	0.16	44,44,44,44	0
54	MG	2A	3168	1/1	0.92	0.13	43,43,43,43	0
54	MG	1A	3187	1/1	0.92	0.18	31,31,31,31	0
54	MG	1A	3486	1/1	0.92	0.14	47,47,47,47	0
54	MG	2A	3723	1/1	0.92	0.06	43,43,43,43	0
54	MG	1A	3741	1/1	0.92	0.06	35,35,35,35	0
54	MG	1A	3563	1/1	0.92	0.08	55,55,55,55	0
54	MG	1A	3975	1/1	0.92	0.22	43,43,43,43	0
54	MG	1A	3116	1/1	0.92	0.13	31,31,31,31	0
54	MG	1a	3082	1/1	0.93	0.11	50,50,50,50	0
54	MG	2A	3725	1/1	0.93	0.10	52,52,52,52	0
54	MG	1A	3477	1/1	0.93	0.08	57,57,57,57	0
54	MG	1A	3594	1/1	0.93	0.40	31,31,31,31	0
54	MG	1a	3086	1/1	0.93	0.16	56,56,56,56	0
54	MG	2A	3421	1/1	0.93	0.41	36,36,36,36	0
54	MG	2A	3424	1/1	0.93	0.15	63,63,63,63	0
54	MG	1A	3059	1/1	0.93	0.11	47,47,47,47	0
54	MG	1A	3369	1/1	0.93	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3483	1/1	0.93	0.08	17,17,17,17	0
54	MG	2A	3167	1/1	0.93	0.16	40,40,40,40	0
54	MG	1A	3484	1/1	0.93	0.13	35,35,35,35	0
54	MG	2A	3169	1/1	0.93	0.18	48,48,48,48	0
54	MG	2A	3438	1/1	0.93	0.14	59,59,59,59	0
54	MG	1A	3752	1/1	0.93	0.14	40,40,40,40	0
54	MG	1A	3923	1/1	0.93	0.07	27,27,27,27	0
54	MG	2A	3441	1/1	0.93	0.21	41,41,41,41	0
54	MG	1A	3605	1/1	0.93	0.23	35,35,35,35	0
54	MG	1a	3095	1/1	0.93	0.15	58,58,58,58	0
54	MG	1A	3135	1/1	0.93	0.44	42,42,42,42	0
54	MG	2B	215	1/1	0.93	0.10	60,60,60,60	0
54	MG	1a	3255	1/1	0.93	0.17	55,55,55,55	0
54	MG	1Q	201	1/1	0.93	0.37	28,28,28,28	0
54	MG	2D	303	1/1	0.93	0.40	40,40,40,40	0
54	MG	2A	3186	1/1	0.93	0.13	47,47,47,47	0
54	MG	1a	3260	1/1	0.93	0.13	54,54,54,54	0
54	MG	1a	3099	1/1	0.93	0.10	43,43,43,43	0
54	MG	2A	3189	1/1	0.93	0.09	45,45,45,45	0
54	MG	2E	308	1/1	0.93	0.16	41,41,41,41	0
54	MG	2A	3454	1/1	0.93	0.09	54,54,54,54	0
54	MG	1A	3612	1/1	0.93	0.10	20,20,20,20	0
54	MG	1a	3102	1/1	0.93	0.11	63,63,63,63	0
54	MG	2A	3192	1/1	0.93	0.18	53,53,53,53	0
54	MG	1A	3375	1/1	0.93	0.09	37,37,37,37	0
54	MG	2O	201	1/1	0.93	0.07	40,40,40,40	0
54	MG	1A	3060	1/1	0.93	0.12	46,46,46,46	0
54	MG	2P	202	1/1	0.93	0.11	51,51,51,51	0
54	MG	1A	3502	1/1	0.93	0.10	19,19,19,19	0
54	MG	1A	3622	1/1	0.93	0.17	53,53,53,53	0
54	MG	2A	3466	1/1	0.93	0.17	50,50,50,50	0
54	MG	2T	202	1/1	0.93	0.09	50,50,50,50	0
54	MG	1A	3771	1/1	0.93	0.14	28,28,28,28	0
54	MG	1U	202	1/1	0.93	0.11	35,35,35,35	0
54	MG	1a	3116	1/1	0.93	0.09	53,53,53,53	0
54	MG	1A	3503	1/1	0.93	0.13	17,17,17,17	0
54	MG	1V	206	1/1	0.93	0.05	52,52,52,52	0
54	MG	1A	3953	1/1	0.93	0.12	62,62,62,62	0
54	MG	2A	3209	1/1	0.93	0.10	45,45,45,45	0
54	MG	25	103	1/1	0.93	0.12	64,64,64,64	0
54	MG	1A	3029	1/1	0.93	0.12	33,33,33,33	0
54	MG	1A	3776	1/1	0.93	0.08	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3103	1/1	0.93	0.48	32,32,32,32	0
54	MG	2A	3493	1/1	0.93	0.08	34,34,34,34	0
54	MG	2A	3218	1/1	0.93	0.19	55,55,55,55	0
54	MG	1a	3128	1/1	0.93	0.10	39,39,39,39	0
54	MG	1A	3195	1/1	0.93	0.06	29,29,29,29	0
54	MG	1A	3105	1/1	0.93	0.08	54,54,54,54	0
54	MG	1A	3967	1/1	0.93	0.11	52,52,52,52	0
54	MG	2a	3010	1/1	0.93	0.13	75,75,75,75	0
54	MG	2A	3226	1/1	0.93	0.16	41,41,41,41	0
54	MG	2A	3228	1/1	0.93	0.27	59,59,59,59	0
54	MG	1A	3783	1/1	0.93	0.09	48,48,48,48	0
54	MG	1A	3785	1/1	0.93	0.36	46,46,46,46	0
54	MG	1A	3281	1/1	0.93	0.23	44,44,44,44	0
54	MG	2A	3232	1/1	0.93	0.28	41,41,41,41	0
54	MG	1A	3642	1/1	0.93	0.18	48,48,48,48	0
54	MG	1A	3977	1/1	0.93	0.28	52,52,52,52	0
54	MG	1A	3107	1/1	0.93	0.48	25,25,25,25	0
54	MG	2A	3236	1/1	0.93	0.16	48,48,48,48	0
54	MG	1A	3153	1/1	0.93	0.07	26,26,26,26	0
54	MG	1A	3034	1/1	0.93	0.08	42,42,42,42	0
54	MG	2a	3028	1/1	0.93	0.15	74,74,74,74	0
54	MG	1A	3211	1/1	0.93	0.41	36,36,36,36	0
54	MG	1A	3286	1/1	0.93	0.12	53,53,53,53	0
54	MG	2a	3031	1/1	0.93	0.13	56,56,56,56	0
54	MG	2A	3007	1/1	0.93	0.08	41,41,41,41	0
54	MG	1A	3523	1/1	0.93	0.05	37,37,37,37	0
54	MG	2A	3525	1/1	0.93	0.09	53,53,53,53	0
54	MG	2A	3246	1/1	0.93	0.08	47,47,47,47	0
54	MG	2A	3012	1/1	0.93	0.18	52,52,52,52	0
54	MG	1A	3112	1/1	0.93	0.15	50,50,50,50	0
54	MG	1A	3067	1/1	0.93	0.06	14,14,14,14	0
54	MG	2a	3041	1/1	0.93	0.12	72,72,72,72	0
54	MG	2a	3042	1/1	0.93	0.16	64,64,64,64	0
54	MG	2A	3021	1/1	0.93	0.16	39,39,39,39	0
54	MG	1a	3153	1/1	0.93	0.09	54,54,54,54	0
54	MG	2A	3254	1/1	0.93	0.39	45,45,45,45	0
54	MG	1A	3810	1/1	0.93	0.18	51,51,51,51	0
54	MG	1A	3663	1/1	0.93	0.08	59,59,59,59	0
54	MG	1A	3070	1/1	0.93	0.51	28,28,28,28	0
54	MG	1A	3424	1/1	0.93	0.13	17,17,17,17	0
54	MG	1a	3160	1/1	0.93	0.09	36,36,36,36	0
54	MG	2a	3055	1/1	0.93	0.09	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3056	1/1	0.93	0.07	65,65,65,65	0
54	MG	2A	3265	1/1	0.93	0.10	49,49,49,49	0
54	MG	2A	3037	1/1	0.93	0.20	54,54,54,54	0
54	MG	2A	3268	1/1	0.93	0.10	54,54,54,54	0
54	MG	2A	3040	1/1	0.93	0.11	41,41,41,41	0
54	MG	2A	3041	1/1	0.93	0.07	23,23,23,23	0
54	MG	1A	3241	1/1	0.93	0.25	34,34,34,34	0
54	MG	1A	3304	1/1	0.93	0.16	33,33,33,33	0
54	MG	1A	3242	1/1	0.93	0.06	51,51,51,51	0
54	MG	1A	4008	1/1	0.93	0.11	46,46,46,46	0
54	MG	1A	4010	1/1	0.93	0.20	42,42,42,42	0
54	MG	1A	4011	1/1	0.93	0.11	53,53,53,53	0
54	MG	2A	3286	1/1	0.93	0.08	30,30,30,30	0
54	MG	1B	201	1/1	0.93	0.17	50,50,50,50	0
54	MG	2A	3583	1/1	0.93	0.10	73,73,73,73	0
54	MG	2A	3589	1/1	0.93	0.10	70,70,70,70	0
54	MG	2A	3591	1/1	0.93	0.09	35,35,35,35	0
54	MG	1A	3243	1/1	0.93	0.13	64,64,64,64	0
54	MG	1B	203	1/1	0.93	0.17	43,43,43,43	0
54	MG	2A	3597	1/1	0.93	0.10	36,36,36,36	0
54	MG	1A	3832	1/1	0.93	0.15	34,34,34,34	0
54	MG	1A	3837	1/1	0.93	0.11	17,17,17,17	0
54	MG	2a	3088	1/1	0.93	0.09	61,61,61,61	0
54	MG	1A	3545	1/1	0.93	0.07	39,39,39,39	0
54	MG	2A	3298	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3075	1/1	0.93	0.08	37,37,37,37	0
54	MG	1B	215	1/1	0.93	0.09	52,52,52,52	0
54	MG	1A	3688	1/1	0.93	0.11	49,49,49,49	0
54	MG	1A	3318	1/1	0.93	0.12	30,30,30,30	0
54	MG	1A	3553	1/1	0.93	0.08	37,37,37,37	0
54	MG	1A	3246	1/1	0.93	0.33	40,40,40,40	0
54	MG	1a	3044	1/1	0.93	0.12	45,45,45,45	0
54	MG	1A	3445	1/1	0.93	0.07	30,30,30,30	0
54	MG	1B	226	1/1	0.93	0.17	65,65,65,65	0
54	MG	2A	3091	1/1	0.93	0.09	64,64,64,64	0
54	MG	1A	3446	1/1	0.93	0.08	40,40,40,40	0
54	MG	2a	3119	1/1	0.93	0.20	52,52,52,52	0
54	MG	1A	3854	1/1	0.93	0.07	28,28,28,28	0
54	MG	2A	3333	1/1	0.93	0.14	58,58,58,58	0
54	MG	1B	229	1/1	0.93	0.17	49,49,49,49	0
54	MG	2A	3338	1/1	0.93	0.07	30,30,30,30	0
54	MG	2A	3340	1/1	0.93	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3634	1/1	0.93	0.08	66,66,66,66	0
54	MG	1A	3320	1/1	0.93	0.09	19,19,19,19	0
54	MG	2A	3342	1/1	0.93	0.22	38,38,38,38	0
54	MG	2a	3132	1/1	0.93	0.09	73,73,73,73	0
54	MG	2A	3343	1/1	0.93	0.14	52,52,52,52	0
54	MG	2a	3146	1/1	0.93	0.17	64,64,64,64	0
54	MG	1D	302	1/1	0.93	0.78	23,23,23,23	0
54	MG	2A	3103	1/1	0.93	0.19	35,35,35,35	0
54	MG	1a	3203	1/1	0.93	0.12	70,70,70,70	0
54	MG	1A	3326	1/1	0.93	0.13	11,11,11,11	0
54	MG	1A	3329	1/1	0.93	0.12	44,44,44,44	0
54	MG	1a	3209	1/1	0.93	0.10	61,61,61,61	0
54	MG	2A	3652	1/1	0.93	0.07	48,48,48,48	0
54	MG	1D	311	1/1	0.93	0.16	33,33,33,33	0
54	MG	2A	3361	1/1	0.93	0.09	59,59,59,59	0
54	MG	2A	3656	1/1	0.93	0.10	35,35,35,35	0
54	MG	2a	3160	1/1	0.93	0.09	62,62,62,62	0
54	MG	1A	3126	1/1	0.93	0.16	41,41,41,41	0
54	MG	1A	3870	1/1	0.93	0.14	37,37,37,37	0
54	MG	2A	3669	1/1	0.93	0.09	52,52,52,52	0
54	MG	2A	3116	1/1	0.93	0.08	43,43,43,43	0
54	MG	2A	3370	1/1	0.93	0.12	58,58,58,58	0
54	MG	1A	3043	1/1	0.93	0.16	8,8,8,8	0
54	MG	1D	317	1/1	0.93	0.12	44,44,44,44	0
54	MG	2A	3679	1/1	0.93	0.12	51,51,51,51	0
54	MG	2A	3373	1/1	0.93	0.07	40,40,40,40	0
54	MG	2a	3182	1/1	0.93	0.25	70,70,70,70	0
54	MG	2A	3682	1/1	0.93	0.19	82,82,82,82	0
54	MG	2A	3375	1/1	0.93	0.13	38,38,38,38	0
54	MG	1A	3174	1/1	0.93	0.11	31,31,31,31	0
54	MG	1A	3460	1/1	0.93	0.09	29,29,29,29	0
54	MG	1A	3261	1/1	0.93	0.10	32,32,32,32	0
54	MG	2A	3693	1/1	0.93	0.22	47,47,47,47	0
54	MG	2A	3127	1/1	0.93	0.26	53,53,53,53	0
54	MG	2e	201	1/1	0.93	0.28	51,51,51,51	0
54	MG	1A	3886	1/1	0.93	0.13	22,22,22,22	0
54	MG	1A	3128	1/1	0.93	0.17	46,46,46,46	0
54	MG	1a	3221	1/1	0.93	0.12	41,41,41,41	0
54	MG	2r	101	1/1	0.93	0.11	67,67,67,67	0
54	MG	1A	3473	1/1	0.93	0.09	36,36,36,36	0
54	MG	1A	3088	1/1	0.93	0.47	41,41,41,41	0
54	MG	1A	3588	1/1	0.93	0.07	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3591	1/1	0.93	0.11	50,50,50,50	0
54	MG	2A	3142	1/1	0.93	0.11	38,38,38,38	0
54	MG	2A	3712	1/1	0.93	0.18	78,78,78,78	0
54	MG	1F	313	1/1	0.93	0.09	39,39,39,39	0
54	MG	1A	3730	1/1	0.93	0.10	41,41,41,41	0
54	MG	2A	3721	1/1	0.93	0.10	43,43,43,43	0
54	MG	1A	3737	1/1	0.93	0.08	18,18,18,18	0
54	MG	1A	3386	1/1	0.94	0.08	19,19,19,19	0
54	MG	1A	3552	1/1	0.94	0.09	43,43,43,43	0
54	MG	2A	3717	1/1	0.94	0.10	48,48,48,48	0
54	MG	2A	3718	1/1	0.94	0.17	52,52,52,52	0
54	MG	1a	3232	1/1	0.94	0.11	54,54,54,54	0
54	MG	2A	3151	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3042	1/1	0.94	0.08	25,25,25,25	0
54	MG	1A	3309	1/1	0.94	0.18	32,32,32,32	0
54	MG	2A	3154	1/1	0.94	0.12	34,34,34,34	0
54	MG	1A	3170	1/1	0.94	0.11	40,40,40,40	0
54	MG	1A	3200	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3415	1/1	0.94	0.07	35,35,35,35	0
54	MG	2A	3416	1/1	0.94	0.18	60,60,60,60	0
54	MG	1a	3237	1/1	0.94	0.13	57,57,57,57	0
54	MG	2A	3420	1/1	0.94	0.08	46,46,46,46	0
54	MG	1A	3312	1/1	0.94	0.14	47,47,47,47	0
54	MG	2A	3166	1/1	0.94	0.14	46,46,46,46	0
54	MG	1N	202	1/1	0.94	0.15	61,61,61,61	0
54	MG	1A	3944	1/1	0.94	0.09	35,35,35,35	0
54	MG	2A	3430	1/1	0.94	0.12	54,54,54,54	0
54	MG	1a	3244	1/1	0.94	0.07	66,66,66,66	0
54	MG	2A	3171	1/1	0.94	0.11	40,40,40,40	0
54	MG	1A	3667	1/1	0.94	0.08	26,26,26,26	0
54	MG	1A	3947	1/1	0.94	0.09	31,31,31,31	0
54	MG	2A	3437	1/1	0.94	0.15	48,48,48,48	0
54	MG	1P	205	1/1	0.94	0.15	43,43,43,43	0
54	MG	2A	3180	1/1	0.94	0.07	72,72,72,72	0
54	MG	1A	3201	1/1	0.94	0.08	28,28,28,28	0
54	MG	1a	3096	1/1	0.94	0.11	59,59,59,59	0
54	MG	2A	3442	1/1	0.94	0.08	65,65,65,65	0
54	MG	1a	3253	1/1	0.94	0.08	47,47,47,47	0
54	MG	1A	3952	1/1	0.94	0.13	34,34,34,34	0
54	MG	1Q	204	1/1	0.94	0.07	25,25,25,25	0
54	MG	1R	205	1/1	0.94	0.08	48,48,48,48	0
54	MG	1a	3262	1/1	0.94	0.08	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3100	1/1	0.94	0.07	47,47,47,47	0
54	MG	1A	3793	1/1	0.94	0.15	23,23,23,23	0
54	MG	2A	3451	1/1	0.94	0.10	64,64,64,64	0
54	MG	1S	201	1/1	0.94	0.12	61,61,61,61	0
54	MG	1A	3795	1/1	0.94	0.08	31,31,31,31	0
54	MG	1A	3961	1/1	0.94	0.14	61,61,61,61	0
54	MG	2N	201	1/1	0.94	0.07	48,48,48,48	0
54	MG	1A	3407	1/1	0.94	0.08	30,30,30,30	0
54	MG	1A	3568	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3317	1/1	0.94	0.15	56,56,56,56	0
54	MG	1A	3571	1/1	0.94	0.12	39,39,39,39	0
54	MG	1a	3115	1/1	0.94	0.07	35,35,35,35	0
54	MG	1U	205	1/1	0.94	0.37	63,63,63,63	0
54	MG	2R	202	1/1	0.94	0.07	34,34,34,34	0
54	MG	2A	3464	1/1	0.94	0.08	45,45,45,45	0
54	MG	1V	203	1/1	0.94	0.22	44,44,44,44	0
54	MG	1a	3118	1/1	0.94	0.09	43,43,43,43	0
54	MG	1A	3204	1/1	0.94	0.14	55,55,55,55	0
54	MG	1A	3968	1/1	0.94	0.10	35,35,35,35	0
54	MG	2Y	201	1/1	0.94	0.16	48,48,48,48	0
54	MG	1W	201	1/1	0.94	0.16	33,33,33,33	0
54	MG	2A	3478	1/1	0.94	0.11	49,49,49,49	0
54	MG	2A	3212	1/1	0.94	0.10	53,53,53,53	0
54	MG	1W	203	1/1	0.94	0.16	28,28,28,28	0
54	MG	1A	3143	1/1	0.94	0.09	37,37,37,37	0
54	MG	2A	3487	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3217	1/1	0.94	0.06	42,42,42,42	0
54	MG	1A	3495	1/1	0.94	0.10	41,41,41,41	0
54	MG	1a	3129	1/1	0.94	0.09	43,43,43,43	0
54	MG	1l	202	1/1	0.94	0.09	61,61,61,61	0
54	MG	2A	3222	1/1	0.94	0.15	53,53,53,53	0
54	MG	1A	3578	1/1	0.94	0.10	51,51,51,51	0
54	MG	1A	3690	1/1	0.94	0.08	33,33,33,33	0
54	MG	1A	3415	1/1	0.94	0.09	20,20,20,20	0
54	MG	1l	101	1/1	0.94	0.26	46,46,46,46	0
54	MG	1a	3134	1/1	0.94	0.10	47,47,47,47	0
54	MG	1A	3978	1/1	0.94	0.18	42,42,42,42	0
54	MG	1A	3416	1/1	0.94	0.10	23,23,23,23	0
54	MG	2A	3001	1/1	0.94	0.18	50,50,50,50	0
54	MG	1a	3137	1/1	0.94	0.17	52,52,52,52	0
54	MG	2A	3507	1/1	0.94	0.31	48,48,48,48	0
54	MG	1A	3133	1/1	0.94	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3818	1/1	0.94	0.11	41,41,41,41	0
54	MG	1A	3983	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3238	1/1	0.94	0.26	46,46,46,46	0
54	MG	2a	3025	1/1	0.94	0.15	49,49,49,49	0
54	MG	1A	3321	1/1	0.94	0.08	22,22,22,22	0
54	MG	2A	3011	1/1	0.94	0.16	38,38,38,38	0
54	MG	1A	3826	1/1	0.94	0.16	43,43,43,43	0
54	MG	1A	3420	1/1	0.94	0.06	17,17,17,17	0
54	MG	1A	3152	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3831	1/1	0.94	0.17	26,26,26,26	0
54	MG	1a	3002	1/1	0.94	0.14	69,69,69,69	0
54	MG	1a	3151	1/1	0.94	0.16	46,46,46,46	0
54	MG	1A	3999	1/1	0.94	0.10	68,68,68,68	0
54	MG	2A	3526	1/1	0.94	0.08	26,26,26,26	0
54	MG	1A	3041	1/1	0.94	0.08	45,45,45,45	0
54	MG	2a	3038	1/1	0.94	0.13	56,56,56,56	0
54	MG	2A	3530	1/1	0.94	0.07	42,42,42,42	0
54	MG	1A	3833	1/1	0.94	0.20	59,59,59,59	0
54	MG	2A	3032	1/1	0.94	0.16	48,48,48,48	0
54	MG	2a	3044	1/1	0.94	0.12	65,65,65,65	0
54	MG	2A	3034	1/1	0.94	0.16	53,53,53,53	0
54	MG	2A	3534	1/1	0.94	0.19	88,88,88,88	0
54	MG	1A	3834	1/1	0.94	0.10	53,53,53,53	0
54	MG	1A	3593	1/1	0.94	0.10	23,23,23,23	0
54	MG	2A	3038	1/1	0.94	0.11	45,45,45,45	0
54	MG	2a	3050	1/1	0.94	0.18	46,46,46,46	0
54	MG	1A	3508	1/1	0.94	0.09	37,37,37,37	0
54	MG	1A	3839	1/1	0.94	0.24	33,33,33,33	0
54	MG	1A	3595	1/1	0.94	0.07	70,70,70,70	0
54	MG	2A	3551	1/1	0.94	0.09	62,62,62,62	0
54	MG	1A	3343	1/1	0.94	0.09	66,66,66,66	0
54	MG	1A	4009	1/1	0.94	0.11	33,33,33,33	0
54	MG	2A	3270	1/1	0.94	0.10	44,44,44,44	0
54	MG	1A	3428	1/1	0.94	0.11	34,34,34,34	0
54	MG	1A	3846	1/1	0.94	0.06	58,58,58,58	0
54	MG	2A	3050	1/1	0.94	0.19	43,43,43,43	0
54	MG	1A	3136	1/1	0.94	0.23	31,31,31,31	0
54	MG	1A	3713	1/1	0.94	0.12	54,54,54,54	0
54	MG	1a	3171	1/1	0.94	0.06	70,70,70,70	0
54	MG	2a	3067	1/1	0.94	0.06	55,55,55,55	0
54	MG	1A	3715	1/1	0.94	0.36	43,43,43,43	0
54	MG	1B	205	1/1	0.94	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3070	1/1	0.94	0.11	28,28,28,28	0
54	MG	1A	3852	1/1	0.94	0.07	33,33,33,33	0
54	MG	2A	3574	1/1	0.94	0.17	82,82,82,82	0
54	MG	1A	3717	1/1	0.94	0.19	38,38,38,38	0
54	MG	2A	3578	1/1	0.94	0.08	38,38,38,38	0
54	MG	2A	3060	1/1	0.94	0.11	40,40,40,40	0
54	MG	1A	3223	1/1	0.94	0.13	34,34,34,34	0
54	MG	2A	3062	1/1	0.94	0.14	48,48,48,48	0
54	MG	2A	3586	1/1	0.94	0.07	76,76,76,76	0
54	MG	2a	3080	1/1	0.94	0.21	42,42,42,42	0
54	MG	2A	3292	1/1	0.94	0.09	42,42,42,42	0
54	MG	1A	3235	1/1	0.94	0.23	26,26,26,26	0
54	MG	2A	3064	1/1	0.94	0.42	44,44,44,44	0
54	MG	1A	3356	1/1	0.94	0.09	25,25,25,25	0
54	MG	2a	3091	1/1	0.94	0.14	60,60,60,60	0
54	MG	1A	3155	1/1	0.94	0.27	38,38,38,38	0
54	MG	2A	3303	1/1	0.94	0.12	35,35,35,35	0
54	MG	1A	3186	1/1	0.94	0.15	54,54,54,54	0
54	MG	2a	3096	1/1	0.94	0.11	59,59,59,59	0
54	MG	1B	219	1/1	0.94	0.10	41,41,41,41	0
54	MG	2a	3100	1/1	0.94	0.16	33,33,33,33	0
54	MG	1A	3867	1/1	0.94	0.10	34,34,34,34	0
54	MG	2A	3312	1/1	0.94	0.08	36,36,36,36	0
54	MG	2A	3314	1/1	0.94	0.07	27,27,27,27	0
54	MG	2A	3079	1/1	0.94	0.14	48,48,48,48	0
54	MG	2a	3106	1/1	0.94	0.26	56,56,56,56	0
54	MG	2A	3082	1/1	0.94	0.39	46,46,46,46	0
54	MG	2A	3611	1/1	0.94	0.14	36,36,36,36	0
54	MG	2A	3319	1/1	0.94	0.08	38,38,38,38	0
54	MG	2A	3321	1/1	0.94	0.07	41,41,41,41	0
54	MG	1A	3731	1/1	0.94	0.17	30,30,30,30	0
54	MG	1B	224	1/1	0.94	0.14	44,44,44,44	0
54	MG	2A	3087	1/1	0.94	0.23	60,60,60,60	0
54	MG	1A	3733	1/1	0.94	0.08	25,25,25,25	0
54	MG	2A	3328	1/1	0.94	0.09	34,34,34,34	0
54	MG	1A	3616	1/1	0.94	0.13	52,52,52,52	0
54	MG	1A	3046	1/1	0.94	0.10	32,32,32,32	0
54	MG	2A	3094	1/1	0.94	0.19	53,53,53,53	0
54	MG	1A	3530	1/1	0.94	0.05	32,32,32,32	0
54	MG	2A	3096	1/1	0.94	0.31	52,52,52,52	0
54	MG	1A	3158	1/1	0.94	0.21	47,47,47,47	0
54	MG	2A	3635	1/1	0.94	0.10	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3139	1/1	0.94	0.18	74,74,74,74	0
54	MG	1A	3623	1/1	0.94	0.07	46,46,46,46	0
54	MG	2A	3639	1/1	0.94	0.08	65,65,65,65	0
54	MG	1a	3202	1/1	0.94	0.10	49,49,49,49	0
54	MG	2A	3105	1/1	0.94	0.16	60,60,60,60	0
54	MG	2A	3644	1/1	0.94	0.08	88,88,88,88	0
54	MG	1A	3087	1/1	0.94	0.46	40,40,40,40	0
54	MG	1A	3627	1/1	0.94	0.13	31,31,31,31	0
54	MG	2a	3155	1/1	0.94	0.08	41,41,41,41	0
54	MG	1A	3245	1/1	0.94	0.40	40,40,40,40	0
54	MG	1a	3208	1/1	0.94	0.13	52,52,52,52	0
54	MG	1A	3895	1/1	0.94	0.11	47,47,47,47	0
54	MG	1A	3454	1/1	0.94	0.08	45,45,45,45	0
54	MG	1a	3211	1/1	0.94	0.11	73,73,73,73	0
54	MG	1A	3537	1/1	0.94	0.20	43,43,43,43	0
54	MG	2A	3654	1/1	0.94	0.10	49,49,49,49	0
54	MG	2a	3166	1/1	0.94	0.08	59,59,59,59	0
54	MG	2A	3362	1/1	0.94	0.07	51,51,51,51	0
54	MG	2A	3366	1/1	0.94	0.09	24,24,24,24	0
54	MG	2A	3657	1/1	0.94	0.08	36,36,36,36	0
54	MG	1A	3190	1/1	0.94	0.09	55,55,55,55	0
54	MG	1A	3635	1/1	0.94	0.10	46,46,46,46	0
54	MG	2A	3663	1/1	0.94	0.09	52,52,52,52	0
54	MG	2a	3180	1/1	0.94	0.07	70,70,70,70	0
54	MG	1A	3766	1/1	0.94	0.10	33,33,33,33	0
54	MG	1A	3907	1/1	0.94	0.07	47,47,47,47	0
54	MG	2A	3124	1/1	0.94	0.62	43,43,43,43	0
54	MG	2a	3184	1/1	0.94	0.13	65,65,65,65	0
54	MG	1A	3299	1/1	0.94	0.06	25,25,25,25	0
54	MG	1A	3640	1/1	0.94	0.15	49,49,49,49	0
54	MG	2a	3188	1/1	0.94	0.17	57,57,57,57	0
54	MG	1A	3544	1/1	0.94	0.10	47,47,47,47	0
54	MG	1a	3070	1/1	0.94	0.10	55,55,55,55	0
54	MG	2A	3681	1/1	0.94	0.10	67,67,67,67	0
54	MG	1F	303	1/1	0.94	0.10	28,28,28,28	0
54	MG	2A	3379	1/1	0.94	0.12	53,53,53,53	0
54	MG	2A	3380	1/1	0.94	0.07	28,28,28,28	0
54	MG	1A	3918	1/1	0.94	0.06	48,48,48,48	0
54	MG	1A	3164	1/1	0.94	0.33	26,26,26,26	0
54	MG	1A	3547	1/1	0.94	0.08	40,40,40,40	0
54	MG	2A	3390	1/1	0.94	0.08	56,56,56,56	0
54	MG	2A	3393	1/1	0.94	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	A1CRE	1A	4012	41/41	0.94	0.12	23,29,52,60	0
55	A1CRE	2A	3733	41/41	0.94	0.14	35,45,60,67	0
54	MG	2A	3394	1/1	0.94	0.08	32,32,32,32	0
56	MPD	18	105	8/8	0.94	0.14	24,26,28,33	0
54	MG	1A	3049	1/1	0.94	0.44	38,38,38,38	0
54	MG	1A	3924	1/1	0.94	0.09	35,35,35,35	0
54	MG	1A	3926	1/1	0.94	0.12	52,52,52,52	0
54	MG	2A	3399	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3402	1/1	0.94	0.09	48,48,48,48	0
57	ARG	1B	231	12/12	0.94	0.14	29,40,45,46	0
54	MG	2A	3709	1/1	0.94	0.09	45,45,45,45	0
54	MG	2A	3145	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3461	1/1	0.95	0.08	34,34,34,34	0
54	MG	1A	3368	1/1	0.95	0.07	56,56,56,56	0
54	MG	2A	3210	1/1	0.95	0.13	58,58,58,58	0
54	MG	1A	3219	1/1	0.95	0.08	27,27,27,27	0
54	MG	1y	202	1/1	0.95	0.07	67,67,67,67	0
54	MG	1A	3687	1/1	0.95	0.28	47,47,47,47	0
54	MG	2A	3455	1/1	0.95	0.09	43,43,43,43	0
54	MG	2A	3214	1/1	0.95	0.19	49,49,49,49	0
54	MG	11	104	1/1	0.95	0.12	33,33,33,33	0
54	MG	1A	3819	1/1	0.95	0.10	39,39,39,39	0
54	MG	1A	3984	1/1	0.95	0.07	80,80,80,80	0
54	MG	2A	3461	1/1	0.95	0.06	54,54,54,54	0
54	MG	15	101	1/1	0.95	0.22	32,32,32,32	0
54	MG	2B	219	1/1	0.95	0.12	76,76,76,76	0
54	MG	2D	301	1/1	0.95	0.20	47,47,47,47	0
54	MG	1A	3821	1/1	0.95	0.06	31,31,31,31	0
54	MG	2A	3008	1/1	0.95	0.09	32,32,32,32	0
54	MG	2D	305	1/1	0.95	0.15	40,40,40,40	0
54	MG	1A	3822	1/1	0.95	0.07	35,35,35,35	0
54	MG	17	103	1/1	0.95	0.11	52,52,52,52	0
54	MG	2E	302	1/1	0.95	0.15	33,33,33,33	0
54	MG	2E	303	1/1	0.95	0.07	39,39,39,39	0
54	MG	17	104	1/1	0.95	0.10	32,32,32,32	0
54	MG	2E	305	1/1	0.95	0.07	28,28,28,28	0
54	MG	1A	3472	1/1	0.95	0.08	28,28,28,28	0
54	MG	1A	3570	1/1	0.95	0.18	42,42,42,42	0
54	MG	2A	3476	1/1	0.95	0.06	51,51,51,51	0
54	MG	2A	3020	1/1	0.95	0.06	29,29,29,29	0
54	MG	1A	3992	1/1	0.95	0.15	33,33,33,33	0
54	MG	1A	3371	1/1	0.95	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3998	1/1	0.95	0.18	44,44,44,44	0
54	MG	1A	3177	1/1	0.95	0.45	25,25,25,25	0
54	MG	1a	3004	1/1	0.95	0.08	55,55,55,55	0
54	MG	2A	3028	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3178	1/1	0.95	0.56	29,29,29,29	0
54	MG	2A	3491	1/1	0.95	0.11	54,54,54,54	0
54	MG	1A	3179	1/1	0.95	0.09	40,40,40,40	0
54	MG	1A	3377	1/1	0.95	0.06	19,19,19,19	0
54	MG	2T	201	1/1	0.95	0.08	51,51,51,51	0
54	MG	1A	3378	1/1	0.95	0.08	18,18,18,18	0
54	MG	1A	3380	1/1	0.95	0.07	23,23,23,23	0
54	MG	1A	3581	1/1	0.95	0.07	31,31,31,31	0
54	MG	2A	3039	1/1	0.95	0.18	40,40,40,40	0
54	MG	1A	3232	1/1	0.95	0.36	29,29,29,29	0
54	MG	2A	3247	1/1	0.95	0.12	39,39,39,39	0
54	MG	1A	3287	1/1	0.95	0.12	14,14,14,14	0
54	MG	1a	3015	1/1	0.95	0.10	68,68,68,68	0
54	MG	25	101	1/1	0.95	0.15	44,44,44,44	0
54	MG	2A	3505	1/1	0.95	0.10	27,27,27,27	0
54	MG	1A	3707	1/1	0.95	0.06	83,83,83,83	0
54	MG	1a	3165	1/1	0.95	0.11	51,51,51,51	0
54	MG	28	101	1/1	0.95	0.16	48,48,48,48	0
54	MG	1A	3586	1/1	0.95	0.11	40,40,40,40	0
54	MG	2A	3047	1/1	0.95	0.09	47,47,47,47	0
54	MG	1A	3490	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3182	1/1	0.95	0.15	33,33,33,33	0
54	MG	1A	3150	1/1	0.95	0.09	30,30,30,30	0
54	MG	1A	3849	1/1	0.95	0.23	43,43,43,43	0
54	MG	2a	3007	1/1	0.95	0.12	41,41,41,41	0
54	MG	1A	3130	1/1	0.95	0.06	43,43,43,43	0
54	MG	1a	3025	1/1	0.95	0.06	54,54,54,54	0
54	MG	1a	3026	1/1	0.95	0.17	43,43,43,43	0
54	MG	1A	3012	1/1	0.95	0.17	23,23,23,23	0
54	MG	1A	3301	1/1	0.95	0.12	46,46,46,46	0
54	MG	1a	3029	1/1	0.95	0.14	49,49,49,49	0
54	MG	1A	3718	1/1	0.95	0.10	37,37,37,37	0
54	MG	1A	3596	1/1	0.95	0.13	44,44,44,44	0
54	MG	1B	210	1/1	0.95	0.17	55,55,55,55	0
54	MG	1a	3184	1/1	0.95	0.08	65,65,65,65	0
54	MG	2A	3279	1/1	0.95	0.21	44,44,44,44	0
54	MG	2A	3065	1/1	0.95	0.17	31,31,31,31	0
54	MG	1B	211	1/1	0.95	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3282	1/1	0.95	0.16	54,54,54,54	0
54	MG	2A	3069	1/1	0.95	0.16	30,30,30,30	0
54	MG	1A	3721	1/1	0.95	0.20	42,42,42,42	0
54	MG	2A	3538	1/1	0.95	0.07	65,65,65,65	0
54	MG	1a	3187	1/1	0.95	0.07	69,69,69,69	0
54	MG	2A	3540	1/1	0.95	0.10	86,86,86,86	0
54	MG	1B	216	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3724	1/1	0.95	0.10	38,38,38,38	0
54	MG	1a	3191	1/1	0.95	0.15	47,47,47,47	0
54	MG	1A	3020	1/1	0.95	0.28	32,32,32,32	0
54	MG	2A	3552	1/1	0.95	0.10	76,76,76,76	0
54	MG	1a	3041	1/1	0.95	0.16	55,55,55,55	0
54	MG	2A	3294	1/1	0.95	0.10	50,50,50,50	0
54	MG	2A	3555	1/1	0.95	0.09	26,26,26,26	0
54	MG	2A	3556	1/1	0.95	0.08	70,70,70,70	0
54	MG	2A	3557	1/1	0.95	0.12	28,28,28,28	0
54	MG	1A	3726	1/1	0.95	0.08	41,41,41,41	0
54	MG	2a	3043	1/1	0.95	0.14	45,45,45,45	0
54	MG	2A	3297	1/1	0.95	0.15	33,33,33,33	0
54	MG	1A	3072	1/1	0.95	0.07	34,34,34,34	0
54	MG	2A	3088	1/1	0.95	0.06	44,44,44,44	0
54	MG	2A	3300	1/1	0.95	0.07	51,51,51,51	0
54	MG	2A	3089	1/1	0.95	0.21	49,49,49,49	0
54	MG	2A	3304	1/1	0.95	0.07	34,34,34,34	0
54	MG	2A	3090	1/1	0.95	0.05	59,59,59,59	0
54	MG	2A	3307	1/1	0.95	0.07	44,44,44,44	0
54	MG	2A	3572	1/1	0.95	0.08	55,55,55,55	0
54	MG	1A	3134	1/1	0.95	0.07	24,24,24,24	0
54	MG	1a	3201	1/1	0.95	0.10	58,58,58,58	0
54	MG	1A	3044	1/1	0.95	0.32	26,26,26,26	0
54	MG	1a	3046	1/1	0.95	0.23	56,56,56,56	0
54	MG	1A	3247	1/1	0.95	0.21	63,63,63,63	0
54	MG	2A	3580	1/1	0.95	0.07	50,50,50,50	0
54	MG	2A	3581	1/1	0.95	0.09	32,32,32,32	0
54	MG	1A	3606	1/1	0.95	0.14	31,31,31,31	0
54	MG	2A	3097	1/1	0.95	0.21	39,39,39,39	0
54	MG	2a	3064	1/1	0.95	0.05	51,51,51,51	0
54	MG	1A	3734	1/1	0.95	0.31	34,34,34,34	0
54	MG	2A	3100	1/1	0.95	0.31	61,61,61,61	0
54	MG	1a	3050	1/1	0.95	0.15	55,55,55,55	0
54	MG	1a	3052	1/1	0.95	0.13	39,39,39,39	0
54	MG	2A	3104	1/1	0.95	0.12	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3735	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3512	1/1	0.95	0.13	20,20,20,20	0
54	MG	1A	3891	1/1	0.95	0.07	27,27,27,27	0
54	MG	1A	3739	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3191	1/1	0.95	0.22	50,50,50,50	0
54	MG	2A	3336	1/1	0.95	0.09	38,38,38,38	0
54	MG	1a	3060	1/1	0.95	0.24	62,62,62,62	0
54	MG	1A	3414	1/1	0.95	0.09	20,20,20,20	0
54	MG	2A	3608	1/1	0.95	0.09	77,77,77,77	0
54	MG	2A	3609	1/1	0.95	0.09	55,55,55,55	0
54	MG	1A	3253	1/1	0.95	0.14	38,38,38,38	0
54	MG	1A	3743	1/1	0.95	0.14	45,45,45,45	0
54	MG	1A	3617	1/1	0.95	0.09	38,38,38,38	0
54	MG	2A	3613	1/1	0.95	0.07	50,50,50,50	0
54	MG	2A	3119	1/1	0.95	0.11	49,49,49,49	0
54	MG	1A	3746	1/1	0.95	0.10	31,31,31,31	0
54	MG	1A	3519	1/1	0.95	0.06	29,29,29,29	0
54	MG	1A	3011	1/1	0.95	0.08	40,40,40,40	0
54	MG	2a	3095	1/1	0.95	0.08	46,46,46,46	0
54	MG	1A	3162	1/1	0.95	0.33	30,30,30,30	0
54	MG	2A	3125	1/1	0.95	0.29	52,52,52,52	0
54	MG	2A	3357	1/1	0.95	0.06	28,28,28,28	0
54	MG	2A	3621	1/1	0.95	0.05	32,32,32,32	0
54	MG	1A	3118	1/1	0.95	0.23	30,30,30,30	0
54	MG	2A	3623	1/1	0.95	0.07	76,76,76,76	0
54	MG	1A	3758	1/1	0.95	0.12	18,18,18,18	0
54	MG	2A	3128	1/1	0.95	0.14	52,52,52,52	0
54	MG	1A	3915	1/1	0.95	0.09	45,45,45,45	0
54	MG	2A	3130	1/1	0.95	0.17	51,51,51,51	0
54	MG	2a	3109	1/1	0.95	0.11	55,55,55,55	0
54	MG	2a	3111	1/1	0.95	0.08	39,39,39,39	0
54	MG	1A	3917	1/1	0.95	0.25	43,43,43,43	0
54	MG	2a	3114	1/1	0.95	0.19	71,71,71,71	0
54	MG	2A	3133	1/1	0.95	0.09	35,35,35,35	0
54	MG	1A	3526	1/1	0.95	0.11	42,42,42,42	0
54	MG	1A	3919	1/1	0.95	0.14	55,55,55,55	0
54	MG	1a	3075	1/1	0.95	0.21	50,50,50,50	0
54	MG	1A	3263	1/1	0.95	0.17	38,38,38,38	0
54	MG	2A	3138	1/1	0.95	0.12	48,48,48,48	0
54	MG	1A	3423	1/1	0.95	0.09	54,54,54,54	0
54	MG	2A	3141	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3529	1/1	0.95	0.10	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3630	1/1	0.95	0.12	43,43,43,43	0
54	MG	2A	3381	1/1	0.95	0.07	31,31,31,31	0
54	MG	1A	3101	1/1	0.95	0.14	23,23,23,23	0
54	MG	2a	3135	1/1	0.95	0.07	48,48,48,48	0
54	MG	1F	316	1/1	0.95	0.04	51,51,51,51	0
54	MG	1A	3325	1/1	0.95	0.07	22,22,22,22	0
54	MG	2a	3143	1/1	0.95	0.09	48,48,48,48	0
54	MG	2A	3389	1/1	0.95	0.07	41,41,41,41	0
54	MG	2A	3148	1/1	0.95	0.09	49,49,49,49	0
54	MG	1A	3930	1/1	0.95	0.16	27,27,27,27	0
54	MG	2A	3150	1/1	0.95	0.14	47,47,47,47	0
54	MG	1A	3931	1/1	0.95	0.09	26,26,26,26	0
54	MG	1A	3932	1/1	0.95	0.25	24,24,24,24	0
54	MG	2A	3666	1/1	0.95	0.09	62,62,62,62	0
54	MG	1a	3249	1/1	0.95	0.10	48,48,48,48	0
54	MG	1A	3077	1/1	0.95	0.36	28,28,28,28	0
54	MG	2A	3674	1/1	0.95	0.10	50,50,50,50	0
54	MG	2A	3401	1/1	0.95	0.16	51,51,51,51	0
54	MG	2A	3155	1/1	0.95	0.06	51,51,51,51	0
54	MG	1A	3534	1/1	0.95	0.09	31,31,31,31	0
54	MG	1A	3637	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3938	1/1	0.95	0.10	55,55,55,55	0
54	MG	1A	3269	1/1	0.95	0.16	30,30,30,30	0
54	MG	1A	3330	1/1	0.95	0.12	25,25,25,25	0
54	MG	1a	3259	1/1	0.95	0.18	87,87,87,87	0
54	MG	2A	3686	1/1	0.95	0.15	63,63,63,63	0
54	MG	1A	3645	1/1	0.95	0.21	43,43,43,43	0
54	MG	2a	3176	1/1	0.95	0.07	81,81,81,81	0
54	MG	2A	3688	1/1	0.95	0.09	48,48,48,48	0
54	MG	1A	3646	1/1	0.95	0.07	20,20,20,20	0
54	MG	1A	3945	1/1	0.95	0.12	52,52,52,52	0
54	MG	1A	3331	1/1	0.95	0.08	36,36,36,36	0
54	MG	2A	3694	1/1	0.95	0.20	66,66,66,66	0
54	MG	1A	3339	1/1	0.95	0.07	33,33,33,33	0
54	MG	1A	3080	1/1	0.95	0.28	29,29,29,29	0
54	MG	2A	3178	1/1	0.95	0.07	44,44,44,44	0
54	MG	2a	3186	1/1	0.95	0.06	67,67,67,67	0
54	MG	2A	3419	1/1	0.95	0.10	51,51,51,51	0
54	MG	1A	3348	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3106	1/1	0.95	0.30	20,20,20,20	0
54	MG	1A	3144	1/1	0.95	0.23	40,40,40,40	0
54	MG	1a	3105	1/1	0.95	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3957	1/1	0.95	0.16	48,48,48,48	0
54	MG	2A	3427	1/1	0.95	0.06	51,51,51,51	0
54	MG	2e	202	1/1	0.95	0.06	73,73,73,73	0
54	MG	1A	3794	1/1	0.95	0.30	56,56,56,56	0
54	MG	1A	3273	1/1	0.95	0.14	30,30,30,30	0
54	MG	2l	201	1/1	0.95	0.25	48,48,48,48	0
54	MG	2o	101	1/1	0.95	0.06	48,48,48,48	0
54	MG	1U	201	1/1	0.95	0.10	20,20,20,20	0
54	MG	1e	202	1/1	0.95	0.21	59,59,59,59	0
54	MG	2A	3434	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3148	1/1	0.95	0.14	30,30,30,30	0
54	MG	2A	3722	1/1	0.95	0.13	42,42,42,42	0
54	MG	1A	3129	1/1	0.95	0.10	35,35,35,35	0
54	MG	1A	3361	1/1	0.95	0.12	38,38,38,38	0
54	MG	1A	3554	1/1	0.95	0.16	63,63,63,63	0
54	MG	1A	3363	1/1	0.95	0.06	32,32,32,32	0
54	MG	1A	3214	1/1	0.95	0.35	34,34,34,34	0
54	MG	1W	202	1/1	0.95	0.08	34,34,34,34	0
54	MG	1a	3122	1/1	0.95	0.09	35,35,35,35	0
54	MG	1A	3674	1/1	0.95	0.08	52,52,52,52	0
54	MG	1A	3215	1/1	0.95	0.26	26,26,26,26	0
54	MG	1A	3216	1/1	0.95	0.15	47,47,47,47	0
58	ZN	14	501	1/1	0.95	0.12	126,126,126,126	0
54	MG	1A	3812	1/1	0.95	0.09	31,31,31,31	0
54	MG	1A	3540	1/1	0.96	0.05	26,26,26,26	0
54	MG	1A	3934	1/1	0.96	0.07	52,52,52,52	0
54	MG	1Q	206	1/1	0.96	0.24	39,39,39,39	0
54	MG	1R	201	1/1	0.96	0.28	31,31,31,31	0
54	MG	1R	202	1/1	0.96	0.11	47,47,47,47	0
54	MG	2B	204	1/1	0.96	0.07	56,56,56,56	0
54	MG	1A	3542	1/1	0.96	0.08	32,32,32,32	0
54	MG	2A	3198	1/1	0.96	0.08	45,45,45,45	0
54	MG	1o	101	1/1	0.96	0.08	61,61,61,61	0
54	MG	1o	102	1/1	0.96	0.06	29,29,29,29	0
54	MG	1A	3099	1/1	0.96	0.08	38,38,38,38	0
54	MG	1A	3207	1/1	0.96	0.10	30,30,30,30	0
54	MG	1A	3449	1/1	0.96	0.10	65,65,65,65	0
54	MG	2A	3206	1/1	0.96	0.15	55,55,55,55	0
54	MG	2A	3208	1/1	0.96	0.14	51,51,51,51	0
54	MG	1A	3546	1/1	0.96	0.07	46,46,46,46	0
54	MG	1A	3787	1/1	0.96	0.12	55,55,55,55	0
54	MG	1A	3653	1/1	0.96	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
54	MG	1A	3452	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3030	1/1	0.96	0.07	26,26,26,26	0
54	MG	1A	3657	1/1	0.96	0.10	49,49,49,49	0
54	MG	2A	3215	1/1	0.96	0.06	45,45,45,45	0
54	MG	1U	204	1/1	0.96	0.15	30,30,30,30	0
54	MG	1a	3127	1/1	0.96	0.10	65,65,65,65	0
54	MG	2A	3469	1/1	0.96	0.09	49,49,49,49	0
54	MG	2A	3470	1/1	0.96	0.11	31,31,31,31	0
54	MG	1A	3658	1/1	0.96	0.21	27,27,27,27	0
54	MG	2A	3009	1/1	0.96	0.12	39,39,39,39	0
54	MG	1A	3951	1/1	0.96	0.07	28,28,28,28	0
54	MG	2A	3221	1/1	0.96	0.13	56,56,56,56	0
54	MG	1A	3251	1/1	0.96	0.44	33,33,33,33	0
54	MG	2F	304	1/1	0.96	0.18	45,45,45,45	0
54	MG	1A	3374	1/1	0.96	0.11	37,37,37,37	0
54	MG	2A	3482	1/1	0.96	0.09	32,32,32,32	0
54	MG	1A	3798	1/1	0.96	0.07	36,36,36,36	0
54	MG	2A	3485	1/1	0.96	0.09	46,46,46,46	0
54	MG	2A	3015	1/1	0.96	0.18	43,43,43,43	0
54	MG	2A	3227	1/1	0.96	0.31	50,50,50,50	0
54	MG	1A	3799	1/1	0.96	0.08	50,50,50,50	0
54	MG	2A	3019	1/1	0.96	0.12	40,40,40,40	0
54	MG	1A	3015	1/1	0.96	0.26	37,37,37,37	0
54	MG	1A	3801	1/1	0.96	0.07	20,20,20,20	0
54	MG	2Q	203	1/1	0.96	0.10	47,47,47,47	0
54	MG	1A	3665	1/1	0.96	0.07	20,20,20,20	0
54	MG	10	101	1/1	0.96	0.09	34,34,34,34	0
54	MG	1A	3255	1/1	0.96	0.10	33,33,33,33	0
54	MG	1a	3139	1/1	0.96	0.07	43,43,43,43	0
54	MG	2A	3026	1/1	0.96	0.08	51,51,51,51	0
54	MG	2A	3237	1/1	0.96	0.22	44,44,44,44	0
54	MG	1A	3459	1/1	0.96	0.08	50,50,50,50	0
54	MG	2A	3029	1/1	0.96	0.11	43,43,43,43	0
54	MG	2A	3030	1/1	0.96	0.06	25,25,25,25	0
54	MG	2A	3503	1/1	0.96	0.09	50,50,50,50	0
54	MG	1A	3966	1/1	0.96	0.09	43,43,43,43	0
54	MG	2A	3242	1/1	0.96	0.09	47,47,47,47	0
54	MG	1A	3305	1/1	0.96	0.18	32,32,32,32	0
54	MG	2A	3033	1/1	0.96	0.06	43,43,43,43	0
54	MG	2A	3508	1/1	0.96	0.15	48,48,48,48	0
54	MG	1A	3183	1/1	0.96	0.22	29,29,29,29	0
54	MG	1a	3145	1/1	0.96	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3463	1/1	0.96	0.08	39,39,39,39	0
54	MG	13	101	1/1	0.96	0.25	23,23,23,23	0
54	MG	1A	3970	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3379	1/1	0.96	0.07	11,11,11,11	0
54	MG	1A	3679	1/1	0.96	0.22	25,25,25,25	0
54	MG	1A	3680	1/1	0.96	0.10	44,44,44,44	0
54	MG	1A	3814	1/1	0.96	0.07	42,42,42,42	0
54	MG	2A	3520	1/1	0.96	0.15	44,44,44,44	0
54	MG	1a	3155	1/1	0.96	0.09	61,61,61,61	0
54	MG	2A	3258	1/1	0.96	0.23	44,44,44,44	0
54	MG	17	101	1/1	0.96	0.27	26,26,26,26	0
54	MG	2A	3524	1/1	0.96	0.06	52,52,52,52	0
54	MG	2A	3046	1/1	0.96	0.12	47,47,47,47	0
54	MG	2a	3015	1/1	0.96	0.08	50,50,50,50	0
54	MG	1A	3565	1/1	0.96	0.08	39,39,39,39	0
54	MG	2A	3528	1/1	0.96	0.05	24,24,24,24	0
54	MG	2a	3018	1/1	0.96	0.09	45,45,45,45	0
54	MG	1A	3123	1/1	0.96	0.04	21,21,21,21	0
54	MG	1A	3471	1/1	0.96	0.10	24,24,24,24	0
54	MG	1A	3685	1/1	0.96	0.17	27,27,27,27	0
54	MG	18	103	1/1	0.96	0.10	45,45,45,45	0
54	MG	1A	3982	1/1	0.96	0.14	52,52,52,52	0
54	MG	1A	3260	1/1	0.96	0.05	67,67,67,67	0
54	MG	1A	3125	1/1	0.96	0.07	26,26,26,26	0
54	MG	1A	3384	1/1	0.96	0.06	17,17,17,17	0
54	MG	1a	3003	1/1	0.96	0.09	55,55,55,55	0
54	MG	1A	3314	1/1	0.96	0.08	25,25,25,25	0
54	MG	1A	3691	1/1	0.96	0.22	53,53,53,53	0
54	MG	1A	3829	1/1	0.96	0.18	42,42,42,42	0
54	MG	2A	3542	1/1	0.96	0.09	62,62,62,62	0
54	MG	2A	3543	1/1	0.96	0.08	58,58,58,58	0
54	MG	1A	3140	1/1	0.96	0.28	30,30,30,30	0
54	MG	2A	3548	1/1	0.96	0.10	54,54,54,54	0
54	MG	1A	3694	1/1	0.96	0.06	24,24,24,24	0
54	MG	1a	3009	1/1	0.96	0.08	52,52,52,52	0
54	MG	2a	3039	1/1	0.96	0.18	55,55,55,55	0
54	MG	2A	3066	1/1	0.96	0.16	47,47,47,47	0
54	MG	2A	3067	1/1	0.96	0.18	33,33,33,33	0
54	MG	1A	3576	1/1	0.96	0.21	51,51,51,51	0
54	MG	1A	3316	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3398	1/1	0.96	0.09	30,30,30,30	0
54	MG	1A	4001	1/1	0.96	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3072	1/1	0.96	0.16	52,52,52,52	0
54	MG	1A	3836	1/1	0.96	0.20	38,38,38,38	0
54	MG	2A	3295	1/1	0.96	0.10	58,58,58,58	0
54	MG	1A	3102	1/1	0.96	0.13	28,28,28,28	0
54	MG	1A	3485	1/1	0.96	0.17	40,40,40,40	0
54	MG	2A	3080	1/1	0.96	0.18	49,49,49,49	0
54	MG	1A	3084	1/1	0.96	0.10	34,34,34,34	0
54	MG	1a	3020	1/1	0.96	0.06	48,48,48,48	0
54	MG	2A	3302	1/1	0.96	0.17	50,50,50,50	0
54	MG	1A	3583	1/1	0.96	0.10	30,30,30,30	0
54	MG	2A	3085	1/1	0.96	0.09	32,32,32,32	0
54	MG	2A	3305	1/1	0.96	0.08	28,28,28,28	0
54	MG	2A	3576	1/1	0.96	0.08	57,57,57,57	0
54	MG	2a	3060	1/1	0.96	0.15	45,45,45,45	0
54	MG	1A	3704	1/1	0.96	0.08	43,43,43,43	0
54	MG	1A	3843	1/1	0.96	0.11	55,55,55,55	0
54	MG	1a	3189	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3086	1/1	0.96	0.17	28,28,28,28	0
54	MG	2A	3311	1/1	0.96	0.07	32,32,32,32	0
54	MG	1A	3026	1/1	0.96	0.47	28,28,28,28	0
54	MG	1A	3225	1/1	0.96	0.19	28,28,28,28	0
54	MG	1A	3587	1/1	0.96	0.24	33,33,33,33	0
54	MG	2A	3588	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3496	1/1	0.96	0.07	17,17,17,17	0
54	MG	1A	3850	1/1	0.96	0.08	56,56,56,56	0
54	MG	1a	3030	1/1	0.96	0.12	50,50,50,50	0
54	MG	1A	3589	1/1	0.96	0.05	23,23,23,23	0
54	MG	1a	3033	1/1	0.96	0.12	53,53,53,53	0
54	MG	1A	3497	1/1	0.96	0.07	56,56,56,56	0
54	MG	2A	3599	1/1	0.96	0.11	68,68,68,68	0
54	MG	1A	3498	1/1	0.96	0.07	34,34,34,34	0
54	MG	1a	3205	1/1	0.96	0.05	40,40,40,40	0
54	MG	1A	3716	1/1	0.96	0.08	36,36,36,36	0
54	MG	2a	3081	1/1	0.96	0.08	48,48,48,48	0
54	MG	2a	3082	1/1	0.96	0.09	61,61,61,61	0
54	MG	2a	3083	1/1	0.96	0.17	56,56,56,56	0
54	MG	1A	3322	1/1	0.96	0.11	31,31,31,31	0
54	MG	2a	3085	1/1	0.96	0.07	57,57,57,57	0
54	MG	2A	3331	1/1	0.96	0.06	43,43,43,43	0
54	MG	2A	3332	1/1	0.96	0.06	22,22,22,22	0
54	MG	2A	3106	1/1	0.96	0.09	45,45,45,45	0
54	MG	2A	3107	1/1	0.96	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3858	1/1	0.96	0.17	56,56,56,56	0
54	MG	1A	3410	1/1	0.96	0.07	11,11,11,11	0
54	MG	1B	212	1/1	0.96	0.06	47,47,47,47	0
54	MG	1A	3226	1/1	0.96	0.06	33,33,33,33	0
54	MG	1A	3412	1/1	0.96	0.06	23,23,23,23	0
54	MG	2a	3097	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3227	1/1	0.96	0.24	43,43,43,43	0
54	MG	2A	3114	1/1	0.96	0.12	36,36,36,36	0
54	MG	2a	3101	1/1	0.96	0.06	31,31,31,31	0
54	MG	1A	3868	1/1	0.96	0.07	47,47,47,47	0
54	MG	2A	3351	1/1	0.96	0.10	33,33,33,33	0
54	MG	1A	3869	1/1	0.96	0.17	41,41,41,41	0
54	MG	2A	3353	1/1	0.96	0.07	47,47,47,47	0
54	MG	2A	3117	1/1	0.96	0.13	38,38,38,38	0
54	MG	1A	3598	1/1	0.96	0.30	34,34,34,34	0
54	MG	1A	3599	1/1	0.96	0.31	28,28,28,28	0
54	MG	2A	3624	1/1	0.96	0.15	79,79,79,79	0
54	MG	2A	3625	1/1	0.96	0.06	53,53,53,53	0
54	MG	2a	3112	1/1	0.96	0.07	57,57,57,57	0
54	MG	2A	3628	1/1	0.96	0.09	67,67,67,67	0
54	MG	1B	222	1/1	0.96	0.12	57,57,57,57	0
54	MG	2A	3358	1/1	0.96	0.06	62,62,62,62	0
54	MG	1A	3231	1/1	0.96	0.24	34,34,34,34	0
54	MG	2a	3118	1/1	0.96	0.09	53,53,53,53	0
54	MG	2A	3122	1/1	0.96	0.12	42,42,42,42	0
54	MG	1A	3874	1/1	0.96	0.07	20,20,20,20	0
54	MG	1A	3145	1/1	0.96	0.07	39,39,39,39	0
54	MG	1a	3223	1/1	0.96	0.05	56,56,56,56	0
54	MG	1A	3878	1/1	0.96	0.08	40,40,40,40	0
54	MG	1A	3881	1/1	0.96	0.11	58,58,58,58	0
54	MG	1a	3056	1/1	0.96	0.10	77,77,77,77	0
54	MG	2a	3127	1/1	0.96	0.17	59,59,59,59	0
54	MG	1A	3882	1/1	0.96	0.18	47,47,47,47	0
54	MG	1A	3276	1/1	0.96	0.08	44,44,44,44	0
54	MG	1D	301	1/1	0.96	0.28	34,34,34,34	0
54	MG	2A	3374	1/1	0.96	0.07	39,39,39,39	0
54	MG	2A	3132	1/1	0.96	0.15	35,35,35,35	0
54	MG	1A	3885	1/1	0.96	0.21	27,27,27,27	0
54	MG	2a	3142	1/1	0.96	0.07	59,59,59,59	0
54	MG	1D	303	1/1	0.96	0.13	33,33,33,33	0
54	MG	1D	304	1/1	0.96	0.15	44,44,44,44	0
54	MG	1A	3277	1/1	0.96	0.33	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3233	1/1	0.96	0.33	28,28,28,28	0
54	MG	1A	3419	1/1	0.96	0.10	19,19,19,19	0
54	MG	2a	3150	1/1	0.96	0.08	63,63,63,63	0
54	MG	1A	3610	1/1	0.96	0.06	23,23,23,23	0
54	MG	1a	3238	1/1	0.96	0.06	40,40,40,40	0
54	MG	2A	3661	1/1	0.96	0.11	51,51,51,51	0
54	MG	2a	3154	1/1	0.96	0.07	62,62,62,62	0
54	MG	2A	3388	1/1	0.96	0.07	52,52,52,52	0
54	MG	1A	3234	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3421	1/1	0.96	0.07	13,13,13,13	0
54	MG	2A	3667	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3894	1/1	0.96	0.06	18,18,18,18	0
54	MG	1A	3614	1/1	0.96	0.10	30,30,30,30	0
54	MG	1A	3280	1/1	0.96	0.06	54,54,54,54	0
54	MG	1a	3247	1/1	0.96	0.08	64,64,64,64	0
54	MG	1A	3520	1/1	0.96	0.07	46,46,46,46	0
54	MG	2A	3677	1/1	0.96	0.07	51,51,51,51	0
54	MG	2a	3168	1/1	0.96	0.08	83,83,83,83	0
54	MG	2a	3169	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3171	1/1	0.96	0.21	35,35,35,35	0
54	MG	2A	3400	1/1	0.96	0.06	39,39,39,39	0
54	MG	1A	3073	1/1	0.96	0.14	20,20,20,20	0
54	MG	1A	3745	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3906	1/1	0.96	0.15	55,55,55,55	0
54	MG	2a	3178	1/1	0.96	0.08	56,56,56,56	0
54	MG	1F	305	1/1	0.96	0.18	34,34,34,34	0
54	MG	2A	3685	1/1	0.96	0.08	45,45,45,45	0
54	MG	1A	3239	1/1	0.96	0.18	28,28,28,28	0
54	MG	2A	3156	1/1	0.96	0.08	47,47,47,47	0
54	MG	1a	3256	1/1	0.96	0.07	31,31,31,31	0
54	MG	2A	3158	1/1	0.96	0.08	40,40,40,40	0
54	MG	2A	3162	1/1	0.96	0.15	44,44,44,44	0
54	MG	1A	3358	1/1	0.96	0.08	57,57,57,57	0
54	MG	1F	310	1/1	0.96	0.06	31,31,31,31	0
54	MG	1F	311	1/1	0.96	0.21	37,37,37,37	0
54	MG	1a	3084	1/1	0.96	0.12	57,57,57,57	0
54	MG	1A	3909	1/1	0.96	0.06	44,44,44,44	0
54	MG	2A	3700	1/1	0.96	0.07	60,60,60,60	0
54	MG	2A	3701	1/1	0.96	0.11	47,47,47,47	0
54	MG	1A	3014	1/1	0.96	0.06	32,32,32,32	0
54	MG	1A	3626	1/1	0.96	0.20	21,21,21,21	0
54	MG	2f	201	1/1	0.96	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3170	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3430	1/1	0.96	0.05	20,20,20,20	0
54	MG	1A	3433	1/1	0.96	0.16	40,40,40,40	0
54	MG	1A	3436	1/1	0.96	0.12	41,41,41,41	0
54	MG	1A	3091	1/1	0.96	0.11	37,37,37,37	0
54	MG	1A	3763	1/1	0.96	0.07	19,19,19,19	0
54	MG	2A	3715	1/1	0.96	0.14	42,42,42,42	0
54	MG	2A	3428	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3362	1/1	0.96	0.06	26,26,26,26	0
54	MG	1A	3533	1/1	0.96	0.05	22,22,22,22	0
54	MG	2A	3719	1/1	0.96	0.06	30,30,30,30	0
54	MG	1A	3151	1/1	0.96	0.29	31,31,31,31	0
54	MG	1A	3925	1/1	0.96	0.14	41,41,41,41	0
54	MG	1A	3022	1/1	0.96	0.21	33,33,33,33	0
54	MG	1e	203	1/1	0.96	0.14	43,43,43,43	0
54	MG	2A	3436	1/1	0.96	0.10	46,46,46,46	0
54	MG	1A	3444	1/1	0.96	0.07	37,37,37,37	0
54	MG	1P	202	1/1	0.96	0.52	22,22,22,22	0
54	MG	1A	3290	1/1	0.96	0.27	39,39,39,39	0
54	MG	1A	3203	1/1	0.96	0.04	33,33,33,33	0
54	MG	1A	3539	1/1	0.96	0.11	34,34,34,34	0
58	ZN	2n	501	1/1	0.96	0.07	105,105,105,105	0
54	MG	1A	3861	1/1	0.97	0.06	18,18,18,18	0
54	MG	1A	3450	1/1	0.97	0.07	31,31,31,31	0
54	MG	2D	306	1/1	0.97	0.12	46,46,46,46	0
54	MG	1A	3003	1/1	0.97	0.06	22,22,22,22	0
54	MG	2A	3257	1/1	0.97	0.09	48,48,48,48	0
54	MG	1A	3262	1/1	0.97	0.05	29,29,29,29	0
54	MG	2A	3259	1/1	0.97	0.08	48,48,48,48	0
54	MG	1a	3011	1/1	0.97	0.07	53,53,53,53	0
54	MG	1A	3866	1/1	0.97	0.07	27,27,27,27	0
54	MG	2A	3500	1/1	0.97	0.07	45,45,45,45	0
54	MG	1A	3085	1/1	0.97	0.40	28,28,28,28	0
54	MG	2F	303	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3264	1/1	0.97	0.06	34,34,34,34	0
54	MG	2A	3264	1/1	0.97	0.06	33,33,33,33	0
54	MG	1B	204	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3736	1/1	0.97	0.08	37,37,37,37	0
54	MG	2A	3267	1/1	0.97	0.08	29,29,29,29	0
54	MG	1A	3313	1/1	0.97	0.06	20,20,20,20	0
54	MG	2A	3269	1/1	0.97	0.05	24,24,24,24	0
54	MG	1A	3265	1/1	0.97	0.30	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3073	1/1	0.97	0.08	46,46,46,46	0
54	MG	2A	3074	1/1	0.97	0.11	40,40,40,40	0
54	MG	2Q	201	1/1	0.97	0.09	45,45,45,45	0
54	MG	2A	3513	1/1	0.97	0.05	45,45,45,45	0
54	MG	2A	3075	1/1	0.97	0.06	42,42,42,42	0
54	MG	2A	3076	1/1	0.97	0.10	50,50,50,50	0
54	MG	1A	3050	1/1	0.97	0.24	26,26,26,26	0
54	MG	2A	3278	1/1	0.97	0.09	29,29,29,29	0
54	MG	1A	3157	1/1	0.97	0.19	39,39,39,39	0
54	MG	2A	3519	1/1	0.97	0.06	53,53,53,53	0
54	MG	1A	3224	1/1	0.97	0.08	32,32,32,32	0
54	MG	2V	201	1/1	0.97	0.16	48,48,48,48	0
54	MG	2W	201	1/1	0.97	0.24	35,35,35,35	0
54	MG	1A	3462	1/1	0.97	0.05	45,45,45,45	0
54	MG	2A	3081	1/1	0.97	0.33	39,39,39,39	0
54	MG	1A	3392	1/1	0.97	0.05	15,15,15,15	0
54	MG	20	101	1/1	0.97	0.12	40,40,40,40	0
54	MG	20	102	1/1	0.97	0.09	59,59,59,59	0
54	MG	1a	3193	1/1	0.97	0.09	56,56,56,56	0
54	MG	2A	3287	1/1	0.97	0.07	31,31,31,31	0
54	MG	1B	213	1/1	0.97	0.08	44,44,44,44	0
54	MG	1A	3633	1/1	0.97	0.06	30,30,30,30	0
54	MG	2A	3086	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3465	1/1	0.97	0.09	9,9,9,9	0
54	MG	1A	3747	1/1	0.97	0.07	43,43,43,43	0
54	MG	1a	3199	1/1	0.97	0.09	44,44,44,44	0
54	MG	1A	3467	1/1	0.97	0.06	20,20,20,20	0
54	MG	1A	3111	1/1	0.97	0.27	32,32,32,32	0
54	MG	2A	3535	1/1	0.97	0.07	57,57,57,57	0
54	MG	1A	3888	1/1	0.97	0.05	25,25,25,25	0
54	MG	1a	3032	1/1	0.97	0.10	29,29,29,29	0
54	MG	1A	3751	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3638	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3396	1/1	0.97	0.07	21,21,21,21	0
54	MG	2A	3301	1/1	0.97	0.13	44,44,44,44	0
54	MG	1A	3641	1/1	0.97	0.16	37,37,37,37	0
54	MG	1A	3550	1/1	0.97	0.05	46,46,46,46	0
54	MG	1A	3643	1/1	0.97	0.06	24,24,24,24	0
54	MG	2A	3545	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3762	1/1	0.97	0.26	38,38,38,38	0
54	MG	2A	3102	1/1	0.97	0.06	40,40,40,40	0
54	MG	1A	3551	1/1	0.97	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3159	1/1	0.97	0.14	38,38,38,38	0
54	MG	1A	3051	1/1	0.97	0.20	34,34,34,34	0
54	MG	2A	3310	1/1	0.97	0.09	52,52,52,52	0
54	MG	1A	3114	1/1	0.97	0.21	34,34,34,34	0
54	MG	1A	3904	1/1	0.97	0.06	50,50,50,50	0
54	MG	1A	3905	1/1	0.97	0.07	52,52,52,52	0
54	MG	1D	305	1/1	0.97	0.09	21,21,21,21	0
54	MG	1D	306	1/1	0.97	0.23	26,26,26,26	0
54	MG	2a	3027	1/1	0.97	0.07	60,60,60,60	0
54	MG	1A	3768	1/1	0.97	0.10	35,35,35,35	0
54	MG	2A	3320	1/1	0.97	0.08	22,22,22,22	0
54	MG	2A	3565	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3474	1/1	0.97	0.08	23,23,23,23	0
54	MG	1D	310	1/1	0.97	0.07	39,39,39,39	0
54	MG	1a	3051	1/1	0.97	0.29	53,53,53,53	0
54	MG	2A	3324	1/1	0.97	0.06	26,26,26,26	0
54	MG	1A	3475	1/1	0.97	0.07	25,25,25,25	0
54	MG	1a	3053	1/1	0.97	0.11	50,50,50,50	0
54	MG	1D	313	1/1	0.97	0.13	40,40,40,40	0
54	MG	1A	3561	1/1	0.97	0.07	33,33,33,33	0
54	MG	2A	3575	1/1	0.97	0.10	64,64,64,64	0
54	MG	1A	3052	1/1	0.97	0.14	32,32,32,32	0
54	MG	1A	3911	1/1	0.97	0.09	43,43,43,43	0
54	MG	1a	3231	1/1	0.97	0.12	66,66,66,66	0
54	MG	1A	3773	1/1	0.97	0.07	33,33,33,33	0
54	MG	1A	3913	1/1	0.97	0.07	37,37,37,37	0
54	MG	2A	3335	1/1	0.97	0.04	50,50,50,50	0
54	MG	1A	3053	1/1	0.97	0.29	26,26,26,26	0
54	MG	2A	3337	1/1	0.97	0.07	59,59,59,59	0
54	MG	2A	3585	1/1	0.97	0.10	63,63,63,63	0
54	MG	1A	3036	1/1	0.97	0.07	22,22,22,22	0
54	MG	1A	3481	1/1	0.97	0.05	53,53,53,53	0
54	MG	1A	3092	1/1	0.97	0.19	33,33,33,33	0
54	MG	2A	3590	1/1	0.97	0.05	33,33,33,33	0
54	MG	1E	309	1/1	0.97	0.08	52,52,52,52	0
54	MG	2a	3054	1/1	0.97	0.05	42,42,42,42	0
54	MG	1F	301	1/1	0.97	0.13	28,28,28,28	0
54	MG	1A	3660	1/1	0.97	0.06	60,60,60,60	0
54	MG	2A	3347	1/1	0.97	0.09	64,64,64,64	0
54	MG	1A	3921	1/1	0.97	0.12	61,61,61,61	0
54	MG	1a	3242	1/1	0.97	0.10	76,76,76,76	0
54	MG	1A	3093	1/1	0.97	0.06	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3602	1/1	0.97	0.06	43,43,43,43	0
54	MG	1F	306	1/1	0.97	0.13	28,28,28,28	0
54	MG	1A	3124	1/1	0.97	0.04	21,21,21,21	0
54	MG	1A	3333	1/1	0.97	0.05	17,17,17,17	0
54	MG	1A	3335	1/1	0.97	0.12	34,34,34,34	0
54	MG	1A	3789	1/1	0.97	0.05	43,43,43,43	0
54	MG	2A	3139	1/1	0.97	0.21	45,45,45,45	0
54	MG	1A	3666	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3929	1/1	0.97	0.07	55,55,55,55	0
54	MG	1A	3338	1/1	0.97	0.06	21,21,21,21	0
54	MG	2A	3364	1/1	0.97	0.08	62,62,62,62	0
54	MG	1a	3254	1/1	0.97	0.06	59,59,59,59	0
54	MG	2A	3144	1/1	0.97	0.12	46,46,46,46	0
54	MG	1a	3077	1/1	0.97	0.08	44,44,44,44	0
54	MG	1a	3078	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3792	1/1	0.97	0.07	29,29,29,29	0
54	MG	1A	3573	1/1	0.97	0.07	30,30,30,30	0
54	MG	2a	3078	1/1	0.97	0.25	46,46,46,46	0
54	MG	1A	3489	1/1	0.97	0.08	26,26,26,26	0
54	MG	1A	3575	1/1	0.97	0.05	38,38,38,38	0
54	MG	1G	203	1/1	0.97	0.18	66,66,66,66	0
54	MG	1A	3675	1/1	0.97	0.08	36,36,36,36	0
54	MG	1H	4101	1/1	0.97	0.06	50,50,50,50	0
54	MG	1A	3074	1/1	0.97	0.10	28,28,28,28	0
54	MG	1A	3937	1/1	0.97	0.08	40,40,40,40	0
54	MG	2A	3627	1/1	0.97	0.19	64,64,64,64	0
54	MG	1A	3492	1/1	0.97	0.04	41,41,41,41	0
54	MG	1A	3146	1/1	0.97	0.16	18,18,18,18	0
54	MG	2a	3089	1/1	0.97	0.13	61,61,61,61	0
54	MG	1a	3090	1/1	0.97	0.15	39,39,39,39	0
54	MG	2A	3159	1/1	0.97	0.18	71,71,71,71	0
54	MG	2A	3633	1/1	0.97	0.06	41,41,41,41	0
54	MG	2A	3160	1/1	0.97	0.18	50,50,50,50	0
54	MG	1O	201	1/1	0.97	0.06	36,36,36,36	0
54	MG	1A	3940	1/1	0.97	0.05	36,36,36,36	0
54	MG	1A	3345	1/1	0.97	0.05	20,20,20,20	0
54	MG	2A	3392	1/1	0.97	0.06	51,51,51,51	0
54	MG	1A	3346	1/1	0.97	0.05	21,21,21,21	0
54	MG	1P	203	1/1	0.97	0.30	26,26,26,26	0
54	MG	1A	3943	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3804	1/1	0.97	0.23	22,22,22,22	0
54	MG	1A	3347	1/1	0.97	0.07	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3206	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3684	1/1	0.97	0.08	38,38,38,38	0
54	MG	1A	3500	1/1	0.97	0.06	18,18,18,18	0
54	MG	1A	3686	1/1	0.97	0.05	34,34,34,34	0
54	MG	2A	3403	1/1	0.97	0.10	29,29,29,29	0
54	MG	1A	3032	1/1	0.97	0.11	42,42,42,42	0
54	MG	2A	3176	1/1	0.97	0.07	44,44,44,44	0
54	MG	1R	203	1/1	0.97	0.10	28,28,28,28	0
54	MG	1l	201	1/1	0.97	0.12	48,48,48,48	0
54	MG	2A	3658	1/1	0.97	0.06	30,30,30,30	0
54	MG	1R	204	1/1	0.97	0.19	43,43,43,43	0
54	MG	1A	3008	1/1	0.97	0.08	32,32,32,32	0
54	MG	1A	3209	1/1	0.97	0.23	36,36,36,36	0
54	MG	1R	207	1/1	0.97	0.05	20,20,20,20	0
54	MG	2a	3121	1/1	0.97	0.15	71,71,71,71	0
54	MG	2A	3664	1/1	0.97	0.06	57,57,57,57	0
54	MG	1a	3113	1/1	0.97	0.08	38,38,38,38	0
54	MG	1R	208	1/1	0.97	0.07	39,39,39,39	0
54	MG	2A	3668	1/1	0.97	0.05	61,61,61,61	0
54	MG	1A	3354	1/1	0.97	0.08	18,18,18,18	0
54	MG	2A	3672	1/1	0.97	0.08	32,32,32,32	0
54	MG	1A	3958	1/1	0.97	0.11	44,44,44,44	0
54	MG	2a	3129	1/1	0.97	0.09	65,65,65,65	0
54	MG	2a	3130	1/1	0.97	0.05	48,48,48,48	0
54	MG	1A	3959	1/1	0.97	0.10	41,41,41,41	0
54	MG	1A	3001	1/1	0.97	0.05	28,28,28,28	0
54	MG	2a	3133	1/1	0.97	0.07	65,65,65,65	0
54	MG	2a	3134	1/1	0.97	0.10	51,51,51,51	0
54	MG	1A	3590	1/1	0.97	0.14	48,48,48,48	0
54	MG	1A	3248	1/1	0.97	0.46	30,30,30,30	0
54	MG	2a	3138	1/1	0.97	0.07	53,53,53,53	0
54	MG	2A	3422	1/1	0.97	0.05	56,56,56,56	0
54	MG	2a	3140	1/1	0.97	0.06	73,73,73,73	0
54	MG	1A	3695	1/1	0.97	0.18	26,26,26,26	0
54	MG	2A	3003	1/1	0.97	0.08	32,32,32,32	0
54	MG	1A	3427	1/1	0.97	0.13	51,51,51,51	0
54	MG	1U	203	1/1	0.97	0.45	35,35,35,35	0
54	MG	1A	3509	1/1	0.97	0.07	49,49,49,49	0
54	MG	2A	3429	1/1	0.97	0.11	48,48,48,48	0
54	MG	1A	3359	1/1	0.97	0.05	34,34,34,34	0
54	MG	1V	201	1/1	0.97	0.26	23,23,23,23	0
54	MG	1A	3288	1/1	0.97	0.09	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3203	1/1	0.97	0.09	25,25,25,25	0
54	MG	1A	3048	1/1	0.97	0.18	35,35,35,35	0
54	MG	1A	3828	1/1	0.97	0.09	43,43,43,43	0
54	MG	1A	3514	1/1	0.97	0.06	38,38,38,38	0
54	MG	2A	3207	1/1	0.97	0.07	46,46,46,46	0
54	MG	1A	3432	1/1	0.97	0.08	38,38,38,38	0
54	MG	2A	3016	1/1	0.97	0.12	41,41,41,41	0
54	MG	1A	3292	1/1	0.97	0.45	28,28,28,28	0
54	MG	2A	3018	1/1	0.97	0.21	31,31,31,31	0
54	MG	1A	3976	1/1	0.97	0.07	46,46,46,46	0
54	MG	2A	3703	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3600	1/1	0.97	0.32	22,22,22,22	0
54	MG	2A	3444	1/1	0.97	0.07	22,22,22,22	0
54	MG	1A	3212	1/1	0.97	0.48	35,35,35,35	0
54	MG	2A	3707	1/1	0.97	0.09	63,63,63,63	0
54	MG	1A	3602	1/1	0.97	0.26	27,27,27,27	0
54	MG	10	104	1/1	0.97	0.07	34,34,34,34	0
54	MG	2A	3710	1/1	0.97	0.10	56,56,56,56	0
54	MG	1A	3835	1/1	0.97	0.13	42,42,42,42	0
54	MG	10	106	1/1	0.97	0.08	56,56,56,56	0
54	MG	1A	3294	1/1	0.97	0.05	26,26,26,26	0
54	MG	1A	3710	1/1	0.97	0.09	33,33,33,33	0
54	MG	1A	3252	1/1	0.97	0.30	40,40,40,40	0
54	MG	1A	3366	1/1	0.97	0.11	24,24,24,24	0
54	MG	1A	3213	1/1	0.97	0.19	33,33,33,33	0
54	MG	2A	3224	1/1	0.97	0.15	41,41,41,41	0
54	MG	1A	3607	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	3608	1/1	0.97	0.10	38,38,38,38	0
54	MG	1A	3990	1/1	0.97	0.12	38,38,38,38	0
54	MG	15	103	1/1	0.97	0.27	36,36,36,36	0
54	MG	1A	3844	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3441	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3993	1/1	0.97	0.07	26,26,26,26	0
54	MG	17	102	1/1	0.97	0.29	29,29,29,29	0
54	MG	2A	3729	1/1	0.97	0.07	37,37,37,37	0
54	MG	1A	3994	1/1	0.97	0.06	34,34,34,34	0
54	MG	1A	3180	1/1	0.97	0.19	30,30,30,30	0
54	MG	2A	3468	1/1	0.97	0.13	53,53,53,53	0
54	MG	1A	3997	1/1	0.97	0.12	53,53,53,53	0
54	MG	1A	3256	1/1	0.97	0.13	60,60,60,60	0
54	MG	1A	3720	1/1	0.97	0.05	27,27,27,27	0
54	MG	2A	3472	1/1	0.97	0.16	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3081	1/1	0.97	0.29	28,28,28,28	0
54	MG	19	101	1/1	0.97	0.04	45,45,45,45	0
54	MG	1A	3722	1/1	0.97	0.04	30,30,30,30	0
54	MG	2A	3477	1/1	0.97	0.09	32,32,32,32	0
54	MG	2B	209	1/1	0.97	0.09	62,62,62,62	0
54	MG	2A	3049	1/1	0.97	0.11	46,46,46,46	0
54	MG	1A	3082	1/1	0.97	0.10	34,34,34,34	0
54	MG	1a	3167	1/1	0.97	0.08	75,75,75,75	0
54	MG	1A	3615	1/1	0.97	0.09	16,16,16,16	0
54	MG	1A	3218	1/1	0.97	0.06	36,36,36,36	0
54	MG	1a	3170	1/1	0.97	0.08	55,55,55,55	0
54	MG	1A	3307	1/1	0.97	0.25	30,30,30,30	0
54	MG	1A	3728	1/1	0.97	0.07	40,40,40,40	0
54	MG	2A	3058	1/1	0.97	0.09	33,33,33,33	0
58	ZN	1Y	202	1/1	0.97	0.07	97,97,97,97	0
54	MG	2B	220	1/1	0.97	0.06	66,66,66,66	0
54	MG	1A	3619	1/1	0.97	0.06	24,24,24,24	0
54	MG	1a	3174	1/1	0.97	0.06	53,53,53,53	0
54	MG	1A	3196	1/1	0.98	0.04	34,34,34,34	0
54	MG	1A	3197	1/1	0.98	0.07	41,41,41,41	0
54	MG	2A	3563	1/1	0.98	0.06	55,55,55,55	0
54	MG	11	102	1/1	0.98	0.07	36,36,36,36	0
54	MG	1A	3024	1/1	0.98	0.13	20,20,20,20	0
54	MG	2X	101	1/1	0.98	0.09	45,45,45,45	0
54	MG	1A	3013	1/1	0.98	0.07	25,25,25,25	0
54	MG	2A	3360	1/1	0.98	0.08	41,41,41,41	0
54	MG	1y	203	1/1	0.98	0.14	44,44,44,44	0
54	MG	1y	204	1/1	0.98	0.06	68,68,68,68	0
54	MG	2A	3363	1/1	0.98	0.05	50,50,50,50	0
54	MG	2A	3571	1/1	0.98	0.09	28,28,28,28	0
54	MG	1A	3855	1/1	0.98	0.09	45,45,45,45	0
54	MG	2A	3365	1/1	0.98	0.08	50,50,50,50	0
54	MG	1A	3510	1/1	0.98	0.04	22,22,22,22	0
54	MG	1A	3323	1/1	0.98	0.04	13,13,13,13	0
54	MG	1A	3860	1/1	0.98	0.04	23,23,23,23	0
54	MG	2A	3177	1/1	0.98	0.12	39,39,39,39	0
54	MG	2A	3004	1/1	0.98	0.07	38,38,38,38	0
54	MG	2A	3179	1/1	0.98	0.06	49,49,49,49	0
54	MG	15	102	1/1	0.98	0.20	24,24,24,24	0
54	MG	1A	3058	1/1	0.98	0.06	13,13,13,13	0
54	MG	1A	3117	1/1	0.98	0.17	27,27,27,27	0
54	MG	1A	3328	1/1	0.98	0.04	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3584	1/1	0.98	0.08	57,57,57,57	0
54	MG	2A	3184	1/1	0.98	0.40	41,41,41,41	0
54	MG	2A	3377	1/1	0.98	0.05	32,32,32,32	0
54	MG	1a	3143	1/1	0.98	0.05	61,61,61,61	0
54	MG	1A	3202	1/1	0.98	0.15	38,38,38,38	0
54	MG	1A	3732	1/1	0.98	0.05	29,29,29,29	0
54	MG	1A	3009	1/1	0.98	0.14	23,23,23,23	0
54	MG	2A	3013	1/1	0.98	0.11	22,22,22,22	0
54	MG	2A	3594	1/1	0.98	0.05	54,54,54,54	0
54	MG	1a	3147	1/1	0.98	0.07	55,55,55,55	0
54	MG	2A	3384	1/1	0.98	0.05	31,31,31,31	0
54	MG	2A	3385	1/1	0.98	0.07	51,51,51,51	0
54	MG	1A	3518	1/1	0.98	0.10	38,38,38,38	0
54	MG	2a	3022	1/1	0.98	0.24	55,55,55,55	0
54	MG	1A	3119	1/1	0.98	0.10	33,33,33,33	0
54	MG	2A	3601	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3332	1/1	0.98	0.06	22,22,22,22	0
54	MG	1A	3205	1/1	0.98	0.37	35,35,35,35	0
54	MG	2A	3391	1/1	0.98	0.07	28,28,28,28	0
54	MG	1A	3010	1/1	0.98	0.12	28,28,28,28	0
54	MG	1A	3336	1/1	0.98	0.11	42,42,42,42	0
54	MG	1a	3154	1/1	0.98	0.06	42,42,42,42	0
54	MG	2A	3395	1/1	0.98	0.08	25,25,25,25	0
54	MG	1A	3524	1/1	0.98	0.06	37,37,37,37	0
54	MG	1A	3337	1/1	0.98	0.14	37,37,37,37	0
54	MG	2A	3200	1/1	0.98	0.05	33,33,33,33	0
54	MG	1A	3880	1/1	0.98	0.07	29,29,29,29	0
54	MG	1A	3121	1/1	0.98	0.11	28,28,28,28	0
54	MG	1A	3122	1/1	0.98	0.11	39,39,39,39	0
54	MG	1A	3883	1/1	0.98	0.10	38,38,38,38	0
54	MG	1A	3341	1/1	0.98	0.05	18,18,18,18	0
54	MG	1A	3061	1/1	0.98	0.07	18,18,18,18	0
54	MG	1B	214	1/1	0.98	0.06	42,42,42,42	0
54	MG	1A	3344	1/1	0.98	0.04	20,20,20,20	0
54	MG	1A	3434	1/1	0.98	0.09	38,38,38,38	0
54	MG	1A	3161	1/1	0.98	0.08	20,20,20,20	0
54	MG	2A	3035	1/1	0.98	0.11	41,41,41,41	0
54	MG	1A	3028	1/1	0.98	0.21	23,23,23,23	0
54	MG	1A	3163	1/1	0.98	0.14	28,28,28,28	0
54	MG	1A	3755	1/1	0.98	0.05	28,28,28,28	0
54	MG	2A	3626	1/1	0.98	0.04	57,57,57,57	0
54	MG	1A	3063	1/1	0.98	0.07	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3639	1/1	0.98	0.15	46,46,46,46	0
54	MG	1A	3759	1/1	0.98	0.10	39,39,39,39	0
54	MG	2A	3417	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3165	1/1	0.98	0.20	32,32,32,32	0
54	MG	1A	3350	1/1	0.98	0.07	45,45,45,45	0
54	MG	1A	3900	1/1	0.98	0.07	53,53,53,53	0
54	MG	1A	3090	1/1	0.98	0.13	31,31,31,31	0
54	MG	1A	3167	1/1	0.98	0.07	29,29,29,29	0
54	MG	1A	3541	1/1	0.98	0.05	39,39,39,39	0
54	MG	2A	3640	1/1	0.98	0.07	53,53,53,53	0
54	MG	1a	3179	1/1	0.98	0.06	65,65,65,65	0
54	MG	1A	3016	1/1	0.98	0.27	25,25,25,25	0
54	MG	1A	3169	1/1	0.98	0.05	22,22,22,22	0
54	MG	1A	3357	1/1	0.98	0.07	12,12,12,12	0
54	MG	1A	3649	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3220	1/1	0.98	0.27	34,34,34,34	0
54	MG	1A	3066	1/1	0.98	0.06	30,30,30,30	0
54	MG	2A	3649	1/1	0.98	0.09	54,54,54,54	0
54	MG	1A	3451	1/1	0.98	0.08	13,13,13,13	0
54	MG	1A	3017	1/1	0.98	0.29	17,17,17,17	0
54	MG	1A	3094	1/1	0.98	0.16	30,30,30,30	0
54	MG	1A	3095	1/1	0.98	0.26	21,21,21,21	0
54	MG	1D	312	1/1	0.98	0.09	18,18,18,18	0
54	MG	1A	3914	1/1	0.98	0.13	30,30,30,30	0
54	MG	1A	3068	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3916	1/1	0.98	0.10	51,51,51,51	0
54	MG	1a	3194	1/1	0.98	0.05	62,62,62,62	0
54	MG	1A	3175	1/1	0.98	0.07	32,32,32,32	0
54	MG	2A	3660	1/1	0.98	0.04	63,63,63,63	0
54	MG	1A	3780	1/1	0.98	0.04	28,28,28,28	0
54	MG	1A	3781	1/1	0.98	0.04	20,20,20,20	0
54	MG	1E	301	1/1	0.98	0.19	34,34,34,34	0
54	MG	1A	3659	1/1	0.98	0.05	51,51,51,51	0
54	MG	2A	3665	1/1	0.98	0.06	59,59,59,59	0
54	MG	1a	3200	1/1	0.98	0.13	71,71,71,71	0
54	MG	1E	303	1/1	0.98	0.28	25,25,25,25	0
54	MG	1A	3457	1/1	0.98	0.04	40,40,40,40	0
54	MG	1A	3784	1/1	0.98	0.04	32,32,32,32	0
54	MG	2A	3670	1/1	0.98	0.05	62,62,62,62	0
54	MG	2a	3090	1/1	0.98	0.13	73,73,73,73	0
54	MG	2A	3671	1/1	0.98	0.05	35,35,35,35	0
54	MG	1A	3097	1/1	0.98	0.17	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1E	308	1/1	0.98	0.07	29,29,29,29	0
54	MG	1A	3662	1/1	0.98	0.14	57,57,57,57	0
54	MG	1A	3230	1/1	0.98	0.23	29,29,29,29	0
54	MG	1F	302	1/1	0.98	0.16	27,27,27,27	0
54	MG	1A	3289	1/1	0.98	0.17	33,33,33,33	0
54	MG	1A	3559	1/1	0.98	0.17	25,25,25,25	0
54	MG	2a	3099	1/1	0.98	0.06	44,44,44,44	0
54	MG	1A	3928	1/1	0.98	0.12	47,47,47,47	0
54	MG	2A	3458	1/1	0.98	0.11	46,46,46,46	0
54	MG	1A	3560	1/1	0.98	0.08	37,37,37,37	0
54	MG	1A	3098	1/1	0.98	0.08	13,13,13,13	0
54	MG	1A	3668	1/1	0.98	0.08	49,49,49,49	0
54	MG	2A	3684	1/1	0.98	0.05	41,41,41,41	0
54	MG	1A	3670	1/1	0.98	0.07	52,52,52,52	0
54	MG	1A	3291	1/1	0.98	0.37	30,30,30,30	0
54	MG	1A	3796	1/1	0.98	0.04	38,38,38,38	0
54	MG	1A	3370	1/1	0.98	0.04	22,22,22,22	0
54	MG	2a	3110	1/1	0.98	0.10	42,42,42,42	0
54	MG	1A	3673	1/1	0.98	0.06	26,26,26,26	0
54	MG	1A	3464	1/1	0.98	0.06	34,34,34,34	0
54	MG	2A	3691	1/1	0.98	0.05	43,43,43,43	0
54	MG	2A	3692	1/1	0.98	0.19	37,37,37,37	0
54	MG	1A	3069	1/1	0.98	0.34	43,43,43,43	0
54	MG	1A	3676	1/1	0.98	0.05	24,24,24,24	0
54	MG	1A	3566	1/1	0.98	0.09	23,23,23,23	0
54	MG	1A	3803	1/1	0.98	0.15	41,41,41,41	0
54	MG	2A	3272	1/1	0.98	0.04	45,45,45,45	0
54	MG	2A	3699	1/1	0.98	0.10	54,54,54,54	0
54	MG	1A	3047	1/1	0.98	0.07	26,26,26,26	0
54	MG	2A	3274	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3137	1/1	0.98	0.38	28,28,28,28	0
54	MG	1A	3469	1/1	0.98	0.07	19,19,19,19	0
54	MG	2A	3480	1/1	0.98	0.05	68,68,68,68	0
54	MG	2A	3098	1/1	0.98	0.16	48,48,48,48	0
54	MG	1A	3181	1/1	0.98	0.07	40,40,40,40	0
54	MG	1A	3808	1/1	0.98	0.09	18,18,18,18	0
54	MG	1A	3297	1/1	0.98	0.05	51,51,51,51	0
54	MG	1A	3298	1/1	0.98	0.15	27,27,27,27	0
54	MG	1A	3950	1/1	0.98	0.04	23,23,23,23	0
54	MG	1A	3236	1/1	0.98	0.53	24,24,24,24	0
54	MG	1A	3071	1/1	0.98	0.22	27,27,27,27	0
54	MG	2A	3714	1/1	0.98	0.07	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3031	1/1	0.98	0.05	25,25,25,25	0
54	MG	1A	3240	1/1	0.98	0.35	25,25,25,25	0
54	MG	1A	3303	1/1	0.98	0.25	29,29,29,29	0
54	MG	1A	3018	1/1	0.98	0.16	26,26,26,26	0
54	MG	2a	3141	1/1	0.98	0.06	60,60,60,60	0
54	MG	1A	3479	1/1	0.98	0.04	14,14,14,14	0
54	MG	1Q	202	1/1	0.98	0.21	30,30,30,30	0
54	MG	1Q	203	1/1	0.98	0.07	43,43,43,43	0
54	MG	1a	3243	1/1	0.98	0.07	46,46,46,46	0
54	MG	1A	3960	1/1	0.98	0.08	38,38,38,38	0
54	MG	1Q	205	1/1	0.98	0.04	15,15,15,15	0
54	MG	1A	3480	1/1	0.98	0.06	27,27,27,27	0
54	MG	2A	3501	1/1	0.98	0.07	45,45,45,45	0
54	MG	1Q	207	1/1	0.98	0.09	33,33,33,33	0
54	MG	1A	3820	1/1	0.98	0.04	27,27,27,27	0
54	MG	1A	3692	1/1	0.98	0.11	39,39,39,39	0
54	MG	1A	3385	1/1	0.98	0.05	11,11,11,11	0
54	MG	1A	3823	1/1	0.98	0.33	36,36,36,36	0
54	MG	1A	3582	1/1	0.98	0.05	34,34,34,34	0
54	MG	1A	3104	1/1	0.98	0.12	23,23,23,23	0
54	MG	1A	3388	1/1	0.98	0.05	25,25,25,25	0
54	MG	1A	3391	1/1	0.98	0.14	15,15,15,15	0
54	MG	1A	3306	1/1	0.98	0.04	14,14,14,14	0
54	MG	2a	3162	1/1	0.98	0.07	59,59,59,59	0
54	MG	2a	3163	1/1	0.98	0.08	61,61,61,61	0
54	MG	2a	3164	1/1	0.98	0.04	68,68,68,68	0
54	MG	1a	3258	1/1	0.98	0.04	58,58,58,58	0
54	MG	1A	3971	1/1	0.98	0.06	20,20,20,20	0
54	MG	1A	3019	1/1	0.98	0.18	19,19,19,19	0
54	MG	1a	3261	1/1	0.98	0.06	46,46,46,46	0
54	MG	1A	3973	1/1	0.98	0.12	22,22,22,22	0
54	MG	2A	3313	1/1	0.98	0.06	21,21,21,21	0
54	MG	1A	3487	1/1	0.98	0.04	14,14,14,14	0
54	MG	2a	3174	1/1	0.98	0.07	62,62,62,62	0
54	MG	2A	3315	1/1	0.98	0.09	27,27,27,27	0
54	MG	1A	3394	1/1	0.98	0.04	15,15,15,15	0
54	MG	2A	3317	1/1	0.98	0.06	33,33,33,33	0
54	MG	1a	3265	1/1	0.98	0.06	47,47,47,47	0
54	MG	1A	3395	1/1	0.98	0.06	13,13,13,13	0
54	MG	2B	217	1/1	0.98	0.07	61,61,61,61	0
54	MG	1A	3005	1/1	0.98	0.06	23,23,23,23	0
54	MG	1A	3491	1/1	0.98	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3106	1/1	0.98	0.06	40,40,40,40	0
54	MG	2A	3527	1/1	0.98	0.07	31,31,31,31	0
54	MG	2D	302	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3021	1/1	0.98	0.08	26,26,26,26	0
54	MG	1A	3493	1/1	0.98	0.10	36,36,36,36	0
54	MG	2A	3325	1/1	0.98	0.04	32,32,32,32	0
54	MG	1a	3109	1/1	0.98	0.04	31,31,31,31	0
54	MG	1d	303	1/1	0.98	0.06	73,73,73,73	0
54	MG	1a	3110	1/1	0.98	0.07	35,35,35,35	0
54	MG	1A	3494	1/1	0.98	0.07	36,36,36,36	0
54	MG	1a	3112	1/1	0.98	0.05	39,39,39,39	0
54	MG	1V	202	1/1	0.98	0.14	28,28,28,28	0
54	MG	1A	3108	1/1	0.98	0.29	36,36,36,36	0
54	MG	2E	306	1/1	0.98	0.12	59,59,59,59	0
54	MG	1e	204	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3840	1/1	0.98	0.06	29,29,29,29	0
54	MG	1V	205	1/1	0.98	0.09	43,43,43,43	0
54	MG	1A	3109	1/1	0.98	0.05	28,28,28,28	0
54	MG	1A	3985	1/1	0.98	0.12	8,8,8,8	0
54	MG	1A	3006	1/1	0.98	0.06	19,19,19,19	0
54	MG	2A	3339	1/1	0.98	0.07	26,26,26,26	0
54	MG	1A	3079	1/1	0.98	0.07	45,45,45,45	0
54	MG	2A	3546	1/1	0.98	0.07	27,27,27,27	0
54	MG	2A	3547	1/1	0.98	0.05	54,54,54,54	0
54	MG	1A	3714	1/1	0.98	0.09	38,38,38,38	0
54	MG	1A	3193	1/1	0.98	0.06	33,33,33,33	0
54	MG	2A	3550	1/1	0.98	0.05	43,43,43,43	0
54	MG	1a	3123	1/1	0.98	0.06	61,61,61,61	0
54	MG	1A	3406	1/1	0.98	0.04	29,29,29,29	0
54	MG	1m	201	1/1	0.98	0.04	65,65,65,65	0
54	MG	1A	3194	1/1	0.98	0.12	29,29,29,29	0
54	MG	2R	201	1/1	0.98	0.07	37,37,37,37	0
54	MG	2A	3161	1/1	0.98	0.19	40,40,40,40	0
54	MG	1A	3408	1/1	0.98	0.04	17,17,17,17	0
58	ZN	15	107	1/1	0.98	0.04	64,64,64,64	0
58	ZN	1n	103	1/1	0.98	0.04	74,74,74,74	0
58	ZN	2Y	202	1/1	0.98	0.07	109,109,109,109	0
54	MG	1A	3023	1/1	0.98	0.21	25,25,25,25	0
58	ZN	25	104	1/1	0.98	0.06	87,87,87,87	0
58	ZN	29	501	1/1	0.98	0.04	67,67,67,67	0
54	MG	1A	3254	1/1	0.98	0.06	26,26,26,26	0
54	MG	1A	3324	1/1	0.99	0.04	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3738	1/1	0.99	0.03	26,26,26,26	0
54	MG	2a	3115	1/1	0.99	0.05	65,65,65,65	0
54	MG	1A	3308	1/1	0.99	0.26	23,23,23,23	0
54	MG	1A	3045	1/1	0.99	0.06	11,11,11,11	0
54	MG	2A	3713	1/1	0.99	0.07	51,51,51,51	0
54	MG	2A	3423	1/1	0.99	0.03	39,39,39,39	0
54	MG	2A	3172	1/1	0.99	0.07	46,46,46,46	0
54	MG	1A	3431	1/1	0.99	0.07	33,33,33,33	0
54	MG	2A	3253	1/1	0.99	0.09	17,17,17,17	0
54	MG	1A	3501	1/1	0.99	0.03	13,13,13,13	0
54	MG	1a	3245	1/1	0.99	0.04	53,53,53,53	0
54	MG	2A	3256	1/1	0.99	0.04	24,24,24,24	0
54	MG	1D	308	1/1	0.99	0.05	28,28,28,28	0
54	MG	1A	3399	1/1	0.99	0.03	17,17,17,17	0
54	MG	1A	3327	1/1	0.99	0.03	18,18,18,18	0
54	MG	1A	3401	1/1	0.99	0.04	15,15,15,15	0
54	MG	1A	3372	1/1	0.99	0.04	21,21,21,21	0
54	MG	2A	3346	1/1	0.99	0.04	53,53,53,53	0
54	MG	1A	3249	1/1	0.99	0.08	37,37,37,37	0
54	MG	2A	3348	1/1	0.99	0.03	20,20,20,20	0
54	MG	2A	3349	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3859	1/1	0.99	0.02	28,28,28,28	0
54	MG	2a	3136	1/1	0.99	0.05	56,56,56,56	0
54	MG	1A	3988	1/1	0.99	0.05	39,39,39,39	0
54	MG	2A	3630	1/1	0.99	0.03	43,43,43,43	0
54	MG	2A	3027	1/1	0.99	0.03	22,22,22,22	0
54	MG	1A	3618	1/1	0.99	0.06	18,18,18,18	0
54	MG	1A	3749	1/1	0.99	0.04	19,19,19,19	0
54	MG	1A	3703	1/1	0.99	0.03	13,13,13,13	0
54	MG	1A	3863	1/1	0.99	0.04	36,36,36,36	0
54	MG	2a	3144	1/1	0.99	0.08	40,40,40,40	0
54	MG	2a	3145	1/1	0.99	0.06	51,51,51,51	0
54	MG	1A	3404	1/1	0.99	0.04	19,19,19,19	0
54	MG	2A	3637	1/1	0.99	0.03	33,33,33,33	0
54	MG	2A	3638	1/1	0.99	0.05	40,40,40,40	0
54	MG	1A	3217	1/1	0.99	0.11	28,28,28,28	0
54	MG	1A	3995	1/1	0.99	0.10	21,21,21,21	0
54	MG	1A	3753	1/1	0.99	0.03	26,26,26,26	0
54	MG	1E	306	1/1	0.99	0.09	13,13,13,13	0
54	MG	2A	3643	1/1	0.99	0.03	38,38,38,38	0
54	MG	1A	3754	1/1	0.99	0.03	25,25,25,25	0
54	MG	1A	3706	1/1	0.99	0.07	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3238	1/1	0.99	0.10	19,19,19,19	0
54	MG	1a	3266	1/1	0.99	0.04	53,53,53,53	0
54	MG	1A	3757	1/1	0.99	0.04	17,17,17,17	0
54	MG	10	102	1/1	0.99	0.09	33,33,33,33	0
54	MG	1A	3352	1/1	0.99	0.04	35,35,35,35	0
54	MG	1A	3443	1/1	0.99	0.04	15,15,15,15	0
54	MG	2A	3283	1/1	0.99	0.06	29,29,29,29	0
54	MG	1A	3873	1/1	0.99	0.07	28,28,28,28	0
54	MG	2A	3285	1/1	0.99	0.05	31,31,31,31	0
54	MG	1A	3624	1/1	0.99	0.10	22,22,22,22	0
54	MG	1A	3876	1/1	0.99	0.04	33,33,33,33	0
54	MG	1A	3054	1/1	0.99	0.27	29,29,29,29	0
54	MG	1F	308	1/1	0.99	0.12	29,29,29,29	0
54	MG	2A	3559	1/1	0.99	0.03	46,46,46,46	0
54	MG	2a	3170	1/1	0.99	0.09	47,47,47,47	0
54	MG	2A	3560	1/1	0.99	0.05	19,19,19,19	0
54	MG	1A	3228	1/1	0.99	0.05	25,25,25,25	0
54	MG	2a	3173	1/1	0.99	0.08	57,57,57,57	0
54	MG	1A	3879	1/1	0.99	0.04	21,21,21,21	0
54	MG	1A	3669	1/1	0.99	0.08	36,36,36,36	0
54	MG	2E	307	1/1	0.99	0.04	25,25,25,25	0
54	MG	1A	3355	1/1	0.99	0.03	30,30,30,30	0
54	MG	1A	3765	1/1	0.99	0.07	32,32,32,32	0
54	MG	2F	302	1/1	0.99	0.10	37,37,37,37	0
54	MG	1A	3268	1/1	0.99	0.28	25,25,25,25	0
54	MG	2A	3473	1/1	0.99	0.07	42,42,42,42	0
54	MG	1A	3334	1/1	0.99	0.04	27,27,27,27	0
54	MG	2A	3057	1/1	0.99	0.03	26,26,26,26	0
54	MG	1a	3207	1/1	0.99	0.05	53,53,53,53	0
54	MG	1A	3382	1/1	0.99	0.02	27,27,27,27	0
54	MG	2A	3387	1/1	0.99	0.05	20,20,20,20	0
54	MG	2A	3479	1/1	0.99	0.05	42,42,42,42	0
54	MG	1A	3948	1/1	0.99	0.08	51,51,51,51	0
54	MG	15	105	1/1	0.99	0.04	35,35,35,35	0
54	MG	1A	3229	1/1	0.99	0.32	25,25,25,25	0
54	MG	1A	3064	1/1	0.99	0.04	24,24,24,24	0
54	MG	1A	3556	1/1	0.99	0.08	10,10,10,10	0
54	MG	1A	3889	1/1	0.99	0.05	44,44,44,44	0
54	MG	1A	3634	1/1	0.99	0.13	25,25,25,25	0
54	MG	1A	3557	1/1	0.99	0.07	35,35,35,35	0
54	MG	1A	3955	1/1	0.99	0.07	13,13,13,13	0
54	MG	1A	3774	1/1	0.99	0.07	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3723	1/1	0.99	0.05	31,31,31,31	0
54	MG	1A	3147	1/1	0.99	0.09	29,29,29,29	0
54	MG	1A	3040	1/1	0.99	0.13	34,34,34,34	0
54	MG	2A	3587	1/1	0.99	0.04	38,38,38,38	0
54	MG	1A	3896	1/1	0.99	0.07	20,20,20,20	0
54	MG	1A	3897	1/1	0.99	0.08	46,46,46,46	0
54	MG	1A	3387	1/1	0.99	0.05	22,22,22,22	0
54	MG	1A	3779	1/1	0.99	0.04	78,78,78,78	0
54	MG	2A	3592	1/1	0.99	0.05	41,41,41,41	0
54	MG	2A	3405	1/1	0.99	0.08	33,33,33,33	0
54	MG	1A	3258	1/1	0.99	0.07	21,21,21,21	0
54	MG	1A	3525	1/1	0.99	0.09	44,44,44,44	0
54	MG	2A	3596	1/1	0.99	0.03	25,25,25,25	0
54	MG	2A	3697	1/1	0.99	0.07	61,61,61,61	0
54	MG	1A	3389	1/1	0.99	0.05	32,32,32,32	0
54	MG	1B	223	1/1	0.99	0.05	42,42,42,42	0
54	MG	1A	3390	1/1	0.99	0.10	12,12,12,12	0
54	MG	1A	3340	1/1	0.99	0.08	34,34,34,34	0
54	MG	1A	3644	1/1	0.99	0.04	22,22,22,22	0
54	MG	2a	3001	1/1	0.99	0.07	52,52,52,52	0
54	MG	1A	3786	1/1	0.99	0.10	45,45,45,45	0
54	MG	1A	3113	1/1	0.99	0.15	27,27,27,27	0
54	MG	1A	3342	1/1	0.99	0.06	23,23,23,23	0
54	MG	1A	3083	1/1	0.99	0.06	32,32,32,32	0
58	ZN	26	501	1/1	0.99	0.02	51,51,51,51	0
54	MG	1a	3016	1/1	0.99	0.03	76,76,76,76	0
54	MG	1A	3078	1/1	0.99	0.28	27,27,27,27	0
59	SF4	1d	306	8/8	0.99	0.04	57,64,71,75	0
59	SF4	2d	501	8/8	0.99	0.04	55,77,84,87	0
54	MG	1A	3816	1/1	1.00	0.03	27,27,27,27	0
54	MG	1A	3857	1/1	1.00	0.03	20,20,20,20	0
54	MG	1A	3435	1/1	1.00	0.02	19,19,19,19	0
54	MG	1a	3124	1/1	1.00	0.03	36,36,36,36	0
54	MG	1A	3466	1/1	1.00	0.03	34,34,34,34	0
54	MG	1A	3442	1/1	1.00	0.02	17,17,17,17	0
54	MG	1A	3956	1/1	1.00	0.04	20,20,20,20	0
54	MG	1A	3295	1/1	1.00	0.02	31,31,31,31	0
58	ZN	16	501	1/1	1.00	0.03	40,40,40,40	0
58	ZN	19	103	1/1	1.00	0.01	42,42,42,42	0
54	MG	2A	3344	1/1	1.00	0.03	18,18,18,18	0
54	MG	1A	3422	1/1	1.00	0.05	21,21,21,21	0
54	MG	1A	3611	1/1	1.00	0.03	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3467	1/1	1.00	0.04	26,26,26,26	0
54	MG	2A	3484	1/1	1.00	0.02	25,25,25,25	0
54	MG	1A	3875	1/1	1.00	0.02	32,32,32,32	0
54	MG	1A	3654	1/1	1.00	0.07	34,34,34,34	0
54	MG	1A	3515	1/1	1.00	0.03	17,17,17,17	0
54	MG	1A	3825	1/1	1.00	0.02	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.