



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2025 – 07:24 PM EDT

PDB ID : 9O3I / pdb_00009o3i
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with ketolide telithromycin, mRNA, aminoacylated A-site Lys-tRNA^{Lys}, P-site fMRC-peptidyl-tRNA^{Met}, and deacylated E-site tRNA^{Lys} at 2.80Å resolution
Authors : Syroegin, E.A.; Aleksandrova, E.V.; Kruglov, A.A.; Paranjpe, M.N.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on : 2025-04-07
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

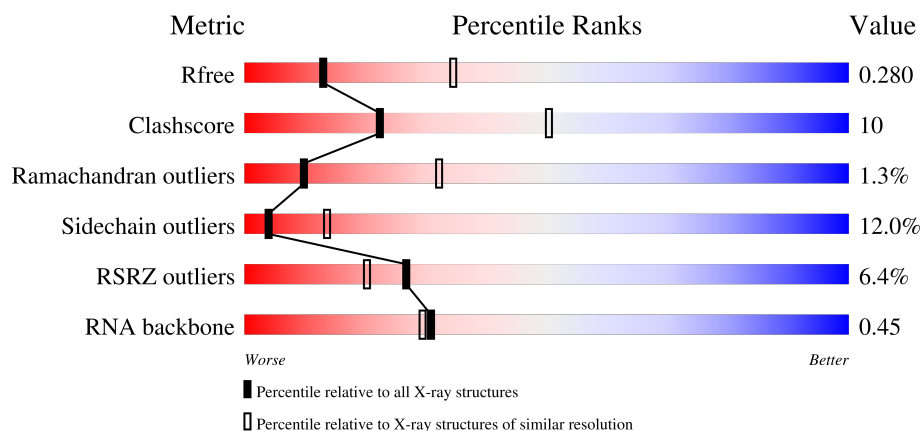
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)
RNA backbone	3690	1037 (3.00-2.60)

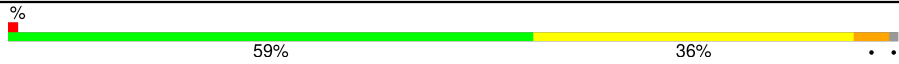
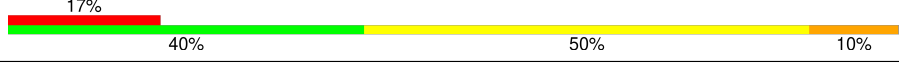
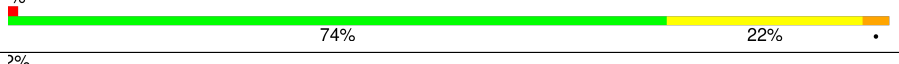


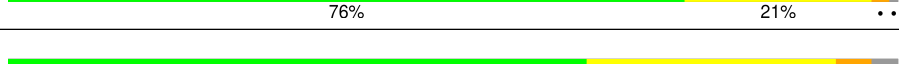

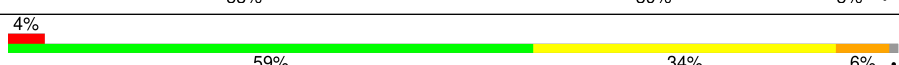



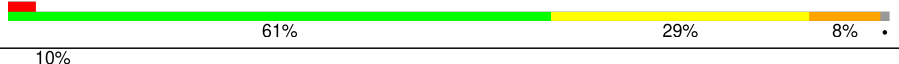
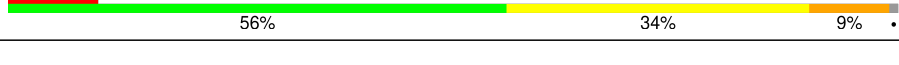

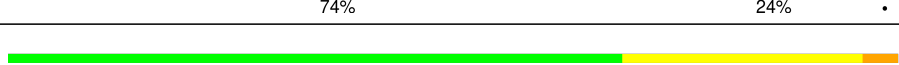










The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>4%</div> <div>59%</div> <div>32%</div> <div>8%</div> </div>
1	2A	2915	<div> <div>3%</div> <div>53%</div> <div>35%</div> <div>8%</div> </div>

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

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Mol	Chain	Length	Quality of chain
2	1B	121	
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	












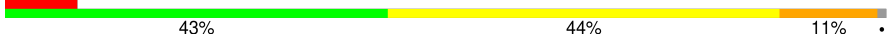

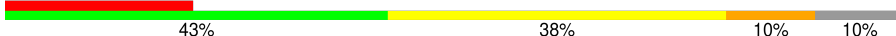











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Mol	Chain	Length	Quality of chain
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	

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Mol	Chain	Length	Quality of chain
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	

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Mol	Chain	Length	Quality of chain
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	

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Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1z	3	
56	2z	3	
57	1y	76	
57	2y	76	

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
58	MG	2A	3715	-	-	-	X
62	SF4	2d	303	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 299377 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	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

- 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
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- 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
			2136	1349	423	361	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
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	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	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	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
			1117	719	207	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			771	495	140	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
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	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
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	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
			588	365	118	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
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	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
			455	285	89	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	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- 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
			1846	1179	331	331	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
			1548	973	301	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
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	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
			1129	714	213	198	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
			810	514	144	149	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
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	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
			1088	689	206	191	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
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- 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
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	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
			829	516	155	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	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	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
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	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
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	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 RNA chain called MET-LYS-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			283	128	59	83	13			
53	2v	13	Total	C	N	O	P	0	0	0
			283	128	59	83	13			

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Lys-tRNAlys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1599	718	282	524	74	1			
54	2w	74	Total	C	N	O	P	S	0	0	0
			1599	718	282	524	74	1			

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMRC-tRNAcys RNA-part.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMRC-tRNAcys Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	3	Total	C	N	O	S	0	0	0
			27	15	6	4	2			
56	2z	3	Total	C	N	O	S	0	0	0
			27	15	6	4	2			

- Molecule 57 is a RNA chain called E-site Deacylated tRNAlys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	1y	74	Total	C	N	O	P	S	0	0	0
			1577	705	277	520	74	1			
57	2y	74	Total	C	N	O	P	S	0	0	0
			1577	705	277	520	74	1			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1080	Total	Mg	0	0
			1080	1080		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	40	Total 40	Mg 40	0	0
58	1D	12	Total 12	Mg 12	0	0
58	1E	12	Total 12	Mg 12	0	0
58	1F	11	Total 11	Mg 11	0	0
58	1G	5	Total 5	Mg 5	0	0
58	1N	6	Total 6	Mg 6	0	0
58	1O	4	Total 4	Mg 4	0	0
58	1P	9	Total 9	Mg 9	0	0
58	1Q	7	Total 7	Mg 7	0	0
58	1R	7	Total 7	Mg 7	0	0
58	1S	1	Total 1	Mg 1	0	0
58	1T	2	Total 2	Mg 2	0	0
58	1U	10	Total 10	Mg 10	0	0
58	1V	8	Total 8	Mg 8	0	0
58	1W	7	Total 7	Mg 7	0	0
58	1X	5	Total 5	Mg 5	0	0
58	1Y	2	Total 2	Mg 2	0	0
58	1Z	3	Total 3	Mg 3	0	0
58	10	11	Total 11	Mg 11	0	0
58	11	5	Total 5	Mg 5	0	0
58	12	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	13	4	Total Mg 4 4	0	0
58	14	1	Total Mg 1 1	0	0
58	15	8	Total Mg 8 8	0	0
58	16	2	Total Mg 2 2	0	0
58	17	7	Total Mg 7 7	0	0
58	18	6	Total Mg 6 6	0	0
58	19	1	Total Mg 1 1	0	0
58	1a	209	Total Mg 209 209	0	0
58	1b	1	Total Mg 1 1	0	0
58	1d	1	Total Mg 1 1	0	0
58	1e	1	Total Mg 1 1	0	0
58	1f	2	Total Mg 2 2	0	0
58	1l	2	Total Mg 2 2	0	0
58	1m	1	Total Mg 1 1	0	0
58	1n	2	Total Mg 2 2	0	0
58	1p	2	Total Mg 2 2	0	0
58	1t	1	Total Mg 1 1	0	0
58	1v	1	Total Mg 1 1	0	0
58	1w	5	Total Mg 5 5	0	0
58	1x	12	Total Mg 12 12	0	0
58	2A	824	Total Mg 824 824	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2B	19	Total 19	Mg 19	0	0
58	2D	8	Total 8	Mg 8	0	0
58	2E	7	Total 7	Mg 7	0	0
58	2F	6	Total 6	Mg 6	0	0
58	2G	1	Total 1	Mg 1	0	0
58	2N	1	Total 1	Mg 1	0	0
58	2O	2	Total 2	Mg 2	0	0
58	2P	2	Total 2	Mg 2	0	0
58	2Q	2	Total 2	Mg 2	0	0
58	2R	2	Total 2	Mg 2	0	0
58	2T	3	Total 3	Mg 3	0	0
58	2U	1	Total 1	Mg 1	0	0
58	2V	2	Total 2	Mg 2	0	0
58	2W	4	Total 4	Mg 4	0	0
58	2X	2	Total 2	Mg 2	0	0
58	2Y	1	Total 1	Mg 1	0	0
58	2Z	1	Total 1	Mg 1	0	0
58	20	2	Total 2	Mg 2	0	0
58	21	4	Total 4	Mg 4	0	0
58	23	3	Total 3	Mg 3	0	0
58	25	3	Total 3	Mg 3	0	0

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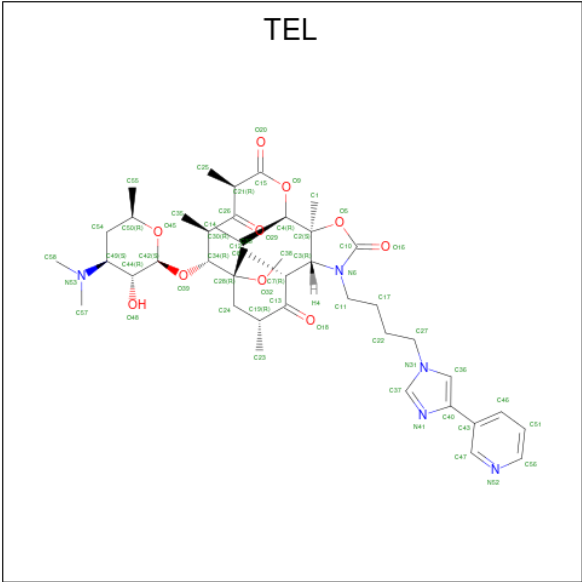
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	27	3	Total 3	Mg 3	0	0
58	28	2	Total 2	Mg 2	0	0
58	2a	211	Total 211	Mg 211	0	0
58	2d	2	Total 2	Mg 2	0	0
58	2e	1	Total 1	Mg 1	0	0
58	2f	1	Total 1	Mg 1	0	0
58	2g	1	Total 1	Mg 1	0	0
58	2j	1	Total 1	Mg 1	0	0
58	2k	1	Total 1	Mg 1	0	0
58	2l	4	Total 4	Mg 4	0	0
58	2q	2	Total 2	Mg 2	0	0
58	2r	1	Total 1	Mg 1	0	0
58	2t	1	Total 1	Mg 1	0	0
58	2v	3	Total 3	Mg 3	0	0
58	2w	2	Total 2	Mg 2	0	0
58	2x	5	Total 5	Mg 5	0	0

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	1	Total 1	K 1	0	0
59	2A	1	Total 1	K 1	0	0

- Molecule 60 is TELITHROMYCIN (CCD ID: TEL) (formula: C₄₃H₆₅N₅O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	1A	1	Total	C	N	O	0	0
			58	43	5	10		
60	2A	1	Total	C	N	O	0	0
			58	43	5	10		

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

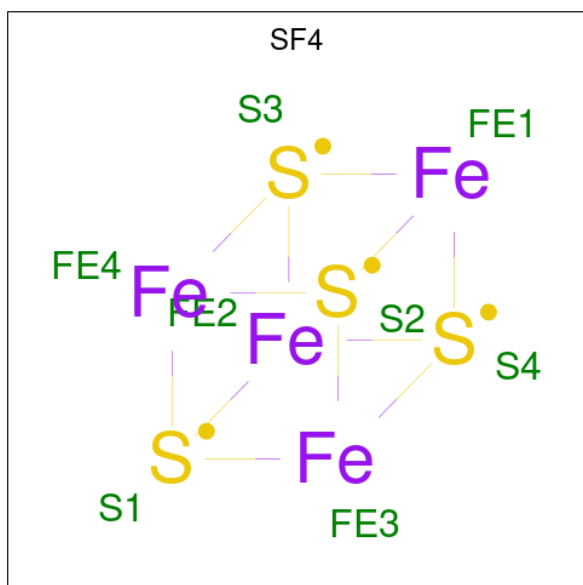
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1Y	1	Total	Zn	0	0
			1	1		
61	14	1	Total	Zn	0	0
			1	1		
61	15	1	Total	Zn	0	0
			1	1		
61	16	1	Total	Zn	0	0
			1	1		
61	19	1	Total	Zn	0	0
			1	1		
61	1n	1	Total	Zn	0	0
			1	1		
61	2Y	1	Total	Zn	0	0
			1	1		
61	24	1	Total	Zn	0	0
			1	1		
61	25	1	Total	Zn	0	0
			1	1		
61	26	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	29	1	Total	Zn	0	0
			1	1		
61	2n	1	Total	Zn	0	0
			1	1		

- Molecule 62 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	1d	1	Total	Fe	S	0	0
			8	4	4		
62	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1A	1780	Total	O	0	0
			1780	1780		
63	1B	57	Total	O	0	0
			57	57		
63	1D	24	Total	O	0	0
			24	24		
63	1E	22	Total	O	0	0
			22	22		
63	1F	14	Total	O	0	0
			14	14		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1G	2	Total	O	0	0
			2	2		
63	1H	2	Total	O	0	0
			2	2		
63	1I	1	Total	O	0	0
			1	1		
63	1N	7	Total	O	0	0
			7	7		
63	1O	4	Total	O	0	0
			4	4		
63	1P	19	Total	O	0	0
			19	19		
63	1Q	6	Total	O	0	0
			6	6		
63	1R	13	Total	O	0	0
			13	13		
63	1S	4	Total	O	0	0
			4	4		
63	1T	11	Total	O	0	0
			11	11		
63	1U	10	Total	O	0	0
			10	10		
63	1V	9	Total	O	0	0
			9	9		
63	1W	10	Total	O	0	0
			10	10		
63	1X	4	Total	O	0	0
			4	4		
63	1Y	1	Total	O	0	0
			1	1		
63	1Z	1	Total	O	0	0
			1	1		
63	10	13	Total	O	0	0
			13	13		
63	11	9	Total	O	0	0
			9	9		
63	12	4	Total	O	0	0
			4	4		
63	13	4	Total	O	0	0
			4	4		
63	15	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	16	2	Total 2	O 2	0	0
63	17	5	Total 5	O 5	0	0
63	18	9	Total 9	O 9	0	0
63	1a	226	Total 226	O 226	0	0
63	1b	1	Total 1	O 1	0	0
63	1e	2	Total 2	O 2	0	0
63	1l	7	Total 7	O 7	0	0
63	1m	1	Total 1	O 1	0	0
63	1n	1	Total 1	O 1	0	0
63	1q	2	Total 2	O 2	0	0
63	1v	5	Total 5	O 5	0	0
63	1w	5	Total 5	O 5	0	0
63	1x	3	Total 3	O 3	0	0
63	1y	1	Total 1	O 1	0	0
63	2A	850	Total 850	O 850	0	0
63	2B	16	Total 16	O 16	0	0
63	2D	18	Total 18	O 18	0	0
63	2E	10	Total 10	O 10	0	0
63	2F	12	Total 12	O 12	0	0
63	2N	1	Total 1	O 1	0	0
63	2O	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2P	1	Total 1	O 1	0	0
63	2Q	1	Total 1	O 1	0	0
63	2R	2	Total 2	O 2	0	0
63	2T	4	Total 4	O 4	0	0
63	2U	2	Total 2	O 2	0	0
63	2W	2	Total 2	O 2	0	0
63	2X	2	Total 2	O 2	0	0
63	2Z	1	Total 1	O 1	0	0
63	20	3	Total 3	O 3	0	0
63	21	5	Total 5	O 5	0	0
63	25	1	Total 1	O 1	0	0
63	27	2	Total 2	O 2	0	0
63	28	2	Total 2	O 2	0	0
63	29	1	Total 1	O 1	0	0
63	2a	148	Total 148	O 148	0	0
63	2d	1	Total 1	O 1	0	0
63	2e	1	Total 1	O 1	0	0
63	2i	1	Total 1	O 1	0	0
63	2l	5	Total 5	O 5	0	0
63	2p	2	Total 2	O 2	0	0
63	2t	2	Total 2	O 2	0	0

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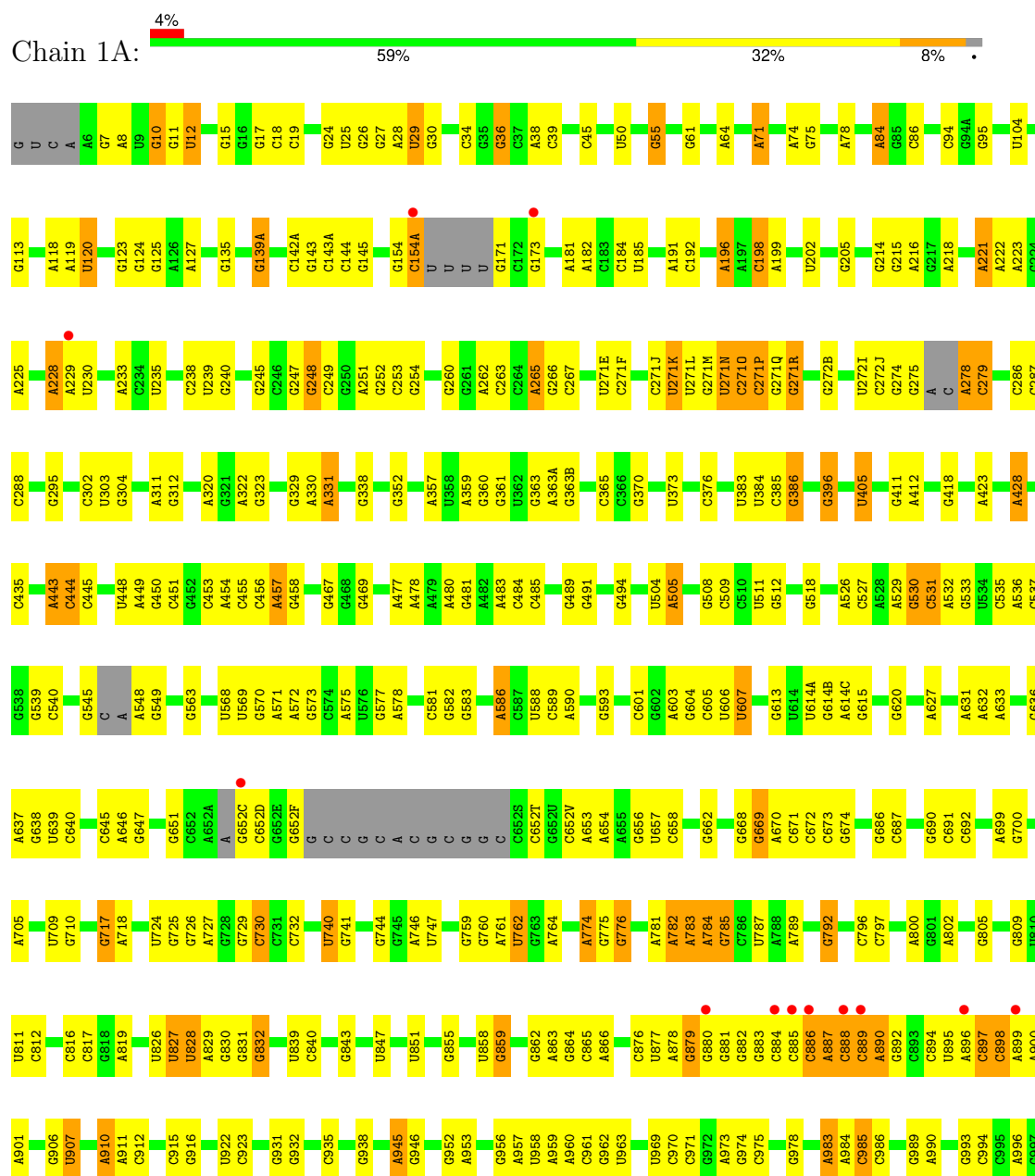
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2v	1	Total	O	0	0
			1	1		
63	2w	4	Total	O	0	0
			4	4		
63	2x	4	Total	O	0	0
			4	4		

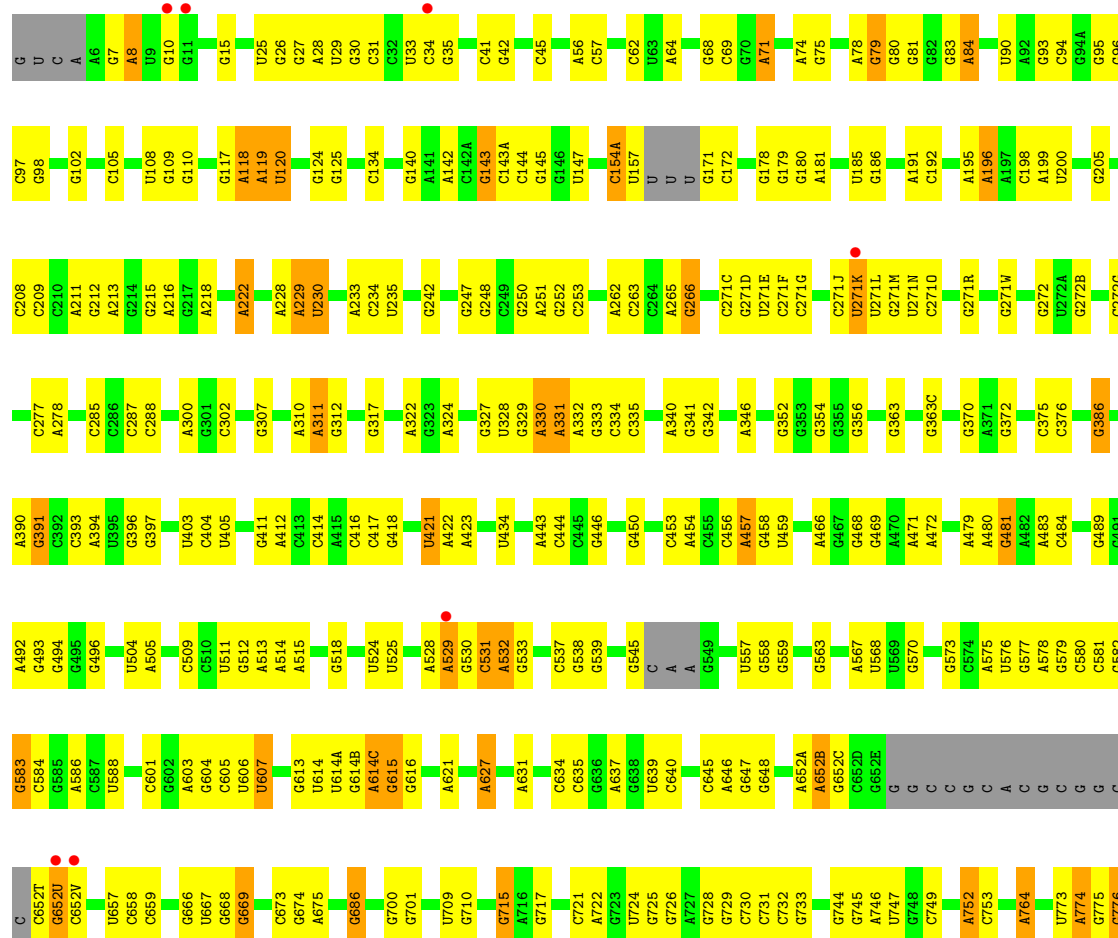
3 Residue-property plots

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.

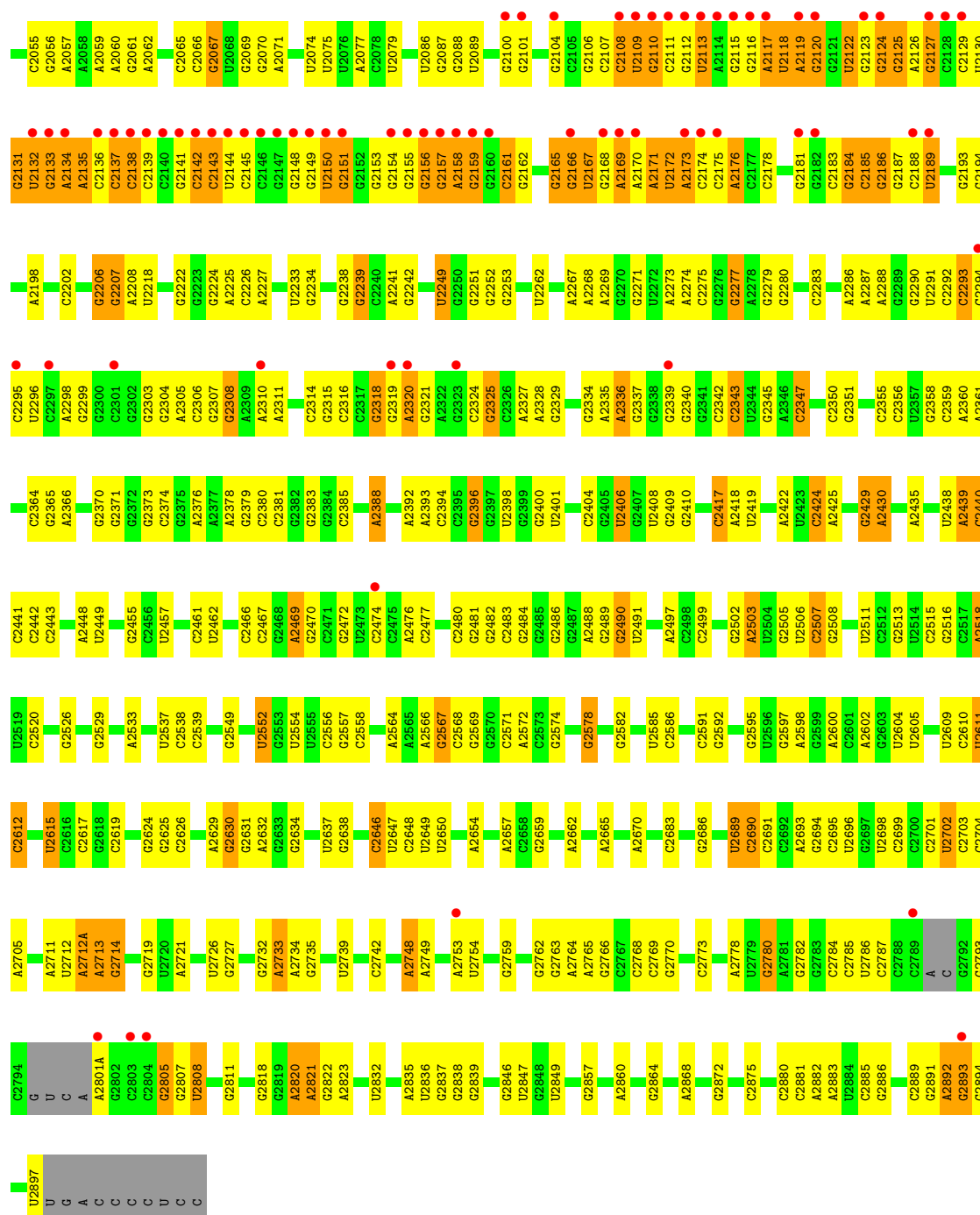
• Molecule 1: 23S Ribosomal RNA



G2308	U2203	C2137	C2063	C1967	G1857	U1757	A1641	A1508	A1393	G1266	U1142	C1071	C999
G2309	C2205	C2138	C2065	G1968	G1858	G1758	G1642	C1509	U1394	A1267	U1142A	C1072	G1003
U2312	G2206	C2140	C2066	A1969	G1865	A1762	G1647	A1509A	U1395	A1268	A1142A	C1073	G1003
C2313	G2207	G2141	G2067	A1970	G1865	G1763	C1648	A1509B	U1396	A1269	A1143	G1074	
C2314	U2208	C2142	U2268	A1972	A1877	G1764	G1649	G1515	C1399	C1270	G1149	G1075	C1007
C2315	U2218	U2143	G2069		G1878		G1650	G1518	U1405	G1271	G1149	C1076	G1068
C2316	G2219	C2144	U2074	C1983	G1878	G1769	G1651	U1518	U1405	A1272		A1077	A1009
C2317	U2075	C2145	U2076	A1986	G1882	G1770	G1651	G1519	U1406	A1273	C1152	A1078	A1010
C2318		G2146			G1883		C1663	G1526	C1407	A1274	C1153	C1079	G1011
C2319		G2147			G1883	A1773	A1664	G1527	U1292	U1081	G1154	C1080	U1012
A2320		G2148	U2079	U1991	G1889		A1665	G1416	U1293	U1082	G1164	U1081	C1013
	G2234	G2149		G1992	A1889	U1777	G1666	C1417	C1293	U1082	U1165	U1082	U1014
G2325	G2235	U2150	U2086	U1993	G1899	U1778	G1667	C1532	C1297	U1083	U1165	U1083	
G2326		G2151	G2087		G1899	U1779	A1668	G		A1084	G1168	A1084	
G2327	G2238	G2152		C1996	A1900	A1780	A1669	U	U1300	A1085	G1168	A1085	
G2328	G2239	G2153	G2093	G1997	G1906	A1783	C1670	A	U1301	A1086	G1170	G1087	G1024
G2329	C2240	G2154	G2094		G1907	A1784	U1671	C	A1301	A1087	G1170	G1087	G1025
G2330	A2241	G2155	U2095	G2012	C1908	A1785	G1674	G1537	G1310	U1088	G1171	A1088	U1026
G2331	G2242	G2157	C2097	A2014	C1908	A1786	G1674	G1539	C1315	U1090	A1174	A1027	A1028
	U2243	A2158	U2098		U1911		G1678	G1543	G1319	G1091	U1175	A1029	G1030
G2334	U2244	G2159	U2099	U2017	G1914	A1789	G1682	C1557	C1320	G1092	A1177	C1092	
A2335	U2245	G2160	G2100		U1915	C1790		C1558	G1431	G1093	C1178	G1093	U1033
A2336	G2246	G2161	G2101	A2020	U1916	A1791	G1686	A1558	U1438	U1094		A1095	U1033
G2337	A2247	G2162	U2102	C2021	U1917	U1794	C1687	A1568	G1325	A1096	G1186	A1096	G1034
	U2248	C2163	C2103	U2022	U1917	G1795	U1688	A1566	G1332	U1097	G1187	U1097	U1035
G2340	U2249	G2164	G2104	G2023	A1918	C1796	U1688	A1567	G1333	A1098	U1188	G1098	G1037
G2341	G2250	G2165	C2105	G2024	A1919	U1796		U1567	G1441	G1099		G1099	C1038
C2342	G2251	G2165	G2106	C2025	C1920	C1797	U1693	G1568	G1442	C1100	C1201	C1100	G1039
C2343	G2252	G2166	G2106		G1921	U1798	C1694	A1569		U1101		U1101	C1040
U2344		U2167	C2107		G1929	G1799	C1695	A1570	A1445	C1102	A1213	C1041	
G2345	G2255	G2168	C2108	U2028	G1930	C1800	G1696	A1571	U1450	A1103		A1103	G1042
A2346	G2259	A2169	U2109	G2029	G1930	G1801	G1697	A1572	G1450	C1218		C1218	C1043
C2347		A2170	G2110	A2030	G1930	A1802	A1698		A1342	U1105	A1226	U1105	G1044
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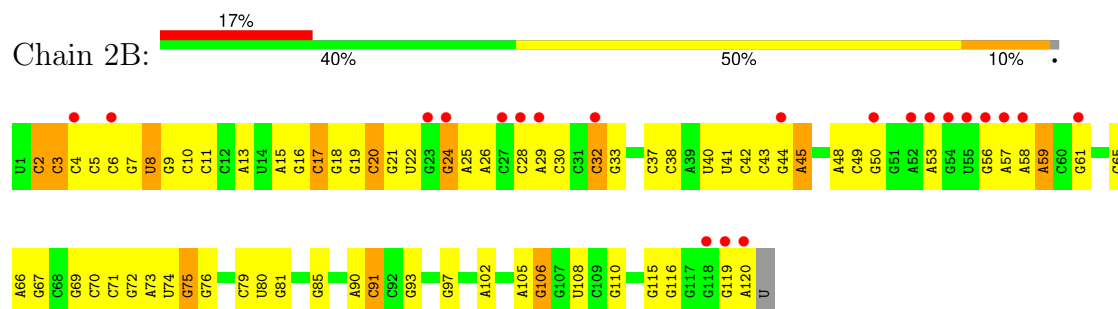
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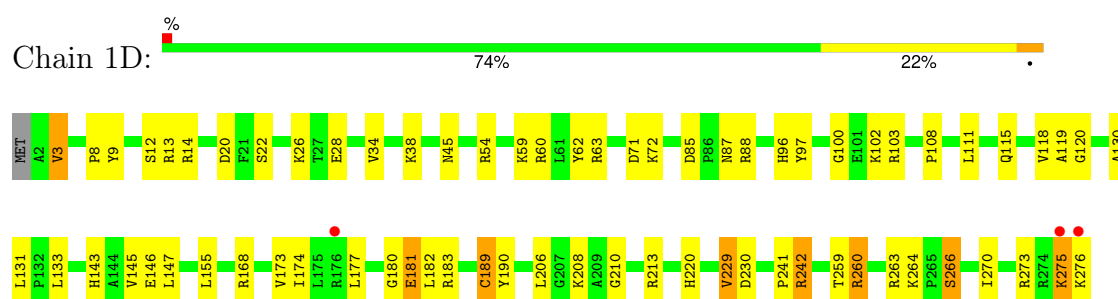
• Molecule 2: 5S Ribosomal RNA



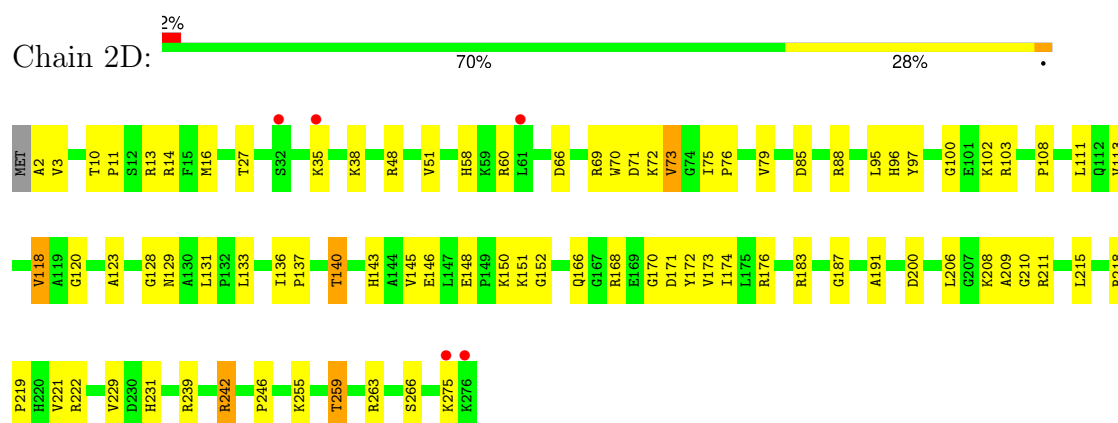
- Molecule 2: 5S Ribosomal RNA



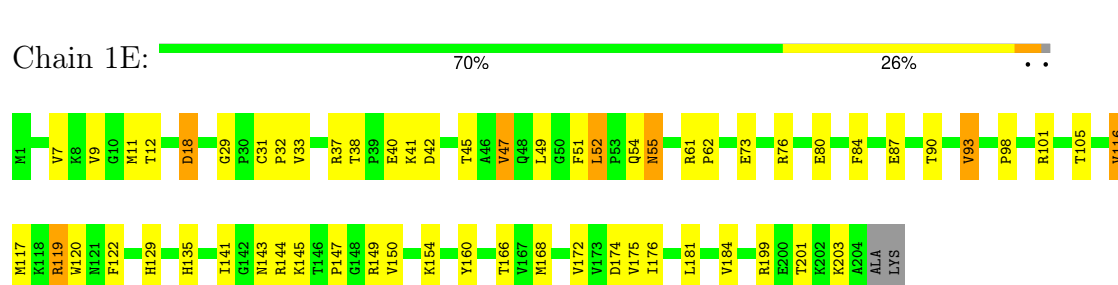
- Molecule 3: 50S ribosomal protein L2



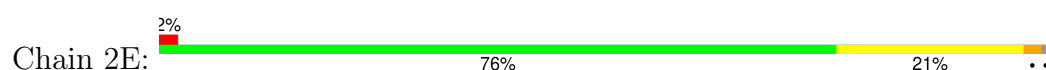
- Molecule 3: 50S ribosomal protein L2

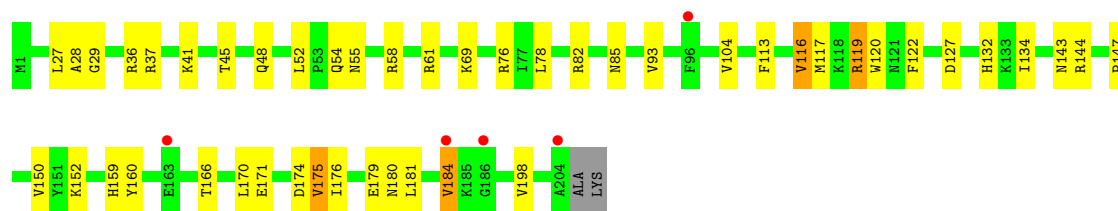


- Molecule 4: 50S ribosomal protein L3



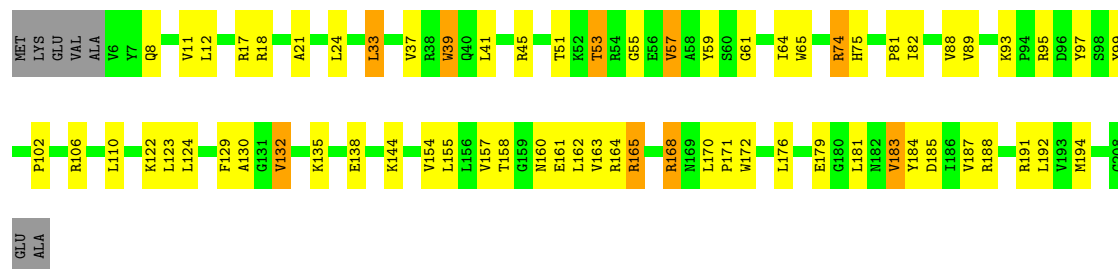
- Molecule 4: 50S ribosomal protein L3





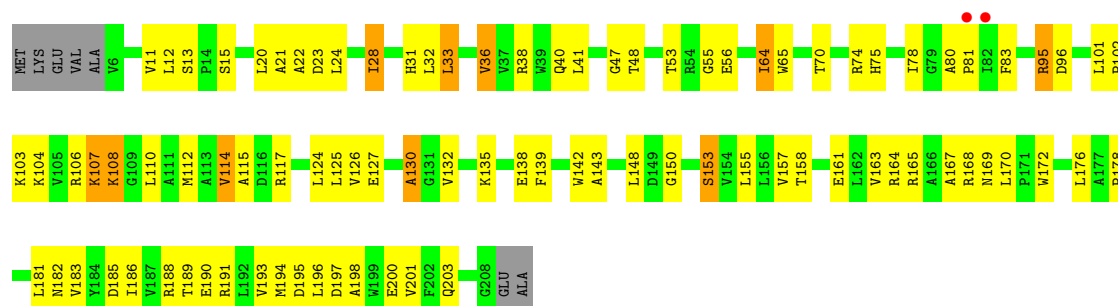
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 65% 28%



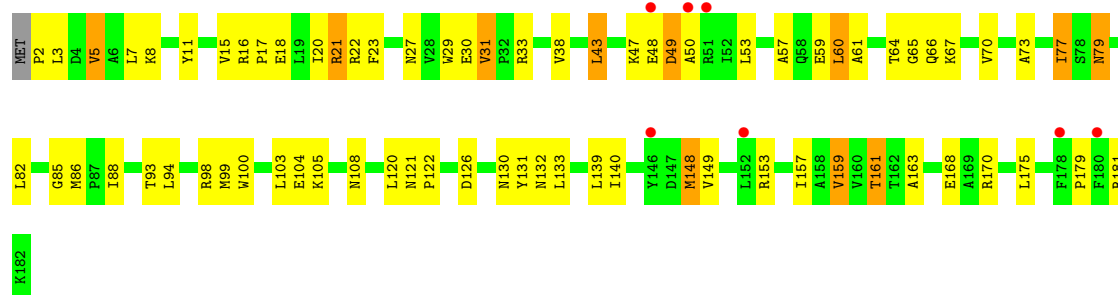
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 53% 39% 5%



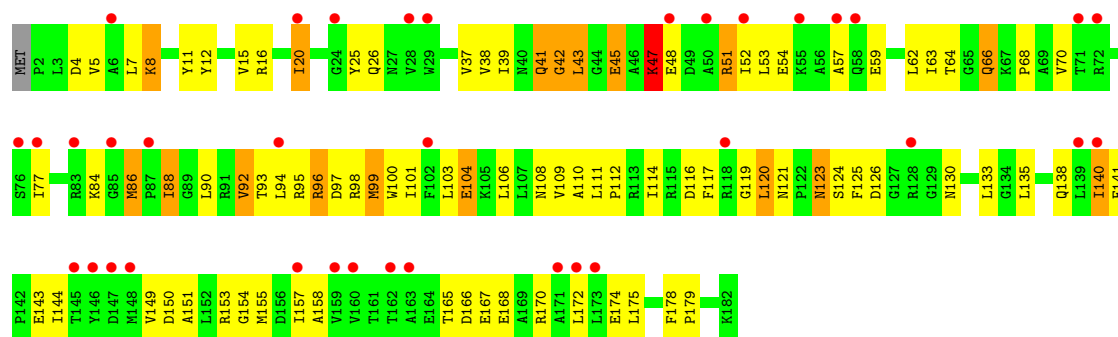
• Molecule 6: 50S ribosomal protein L5

Chain 1G: 59% 34% 6%

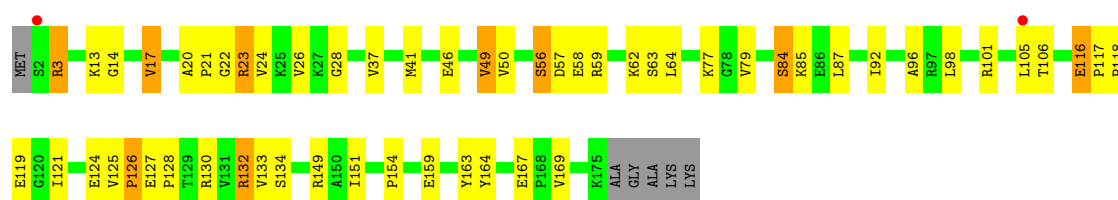


• Molecule 6: 50S ribosomal protein L5

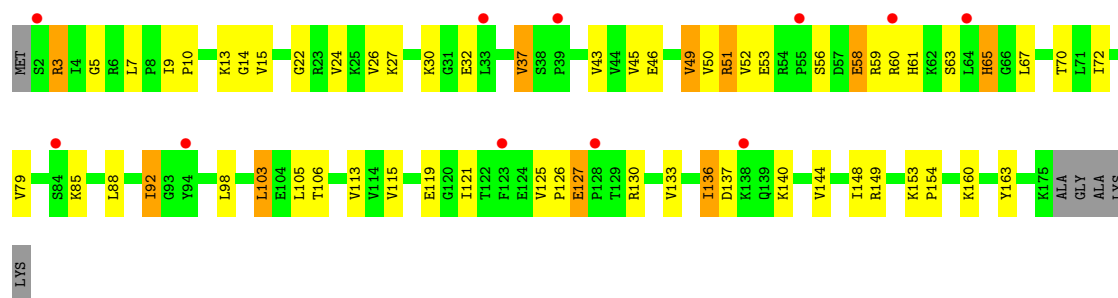
Chain 2G: 49% 40% 9%



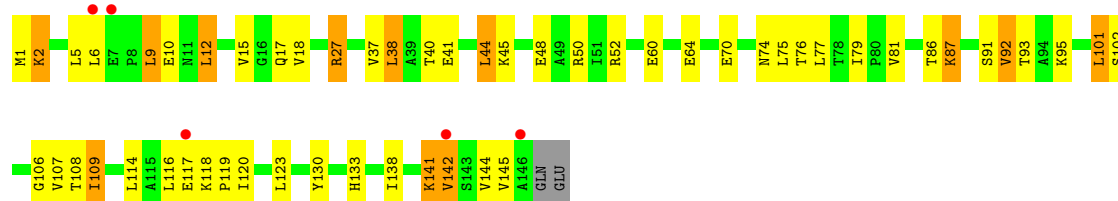
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

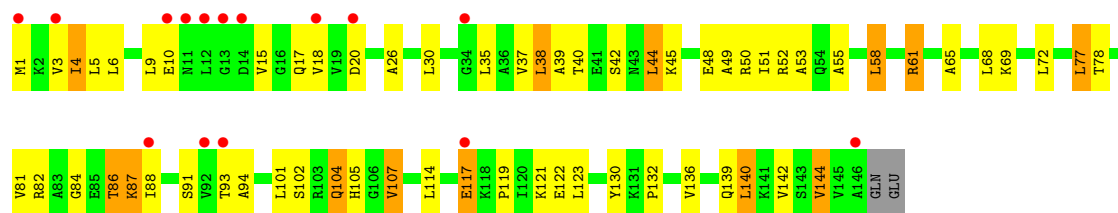


• Molecule 8: 50S ribosomal protein L9

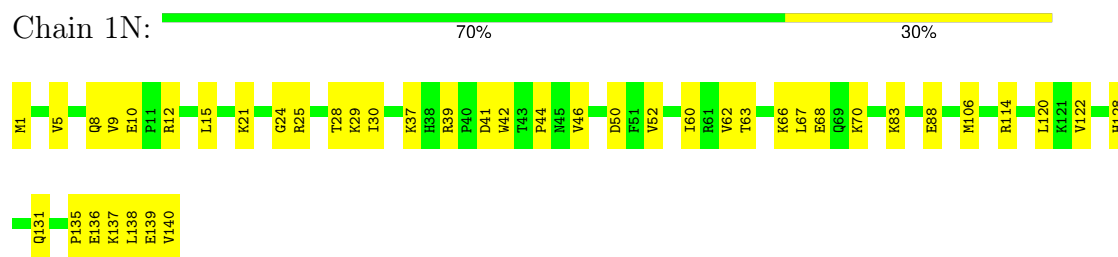


• Molecule 8: 50S ribosomal protein L9

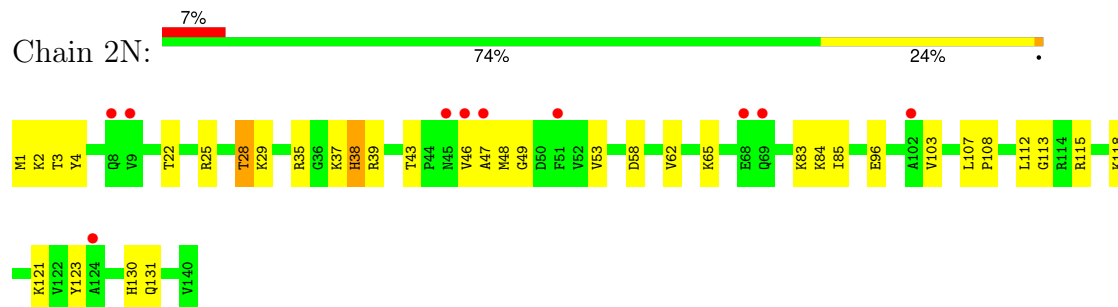




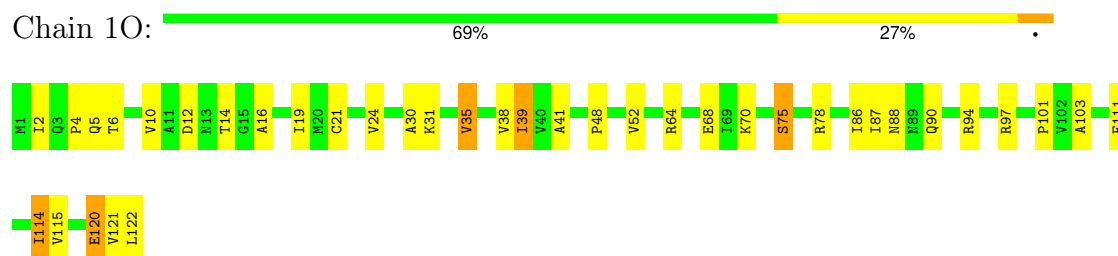
• Molecule 9: 50S ribosomal protein L13



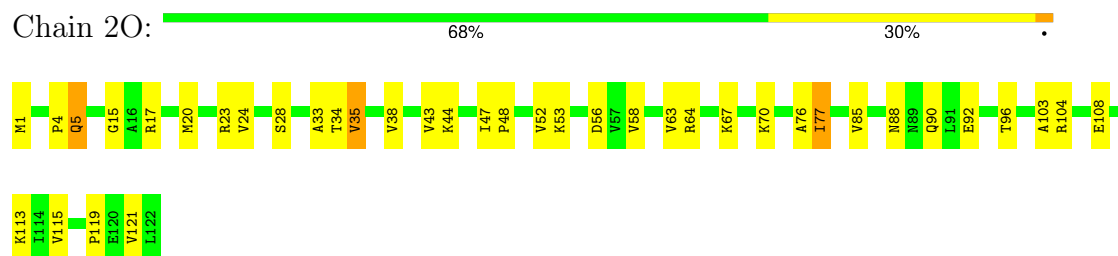
• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14

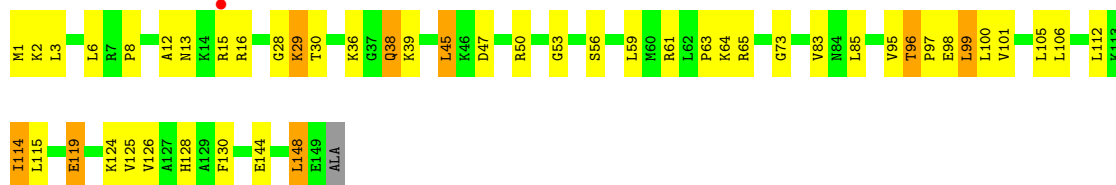


• Molecule 10: 50S ribosomal protein L14



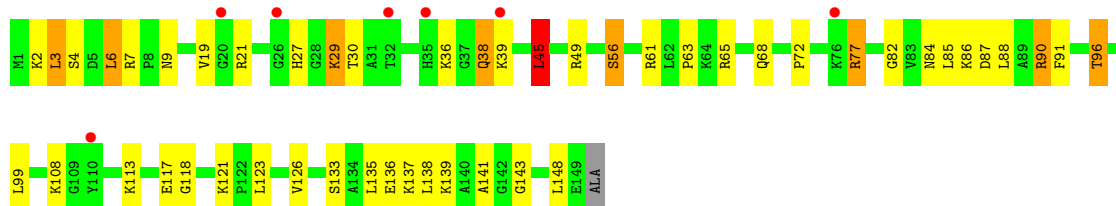
• Molecule 11: 50S ribosomal protein L15

Chain 1P: 



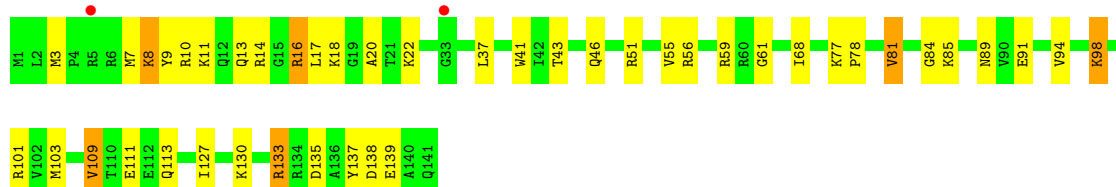
- Molecule 11: 50S ribosomal protein L15

Chain 2P: 



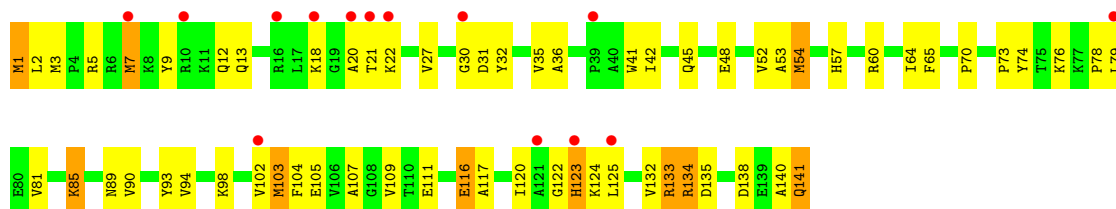
- Molecule 12: 50S ribosomal protein L16

Chain 1Q: 



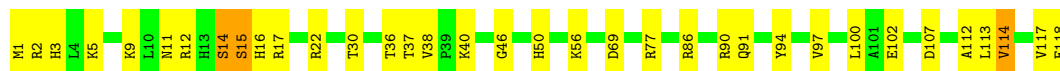
- Molecule 12: 50S ribosomal protein L16

Chain 2Q: 



- Molecule 13: 50S ribosomal protein L17

Chain 1R: 



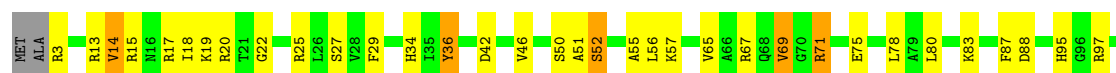
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  70% 30%



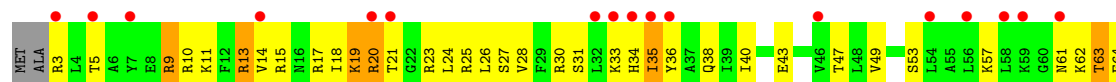
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  63% 29% 5%



- Molecule 14: 50S ribosomal protein L18

Chain 2S:  19% 45% 47% 6%



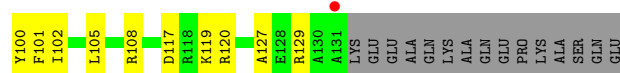
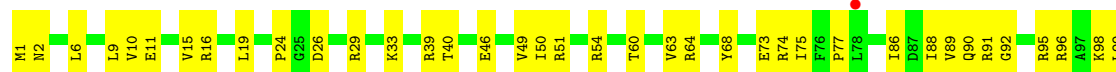
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  56% 33% 10%

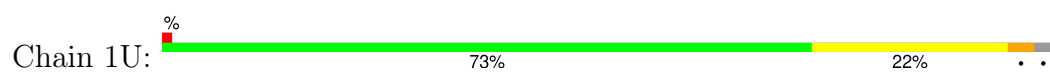


- Molecule 15: 50S ribosomal protein L19

Chain 2T:  57% 33% 10%



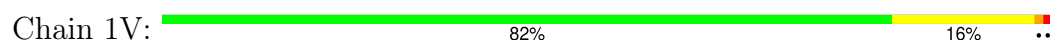
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



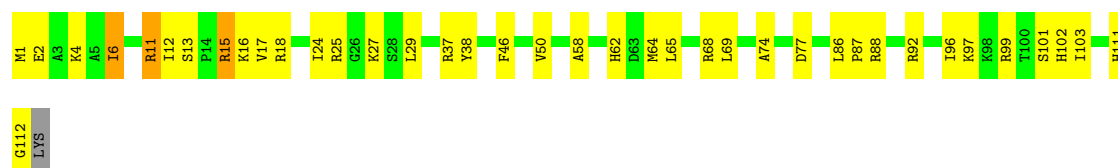
- Molecule 17: 50S ribosomal protein L21



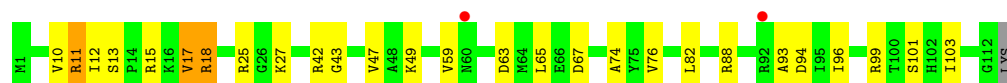
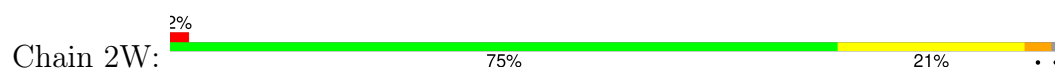
- Molecule 17: 50S ribosomal protein L21



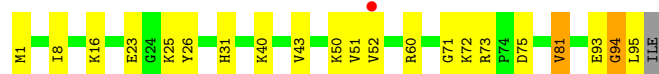
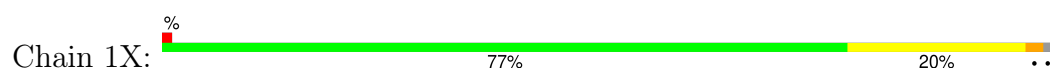
- Molecule 18: 50S ribosomal protein L22



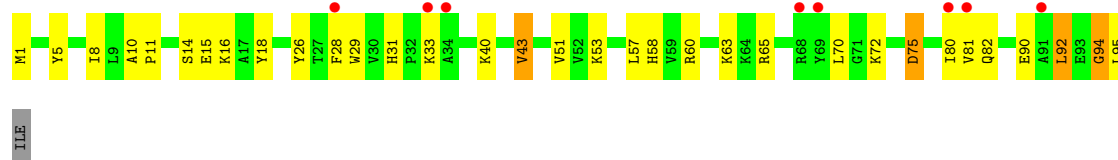
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



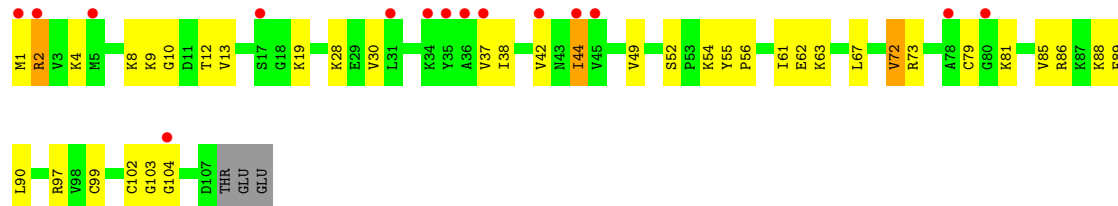
• Molecule 19: 50S ribosomal protein L23



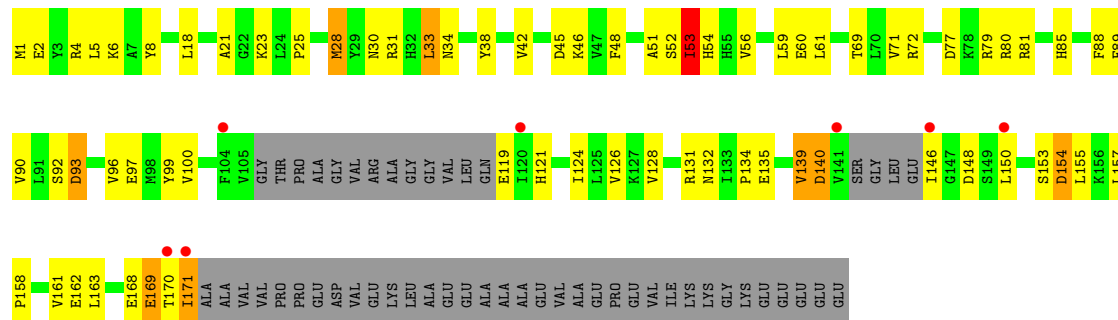
• Molecule 20: 50S ribosomal protein L24



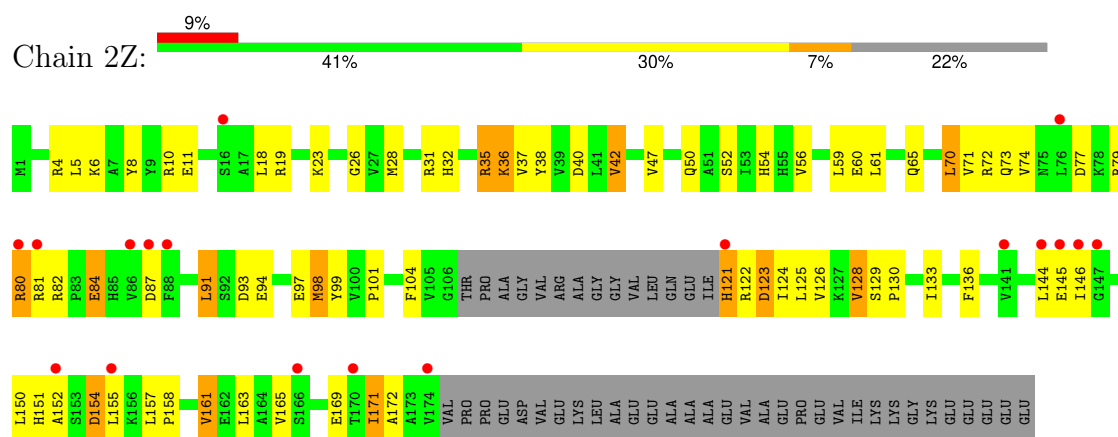
• Molecule 20: 50S ribosomal protein L24



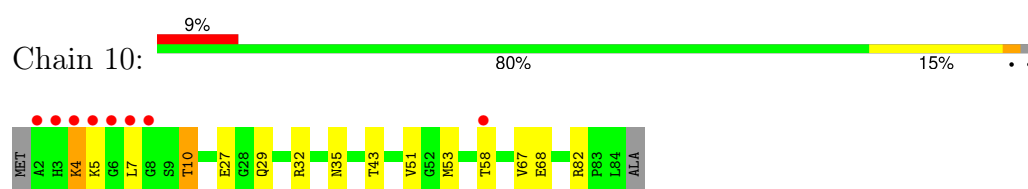
• Molecule 21: 50S ribosomal protein L25



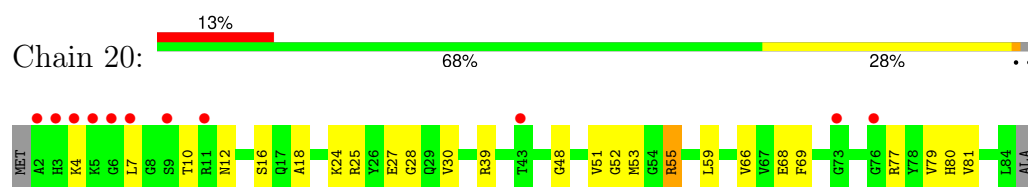
• Molecule 21: 50S ribosomal protein L25



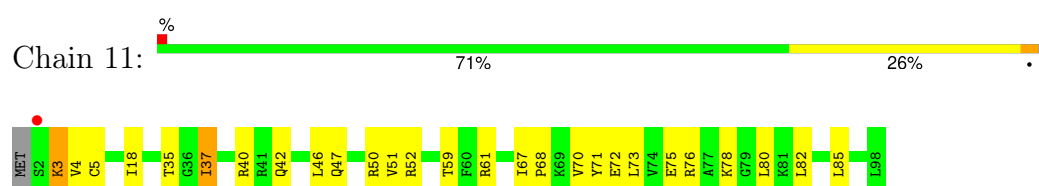
- Molecule 22: 50S ribosomal protein L27



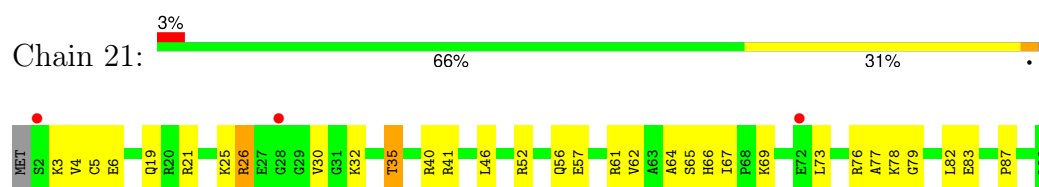
- Molecule 22: 50S ribosomal protein L27



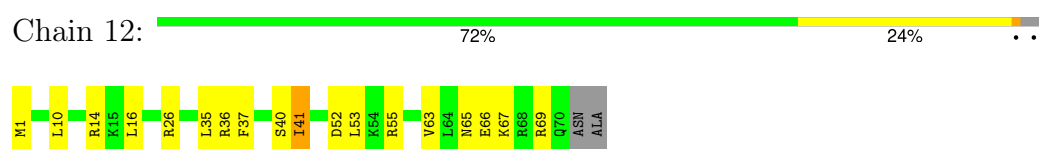
- Molecule 23: 50S ribosomal protein L28



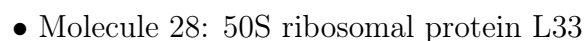
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

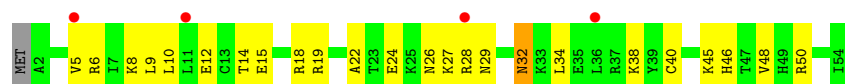


- Molecule 24: 50S ribosomal protein L29





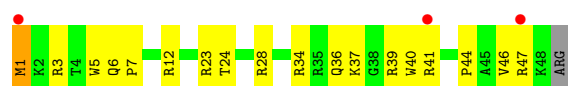
- Molecule 28: 50S ribosomal protein L33



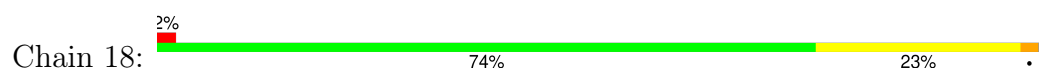
- Molecule 29: 50S ribosomal protein L34



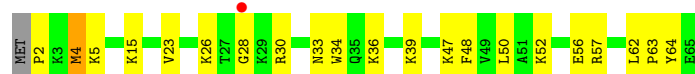
- Molecule 29: 50S ribosomal protein L34



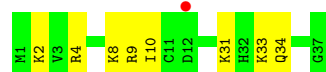
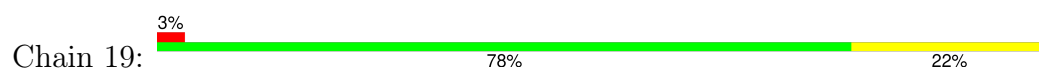
- Molecule 30: 50S ribosomal protein L35



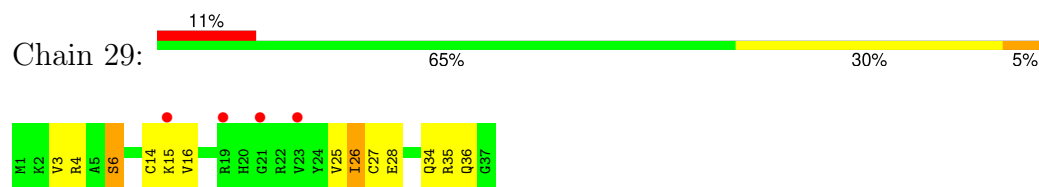
- Molecule 30: 50S ribosomal protein L35



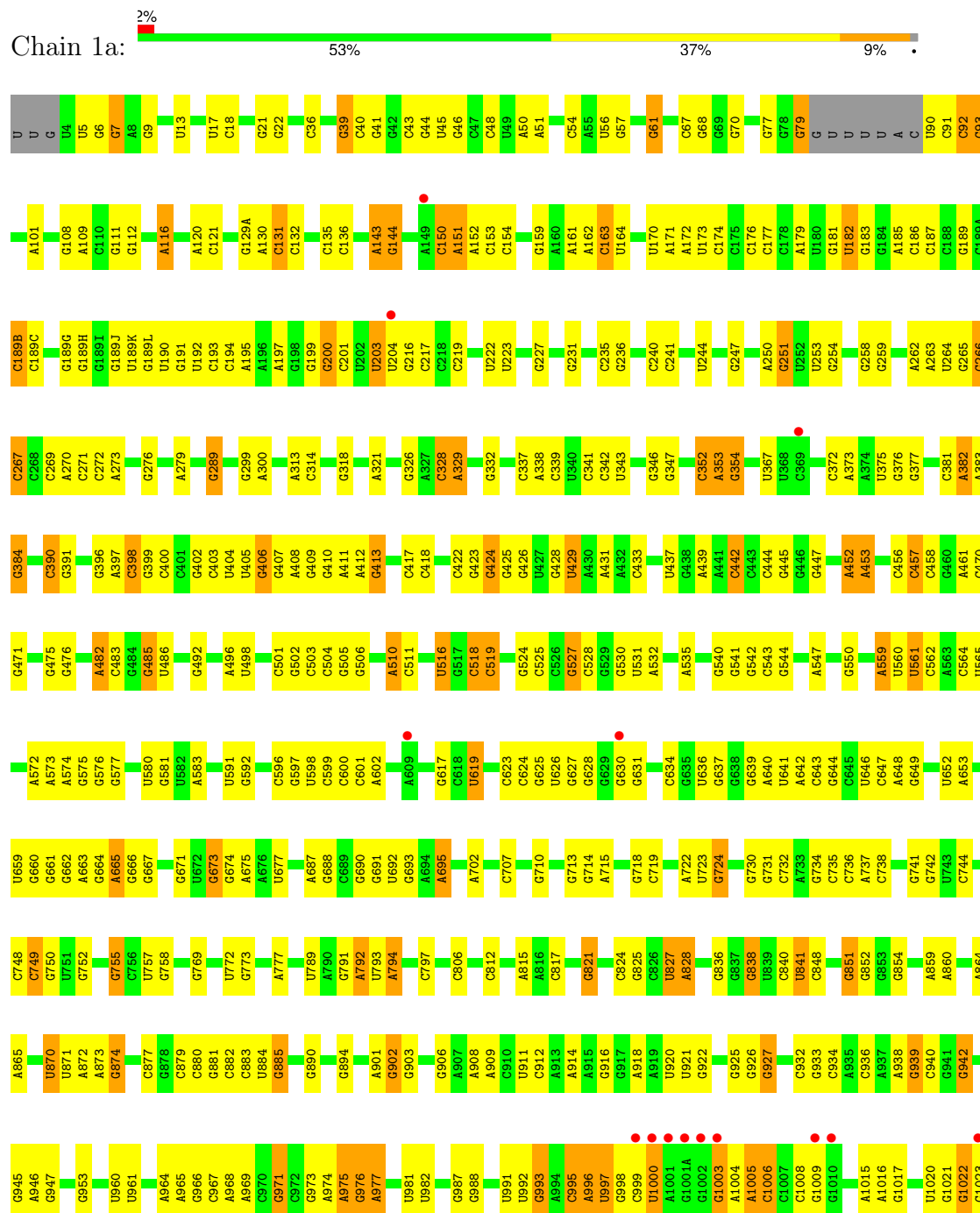
- Molecule 31: 50S ribosomal protein L36



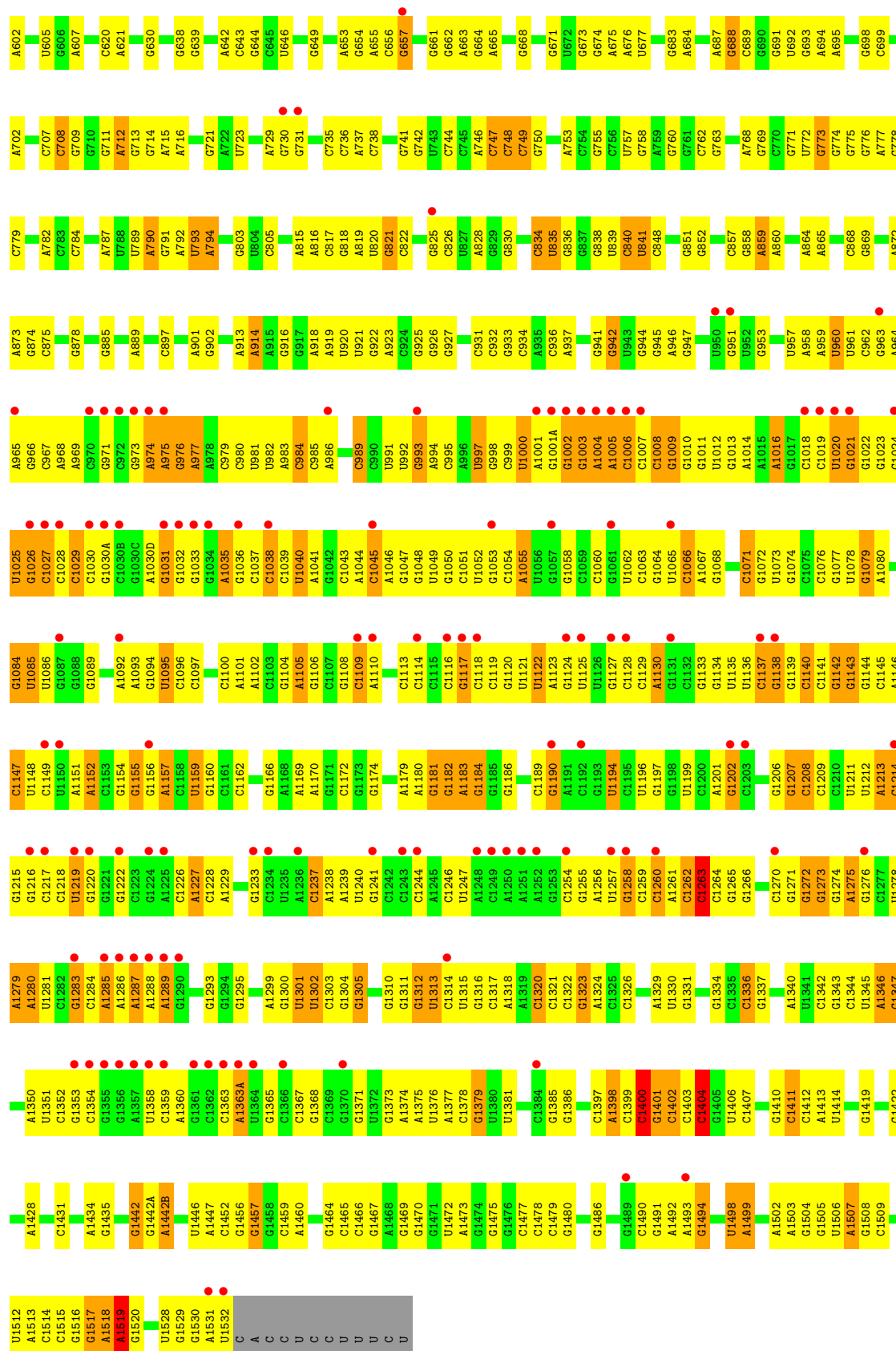
• Molecule 31: 50S ribosomal protein L36

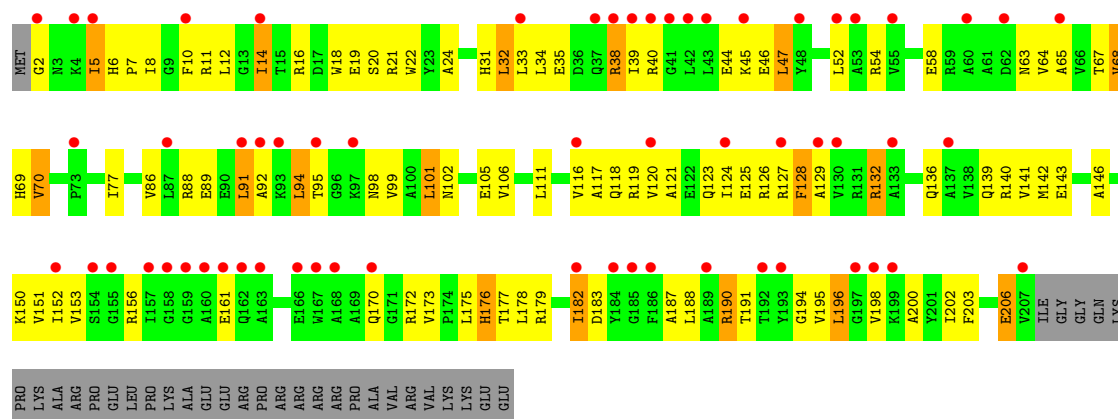


• Molecule 32: 16S Ribosomal RNA

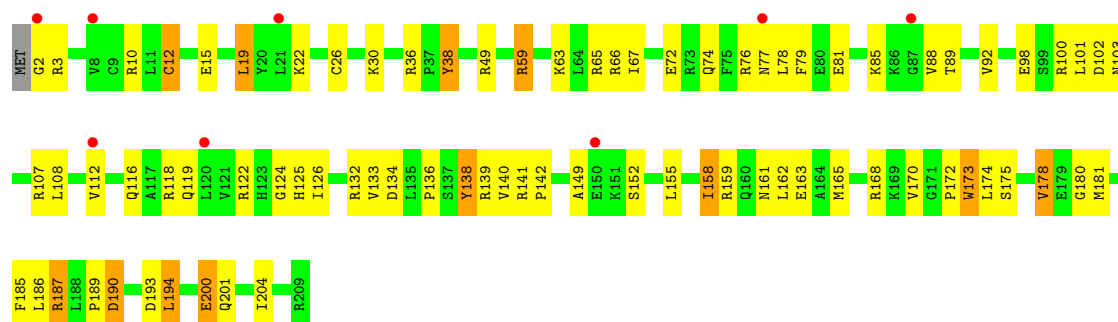




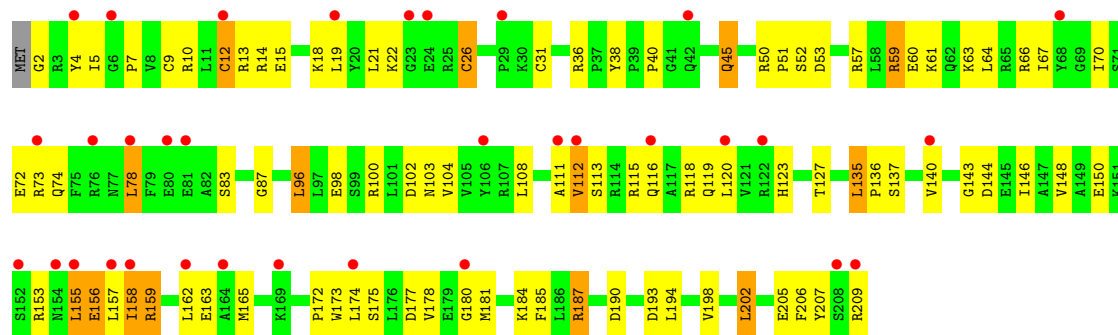




• Molecule 35: 30S ribosomal protein S4



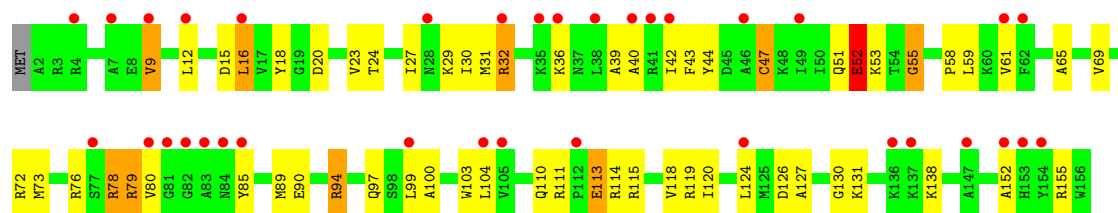
• Molecule 35: 30S ribosomal protein S4



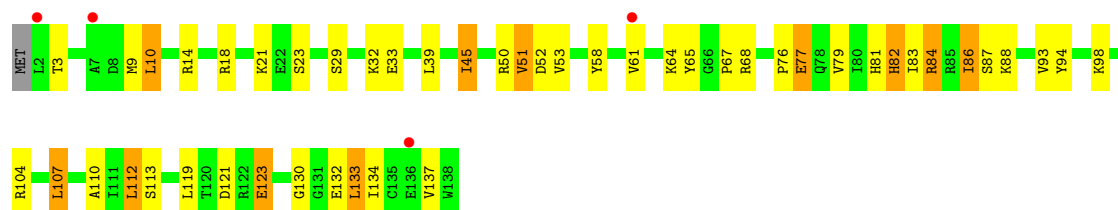
• Molecule 36: 30S ribosomal protein S5



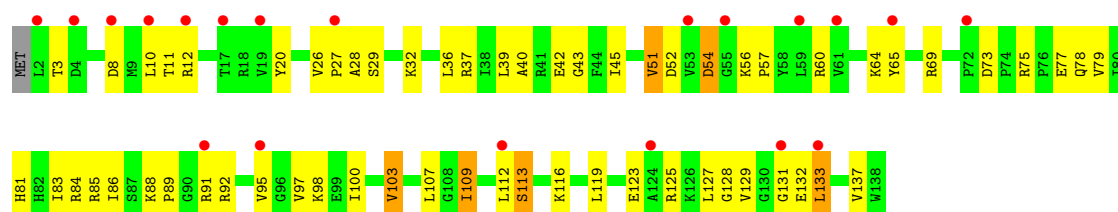




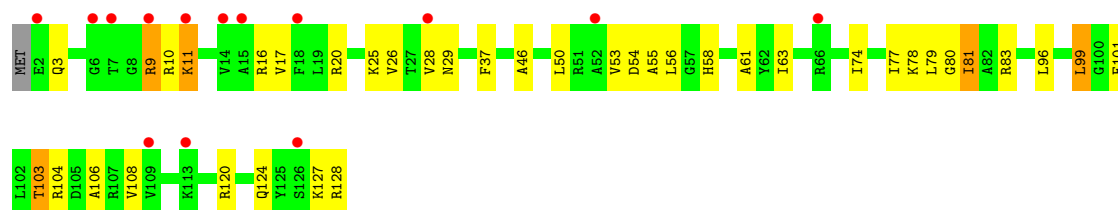
• Molecule 39: 30S ribosomal protein S8



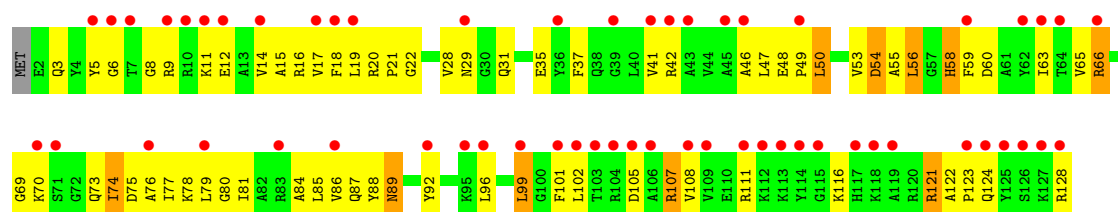
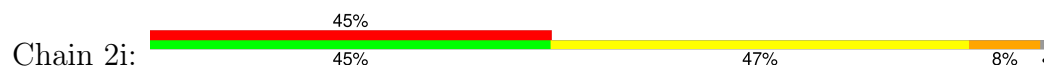
• Molecule 39: 30S ribosomal protein S8



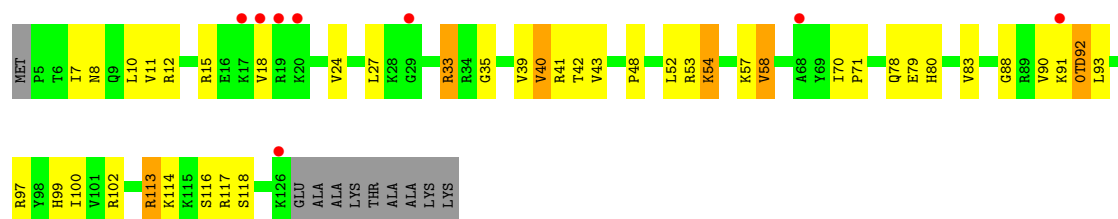
• Molecule 40: 30S ribosomal protein S9



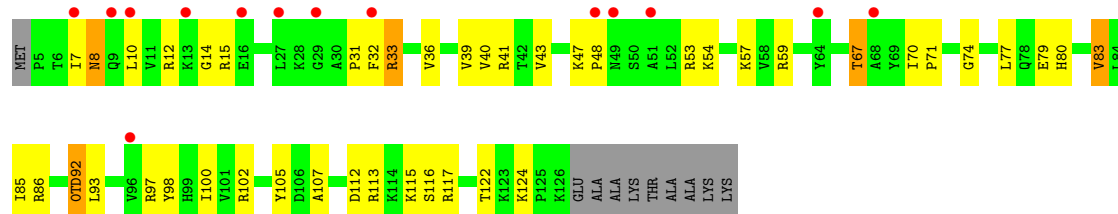
• Molecule 40: 30S ribosomal protein S9



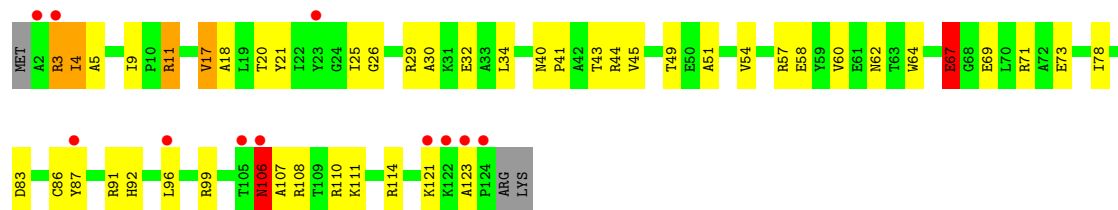
- Chain 11: 



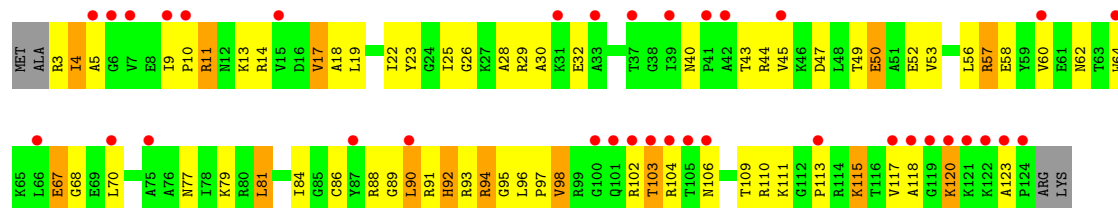
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13



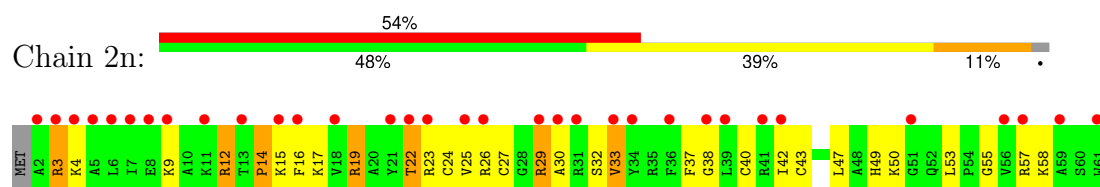
- Molecule 44: 30S ribosomal protein S13



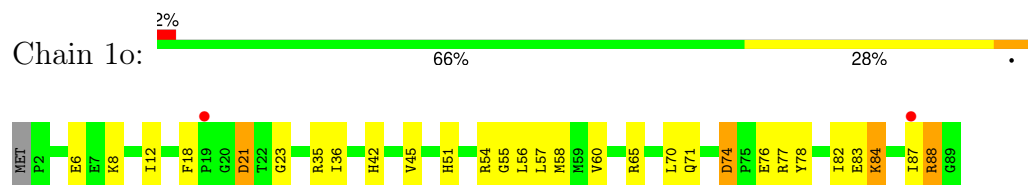
- Molecule 45: 30S ribosomal protein S14 type Z



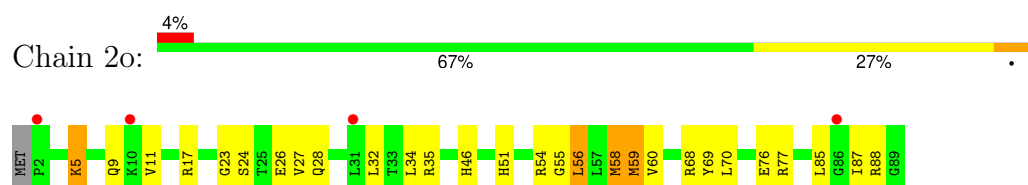
- Molecule 45: 30S ribosomal protein S14 type Z



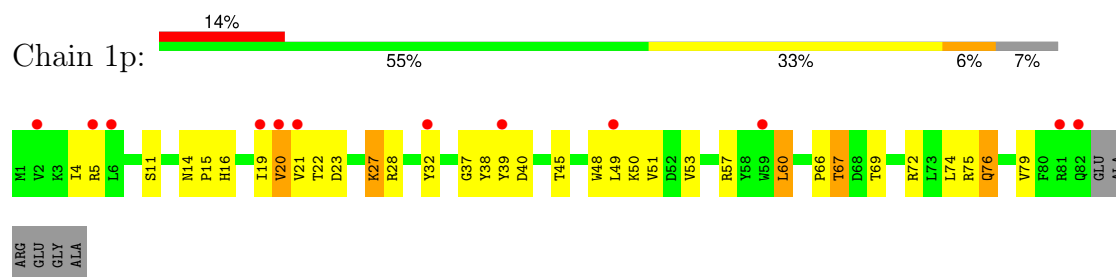
- Molecule 46: 30S ribosomal protein S15



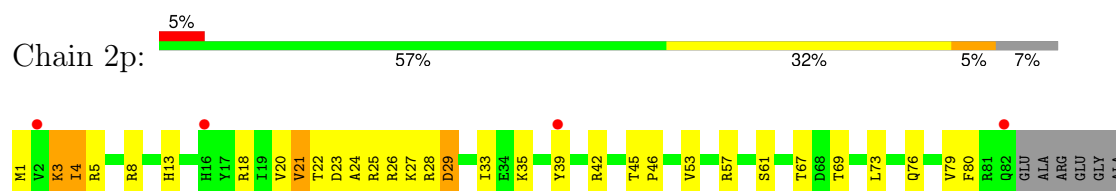
- Molecule 46: 30S ribosomal protein S15



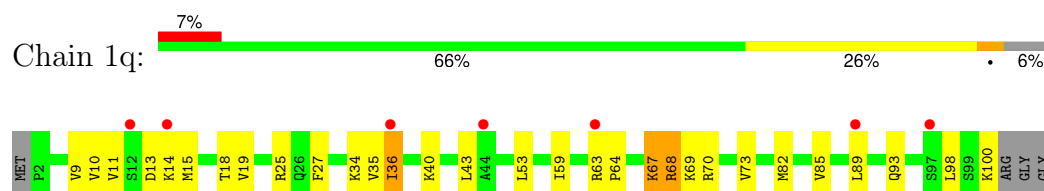
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16

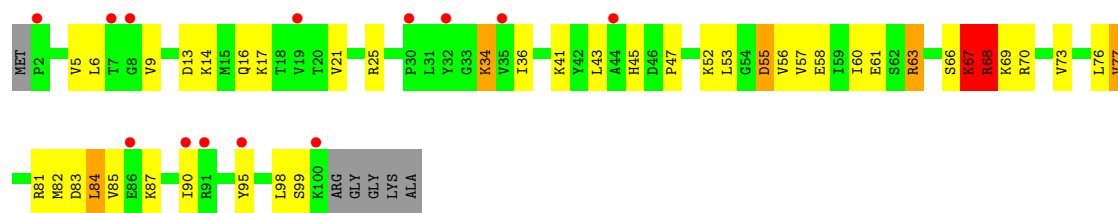


- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17

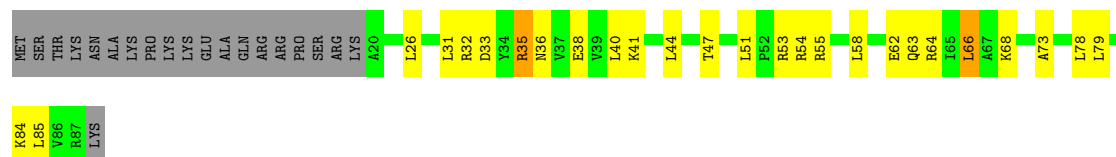




• Molecule 49: 30S ribosomal protein S18



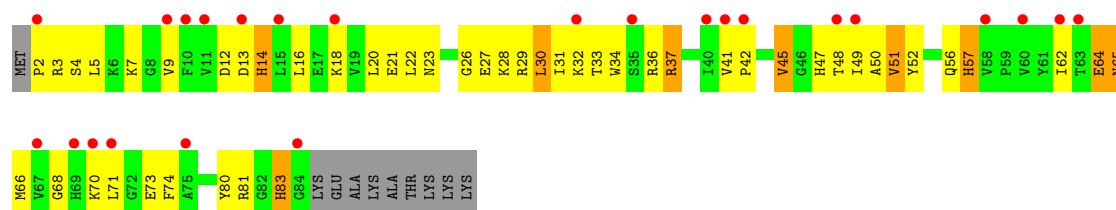
• Molecule 49: 30S ribosomal protein S18



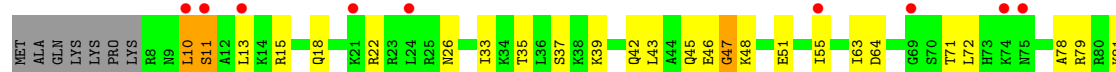
• Molecule 50: 30S ribosomal protein S19



• Molecule 50: 30S ribosomal protein S19

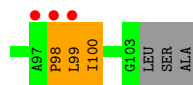


• Molecule 51: 30S ribosomal protein S20

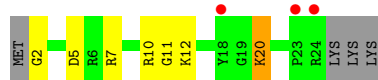




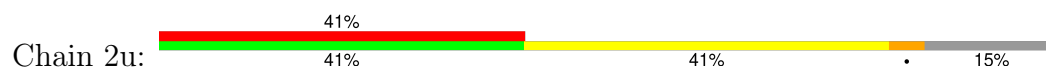
- Molecule 51: 30S ribosomal protein S20



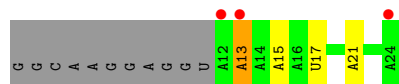
- Molecule 52: 30S ribosomal protein Thx



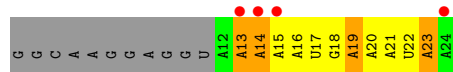
- Molecule 52: 30S ribosomal protein Thx



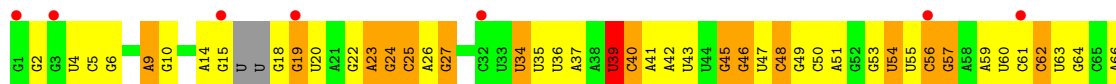
- Molecule 53: MET-LYS-mRNA

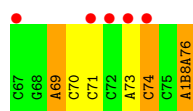


- Molecule 53: MET-LYS-mRNA

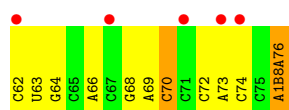
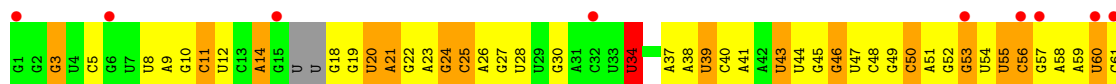


- Molecule 54: A-site Aminoacyl-tRNA Lys-tRNA^{Lys}

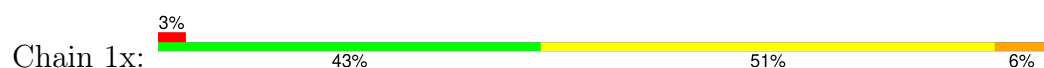




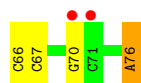
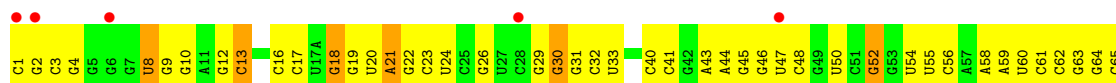
• Molecule 54: A-site Aminoacyl-tRNA Lys-tRNA_{lys}



• Molecule 55: P-site Peptidyl-tRNA fMRC-tRNA_{cys} RNA-part



• Molecule 55: P-site Peptidyl-tRNA fMRC-tRNA_{cys} RNA-part



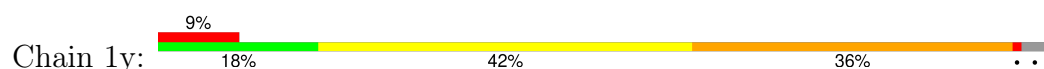
• Molecule 56: P-site Peptidyl-tRNA fMRC-tRNA_{cys} Peptide-part

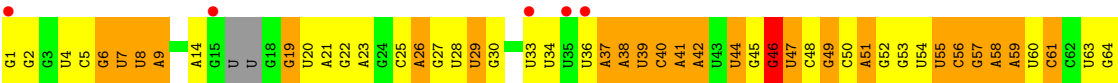


• Molecule 56: P-site Peptidyl-tRNA fMRC-tRNA_{cys} Peptide-part

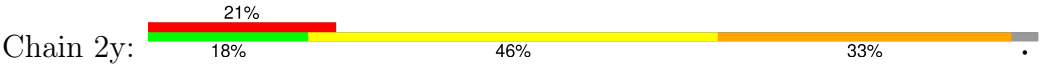


• Molecule 57: E-site Deacylated tRNA_{lys}





• Molecule 57: E-site Deacylated tRNAlys



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.04Å 447.59Å 618.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.58 – 2.80 124.58 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (124.58-2.80) 99.2 (124.58-2.80)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.229 , 0.281 0.229 , 0.280	Depositor DCC
R_{free} test set	70928 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	299377	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FME, G7M, OMU, MA6, 5MU, A1B8A, UR3, 4OC, OMC, M2G, T6A, U8U, TEL, 8AN, K, OMG, SF4, 2MG, 4SU, 2MA, 5MC, PSU, MG, ZN, 0TD

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	0.27	1/69011 (0.0%)	0.46	1/107720 (0.0%)
1	2A	0.21	0/67295	0.40	1/105042 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.19	0/2879	0.38	0/4487
3	1D	0.28	0/2186	0.52	0/2944
3	2D	0.23	0/2186	0.47	0/2944
4	1E	0.26	0/1592	0.50	0/2149
4	2E	0.24	0/1592	0.45	0/2149
5	1F	0.24	0/1619	0.48	0/2193
5	2F	0.21	0/1615	0.47	0/2188
6	1G	0.22	0/1448	0.46	0/1957
6	2G	0.20	0/1453	0.46	0/1963
7	1H	0.22	0/1356	0.41	0/1834
7	2H	0.21	0/1356	0.41	0/1834
8	1I	0.20	0/1112	0.43	0/1514
8	2I	0.19	0/1079	0.40	0/1475
9	1N	0.25	0/1144	0.45	0/1543
9	2N	0.19	0/1144	0.38	0/1543
10	1O	0.25	0/943	0.49	0/1269
10	2O	0.23	0/943	0.48	0/1269
11	1P	0.26	0/1152	0.52	0/1533
11	2P	0.21	0/1152	0.51	0/1533
12	1Q	0.27	0/1143	0.48	0/1527
12	2Q	0.21	0/1143	0.45	0/1527
13	1R	0.26	0/982	0.49	0/1312
13	2R	0.24	0/982	0.53	0/1312
14	1S	0.23	0/883	0.46	0/1176
14	2S	0.20	0/880	0.47	0/1172
15	1T	0.25	0/1105	0.53	1/1477 (0.1%)
15	2T	0.20	0/1097	0.45	0/1468
16	1U	0.26	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.39	0/1301
17	1V	0.24	0/782	0.44	0/1049
17	2V	0.19	0/782	0.42	0/1049
18	1W	0.26	0/897	0.45	0/1205
18	2W	0.22	0/897	0.43	0/1205
19	1X	0.27	0/764	0.55	0/1025
19	2X	0.24	0/764	0.52	0/1025
20	1Y	0.22	0/819	0.48	0/1095
20	2Y	0.21	0/819	0.43	0/1095
21	1Z	0.22	0/1267	0.47	0/1717
21	2Z	0.21	0/1299	0.42	0/1763
22	10	0.25	0/662	0.47	0/881
22	20	0.23	0/662	0.46	0/881
23	11	0.24	0/762	0.43	0/1014
23	21	0.22	0/762	0.44	0/1014
24	12	0.24	0/590	0.45	0/781
24	22	0.20	0/590	0.42	0/781
25	13	0.23	0/474	0.45	0/635
25	23	0.18	0/469	0.39	0/630
26	14	0.22	0/565	0.54	0/761
26	24	0.22	0/545	0.55	0/737
27	15	0.25	0/469	0.51	0/635
27	25	0.23	0/469	0.46	0/635
28	16	0.26	0/460	0.44	0/613
28	26	0.20	0/456	0.40	0/608
29	17	0.26	0/426	0.51	0/561
29	27	0.24	0/426	0.50	0/561
30	18	0.27	0/525	0.49	0/691
30	28	0.21	0/525	0.42	0/691
31	19	0.26	0/310	0.53	0/407
31	29	0.20	0/310	0.40	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.19	1/35886 (0.0%)	0.38	1/56005 (0.0%)
33	1b	0.21	0/1881	0.48	0/2542
33	2b	0.29	1/1860 (0.1%)	0.51	0/2518
34	1c	0.19	0/1572	0.38	0/2126
34	2c	0.25	0/1566	0.51	1/2119 (0.0%)
35	1d	0.20	0/1685	0.44	0/2262
35	2d	0.20	0/1704	0.46	0/2284
36	1e	0.22	0/1145	0.49	0/1543
36	2e	0.21	0/1149	0.49	1/1548 (0.1%)
37	1f	0.22	0/823	0.41	0/1115
37	2f	0.21	0/829	0.40	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.41	0/1679
38	2g	0.19	0/1254	0.44	0/1683
39	1h	0.20	0/1108	0.42	0/1494
39	2h	0.19	0/1108	0.44	0/1494
40	1i	0.21	0/1002	0.50	0/1346
40	2i	0.20	0/997	0.44	0/1343
41	1j	0.19	0/722	0.49	0/982
41	2j	0.22	0/727	0.44	0/988
42	1k	0.20	0/844	0.44	0/1145
42	2k	0.17	0/848	0.42	0/1149
43	1l	0.21	0/937	0.44	0/1260
43	2l	0.21	0/937	0.45	0/1260
44	1m	0.21	0/969	0.47	0/1302
44	2m	0.26	0/961	0.50	0/1291
45	1n	0.18	0/501	0.44	0/664
45	2n	0.20	0/501	0.45	0/664
46	1o	0.19	0/739	0.42	0/985
46	2o	0.19	0/739	0.41	0/985
47	1p	0.21	0/697	0.49	0/939
47	2p	0.21	0/693	0.49	0/935
48	1q	0.18	0/836	0.41	0/1117
48	2q	0.21	0/836	0.47	0/1117
49	1r	0.19	0/560	0.42	0/746
49	2r	0.21	0/560	0.44	0/746
50	1s	0.20	0/667	0.48	0/900
50	2s	0.24	0/661	0.56	0/893
51	1t	0.19	0/730	0.43	0/965
51	2t	0.21	0/729	0.49	0/965
52	1u	0.20	0/203	0.51	0/266
52	2u	0.23	0/203	0.42	0/266
53	1v	0.23	0/319	0.38	0/495
53	2v	0.24	0/319	0.44	0/495
54	1w	0.30	2/1593 (0.1%)	0.38	0/2474
54	2w	0.36	2/1593 (0.1%)	0.54	0/2474
55	1x	0.25	0/1723	0.40	0/2684
55	2x	0.25	1/1723 (0.1%)	0.39	0/2684
56	1z	0.50	0/16	0.68	0/19
56	2z	0.35	0/16	0.79	0/19
57	1y	0.30	0/1618	0.43	0/2513
57	2y	0.32	2/1618 (0.1%)	0.48	0/2513
All	All	0.23	10/316807 (0.0%)	0.43	6/474290 (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
5	2F	0	1
29	27	0	1
33	1b	0	2
All	All	0	4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	10	LEU	CA-C	6.23	1.61	1.52
57	2y	46	G7M	O3'-P	5.51	1.61	1.56
54	2w	46	G7M	O3'-P	5.39	1.61	1.56
54	1w	46	G7M	O3'-P	5.38	1.61	1.56
54	2w	37	T6A	O3'-P	5.26	1.61	1.56

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2c	94	LEU	N-CA-C	-8.65	104.76	114.62
36	2e	109	ILE	N-CA-C	-6.80	104.98	112.80
1	1A	1992	G	C2'-C3'-O3'	6.36	119.04	109.50
1	2A	1992	G	C2'-C3'-O3'	6.10	118.65	109.50
15	1T	129	ARG	N-CA-C	-5.74	106.89	112.97

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	126	GLU	Peptide
33	1b	130	ARG	Peptide
29	27	46	VAL	Peptide
5	2F	20	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31193	700	0
1	2A	60322	0	30424	798	0
2	1B	2577	0	1304	30	0
2	2B	2575	0	1303	56	0
3	1D	2136	0	2218	51	0
3	2D	2136	0	2218	57	0
4	1E	1559	0	1618	40	0
4	2E	1559	0	1618	37	0
5	1F	1584	0	1625	52	0
5	2F	1580	0	1619	61	0
6	1G	1423	0	1436	49	0
6	2G	1428	0	1438	66	0
7	1H	1330	0	1407	28	0
7	2H	1330	0	1407	39	0
8	1I	1097	0	1140	29	0
8	2I	1064	0	1082	34	0
9	1N	1117	0	1184	22	0
9	2N	1117	0	1184	18	0
10	1O	933	0	996	24	0
10	2O	933	0	996	24	0
11	1P	1135	0	1212	37	0
11	2P	1135	0	1212	38	0
12	1Q	1122	0	1179	35	0
12	2Q	1122	0	1179	46	0
13	1R	968	0	1033	22	0
13	2R	968	0	1033	24	0
14	1S	873	0	927	26	0
14	2S	870	0	923	60	0
15	1T	1091	0	1151	33	0
15	2T	1083	0	1136	30	0
16	1U	959	0	1018	22	0
16	2U	959	0	1019	31	0
17	1V	771	0	829	8	0
17	2V	771	0	830	21	0
18	1W	886	0	940	27	0
18	2W	886	0	940	17	0
19	1X	750	0	814	13	0
19	2X	750	0	814	25	0
20	1Y	806	0	881	20	0
20	2Y	806	0	881	22	0
21	1Z	1240	0	1240	39	0
21	2Z	1271	0	1273	49	0
22	10	653	0	674	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	653	0	674	20	0
23	11	755	0	826	17	0
23	21	755	0	826	23	0
24	12	588	0	643	9	0
24	22	588	0	643	22	0
25	13	469	0	518	15	0
25	23	464	0	514	16	0
26	14	552	0	533	18	0
26	24	532	0	503	27	0
27	15	455	0	465	6	0
27	25	455	0	465	10	0
28	16	453	0	473	13	0
28	26	449	0	469	14	0
29	17	418	0	467	11	0
29	27	418	0	467	15	0
30	18	517	0	582	14	0
30	28	517	0	582	18	0
31	19	307	0	335	6	0
31	29	307	0	335	10	0
32	1a	32246	0	16293	454	0
32	2a	32327	0	16338	577	0
33	1b	1846	0	1867	53	0
33	2b	1825	0	1828	81	0
34	1c	1548	0	1535	40	0
34	2c	1542	0	1517	75	0
35	1d	1655	0	1672	56	0
35	2d	1674	0	1713	71	0
36	1e	1129	0	1185	35	0
36	2e	1133	0	1191	47	0
37	1f	810	0	804	16	0
37	2f	816	0	808	17	0
38	1g	1231	0	1238	28	0
38	2g	1235	0	1249	37	0
39	1h	1088	0	1126	30	0
39	2h	1088	0	1126	42	0
40	1i	983	0	986	28	0
40	2i	978	0	966	52	0
41	1j	709	0	650	34	0
41	2j	714	0	672	35	0
42	1k	829	0	825	17	0
42	2k	833	0	834	17	0
43	1l	932	0	981	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	27	0
44	1m	958	0	1002	30	0
44	2m	950	0	988	50	0
45	1n	492	0	529	20	0
45	2n	492	0	529	25	0
46	1o	728	0	760	16	0
46	2o	728	0	760	27	0
47	1p	681	0	697	27	0
47	2p	677	0	686	25	0
48	1q	823	0	891	17	0
48	2q	823	0	891	26	0
49	1r	555	0	618	13	0
49	2r	555	0	618	12	0
50	1s	652	0	662	10	0
50	2s	646	0	644	40	0
51	1t	728	0	798	22	0
51	2t	727	0	796	19	0
52	1u	199	0	208	7	0
52	2u	199	0	208	11	0
53	1v	283	0	141	6	0
53	2v	283	0	141	9	0
54	1w	1599	0	800	31	0
54	2w	1599	0	801	48	0
55	1x	1646	0	839	20	0
55	2x	1646	0	839	32	0
56	1z	27	0	28	1	0
56	2z	27	0	28	5	0
57	1y	1577	0	799	39	0
57	2y	1577	0	798	38	0
58	10	11	0	0	0	0
58	11	5	0	0	0	0
58	12	2	0	0	0	0
58	13	4	0	0	0	0
58	14	1	0	0	0	0
58	15	8	0	0	0	0
58	16	2	0	0	0	0
58	17	7	0	0	0	0
58	18	6	0	0	0	0
58	19	1	0	0	0	0
58	1A	1080	0	0	0	0
58	1B	40	0	0	0	0
58	1D	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1E	12	0	0	0	0
58	1F	11	0	0	0	0
58	1G	5	0	0	0	0
58	1N	6	0	0	0	0
58	1O	4	0	0	0	0
58	1P	9	0	0	0	0
58	1Q	7	0	0	0	0
58	1R	7	0	0	0	0
58	1S	1	0	0	0	0
58	1T	2	0	0	0	0
58	1U	10	0	0	0	0
58	1V	8	0	0	0	0
58	1W	7	0	0	0	0
58	1X	5	0	0	0	0
58	1Y	2	0	0	0	0
58	1Z	3	0	0	0	0
58	1a	209	0	0	0	0
58	1b	1	0	0	0	0
58	1d	1	0	0	0	0
58	1e	1	0	0	0	0
58	1f	2	0	0	0	0
58	1l	2	0	0	0	0
58	1m	1	0	0	0	0
58	1n	2	0	0	0	0
58	1p	2	0	0	0	0
58	1t	1	0	0	0	0
58	1v	1	0	0	0	0
58	1w	5	0	0	0	0
58	1x	12	0	0	0	0
58	20	2	0	0	0	0
58	21	4	0	0	0	0
58	23	3	0	0	0	0
58	25	3	0	0	0	0
58	27	3	0	0	0	0
58	28	2	0	0	0	0
58	2A	824	0	0	0	0
58	2B	19	0	0	0	0
58	2D	8	0	0	0	0
58	2E	7	0	0	0	0
58	2F	6	0	0	0	0
58	2G	1	0	0	0	0
58	2N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2O	2	0	0	0	0
58	2P	2	0	0	0	0
58	2Q	2	0	0	0	0
58	2R	2	0	0	0	0
58	2T	3	0	0	0	0
58	2U	1	0	0	0	0
58	2V	2	0	0	0	0
58	2W	4	0	0	0	0
58	2X	2	0	0	0	0
58	2Y	1	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	211	0	0	0	0
58	2d	2	0	0	0	0
58	2e	1	0	0	0	0
58	2f	1	0	0	0	0
58	2g	1	0	0	0	0
58	2j	1	0	0	0	0
58	2k	1	0	0	0	0
58	2l	4	0	0	0	0
58	2q	2	0	0	1	0
58	2r	1	0	0	0	0
58	2t	1	0	0	0	0
58	2v	3	0	0	0	0
58	2w	2	0	0	0	0
58	2x	5	0	0	0	0
59	1A	1	0	0	0	0
59	2A	1	0	0	0	0
60	1A	58	0	65	4	0
60	2A	58	0	65	4	0
61	14	1	0	0	0	0
61	15	1	0	0	0	0
61	16	1	0	0	0	0
61	19	1	0	0	0	0
61	1Y	1	0	0	0	0
61	1n	1	0	0	0	0
61	24	1	0	0	0	0
61	25	1	0	0	0	0
61	26	1	0	0	0	0
61	29	1	0	0	0	0
61	2Y	1	0	0	0	0
61	2n	1	0	0	0	0
62	1d	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2d	8	0	0	2	0
63	10	13	0	0	1	0
63	11	9	0	0	0	0
63	12	4	0	0	0	0
63	13	4	0	0	0	0
63	15	6	0	0	0	0
63	16	2	0	0	0	0
63	17	5	0	0	0	0
63	18	9	0	0	2	0
63	1A	1780	0	0	101	0
63	1B	57	0	0	3	0
63	1D	24	0	0	1	0
63	1E	22	0	0	3	0
63	1F	14	0	0	3	0
63	1G	2	0	0	0	0
63	1H	2	0	0	0	0
63	1I	1	0	0	0	0
63	1N	7	0	0	0	0
63	1O	4	0	0	0	0
63	1P	19	0	0	1	0
63	1Q	6	0	0	0	0
63	1R	13	0	0	3	0
63	1S	4	0	0	0	0
63	1T	11	0	0	0	0
63	1U	10	0	0	1	0
63	1V	9	0	0	0	0
63	1W	10	0	0	2	0
63	1X	4	0	0	0	0
63	1Y	1	0	0	0	0
63	1Z	1	0	0	0	0
63	1a	226	0	0	22	0
63	1b	1	0	0	0	0
63	1e	2	0	0	0	0
63	1l	7	0	0	0	0
63	1m	1	0	0	0	0
63	1n	1	0	0	0	0
63	1q	2	0	0	0	0
63	1v	5	0	0	0	0
63	1w	5	0	0	1	0
63	1x	3	0	0	0	0
63	1y	1	0	0	1	0
63	20	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	21	5	0	0	1	0
63	25	1	0	0	1	0
63	27	2	0	0	0	0
63	28	2	0	0	1	0
63	29	1	0	0	0	0
63	2A	850	0	0	79	0
63	2B	16	0	0	1	0
63	2D	18	0	0	2	0
63	2E	10	0	0	1	0
63	2F	12	0	0	0	0
63	2N	1	0	0	0	0
63	2O	1	0	0	0	0
63	2P	1	0	0	0	0
63	2Q	1	0	0	0	0
63	2R	2	0	0	0	0
63	2T	4	0	0	0	0
63	2U	2	0	0	0	0
63	2W	2	0	0	0	0
63	2X	2	0	0	0	0
63	2Z	1	0	0	0	0
63	2a	148	0	0	21	0
63	2d	1	0	0	0	0
63	2e	1	0	0	0	0
63	2i	1	0	0	0	0
63	2l	5	0	0	0	0
63	2p	2	0	0	0	0
63	2t	2	0	0	0	0
63	2v	1	0	0	0	0
63	2w	4	0	0	1	0
63	2x	4	0	0	0	0
All	All	299377	0	196882	4932	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 4932 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	1.23	1.34
54:2w:51:A:N6	54:2w:63:U:H3	1.46	1.14
57:2y:10:G:H1	57:2y:25:C:N4	1.47	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2503:2MA:H8	56:2z:2:ARG:HH12	1.17	1.04
54:2w:51:A:H3'	54:2w:64:G:H21	1.17	1.03

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%)	246 (90%)	25 (9%)	2 (1%)	19	48
3	2D	273/276 (99%)	245 (90%)	28 (10%)	0	100	100
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	25	56
4	2E	202/206 (98%)	182 (90%)	17 (8%)	3 (2%)	8	29
5	1F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	25	56
5	2F	201/210 (96%)	186 (92%)	13 (6%)	2 (1%)	13	39
6	1G	179/182 (98%)	152 (85%)	25 (14%)	2 (1%)	12	37
6	2G	179/182 (98%)	155 (87%)	18 (10%)	6 (3%)	3	11
7	1H	172/180 (96%)	158 (92%)	13 (8%)	1 (1%)	22	51
7	2H	172/180 (96%)	149 (87%)	21 (12%)	2 (1%)	11	34
8	1I	144/148 (97%)	123 (85%)	20 (14%)	1 (1%)	19	48
8	2I	144/148 (97%)	119 (83%)	22 (15%)	3 (2%)	5	20
9	1N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
9	2N	138/140 (99%)	122 (88%)	14 (10%)	2 (1%)	9	30
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	103 (86%)	15 (12%)	2 (2%)	7	26
11	1P	147/150 (98%)	130 (88%)	14 (10%)	3 (2%)	6	21
11	2P	147/150 (98%)	124 (84%)	19 (13%)	4 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	4 (3%)	1 (1%)	14	42
13	2R	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	14	42
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	93 (86%)	11 (10%)	4 (4%)	2	9
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	116 (90%)	11 (8%)	2 (2%)	8	27
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	6	21
17	2V	99/101 (98%)	87 (88%)	10 (10%)	2 (2%)	6	21
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	12	37
19	2X	93/96 (97%)	83 (89%)	8 (9%)	2 (2%)	5	20
20	1Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
21	1Z	148/206 (72%)	129 (87%)	14 (10%)	5 (3%)	3	11
21	2Z	156/206 (76%)	128 (82%)	22 (14%)	6 (4%)	2	9
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	73 (90%)	7 (9%)	1 (1%)	11	34
23	11	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
23	21	95/98 (97%)	88 (93%)	6 (6%)	1 (1%)	12	37
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
24	22	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	7	24
26	14	67/71 (94%)	49 (73%)	15 (22%)	3 (4%)	2	7
26	24	67/71 (94%)	47 (70%)	17 (25%)	3 (4%)	2	7
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	25	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	45 (88%)	5 (10%)	1 (2%)	6	21
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%)	60 (97%)	2 (3%)	0	100	100
30	28	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	30 (86%)	5 (14%)	0	100	100
33	1b	229/256 (90%)	195 (85%)	26 (11%)	8 (4%)	3	10
33	2b	229/256 (90%)	177 (77%)	45 (20%)	7 (3%)	3	12
34	1c	204/239 (85%)	184 (90%)	19 (9%)	1 (0%)	25	56
34	2c	204/239 (85%)	170 (83%)	32 (16%)	2 (1%)	13	39
35	1d	206/209 (99%)	180 (87%)	24 (12%)	2 (1%)	13	39
35	2d	206/209 (99%)	176 (85%)	29 (14%)	1 (0%)	25	56
36	1e	146/162 (90%)	130 (89%)	12 (8%)	4 (3%)	4	15
36	2e	146/162 (90%)	128 (88%)	14 (10%)	4 (3%)	4	15
37	1f	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	13	39
37	2f	98/101 (97%)	90 (92%)	8 (8%)	0	100	100
38	1g	153/156 (98%)	130 (85%)	22 (14%)	1 (1%)	19	48
38	2g	153/156 (98%)	133 (87%)	16 (10%)	4 (3%)	4	16
39	1h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
39	2h	135/138 (98%)	118 (87%)	16 (12%)	1 (1%)	19	48
40	1i	125/128 (98%)	109 (87%)	14 (11%)	2 (2%)	8	27
40	2i	125/128 (98%)	106 (85%)	17 (14%)	2 (2%)	8	27
41	1j	95/105 (90%)	78 (82%)	11 (12%)	6 (6%)	1	3
41	2j	94/105 (90%)	77 (82%)	14 (15%)	3 (3%)	3	12
42	1k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	7	24
42	2k	112/129 (87%)	96 (86%)	14 (12%)	2 (2%)	7	24
43	1l	119/132 (90%)	108 (91%)	10 (8%)	1 (1%)	16	44
43	2l	119/132 (90%)	107 (90%)	10 (8%)	2 (2%)	7	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	1m	121/126 (96%)	104 (86%)	15 (12%)	2 (2%)	7	26
44	2m	120/126 (95%)	100 (83%)	19 (16%)	1 (1%)	16	44
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	26
46	1o	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	11	34
46	2o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
47	1p	80/88 (91%)	68 (85%)	12 (15%)	0	100	100
47	2p	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
48	1q	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
48	2q	97/105 (92%)	85 (88%)	10 (10%)	2 (2%)	5	20
49	1r	66/88 (75%)	59 (89%)	7 (11%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
50	2s	81/93 (87%)	63 (78%)	15 (18%)	3 (4%)	2	9
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3	12
51	2t	94/106 (89%)	81 (86%)	9 (10%)	4 (4%)	2	7
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	6
56	1z	1/3 (33%)	0	1 (100%)	0	100	100
56	2z	1/3 (33%)	0	1 (100%)	0	100	100
All	All	11372/12134 (94%)	10129 (89%)	1098 (10%)	145 (1%)	10	32

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	181	ARG
7	1H	126	PRO
21	1Z	53	ILE
26	14	49	PHE

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	204 (95%)	11 (5%)	20	51
3	2D	215/218 (99%)	201 (94%)	14 (6%)	14	40
4	1E	164/166 (99%)	148 (90%)	16 (10%)	6	21
4	2E	164/166 (99%)	154 (94%)	10 (6%)	15	43
5	1F	160/166 (96%)	144 (90%)	16 (10%)	6	20
5	2F	159/166 (96%)	137 (86%)	22 (14%)	3	10
6	1G	143/156 (92%)	126 (88%)	17 (12%)	4	14
6	2G	143/156 (92%)	119 (83%)	24 (17%)	1	6
7	1H	144/148 (97%)	125 (87%)	19 (13%)	3	11
7	2H	144/148 (97%)	125 (87%)	19 (13%)	3	11
8	1I	113/124 (91%)	84 (74%)	29 (26%)	0	1
8	2I	105/124 (85%)	81 (77%)	24 (23%)	0	2
9	1N	118/119 (99%)	106 (90%)	12 (10%)	6	19
9	2N	118/119 (99%)	107 (91%)	11 (9%)	7	23
10	1O	100/100 (100%)	93 (93%)	7 (7%)	12	36
10	2O	100/100 (100%)	92 (92%)	8 (8%)	10	30
11	1P	115/116 (99%)	105 (91%)	10 (9%)	8	26
11	2P	115/116 (99%)	103 (90%)	12 (10%)	5	18
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	8	25
12	2Q	111/111 (100%)	96 (86%)	15 (14%)	3	10
13	1R	101/101 (100%)	94 (93%)	7 (7%)	13	37
13	2R	101/101 (100%)	99 (98%)	2 (2%)	50	81
14	1S	86/88 (98%)	73 (85%)	13 (15%)	2	8
14	2S	85/88 (97%)	69 (81%)	16 (19%)	1	4
15	1T	115/127 (91%)	108 (94%)	7 (6%)	15	43
15	2T	113/127 (89%)	107 (95%)	6 (5%)	19	49
16	1U	93/94 (99%)	83 (89%)	10 (11%)	5	17
16	2U	93/94 (99%)	87 (94%)	6 (6%)	14	40
17	1V	80/82 (98%)	74 (92%)	6 (8%)	11	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	2V	80/82 (98%)	68 (85%)	12 (15%)	2	8
18	1W	90/92 (98%)	86 (96%)	4 (4%)	24	56
18	2W	90/92 (98%)	81 (90%)	9 (10%)	6	20
19	1X	77/78 (99%)	72 (94%)	5 (6%)	14	40
19	2X	77/78 (99%)	70 (91%)	7 (9%)	7	24
20	1Y	85/91 (93%)	73 (86%)	12 (14%)	3	9
20	2Y	85/91 (93%)	73 (86%)	12 (14%)	3	9
21	1Z	135/179 (75%)	113 (84%)	22 (16%)	2	6
21	2Z	137/179 (76%)	109 (80%)	28 (20%)	1	3
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	69
22	20	65/67 (97%)	64 (98%)	1 (2%)	60	86
23	11	80/83 (96%)	74 (92%)	6 (8%)	11	33
23	21	80/83 (96%)	71 (89%)	9 (11%)	4	16
24	12	65/67 (97%)	58 (89%)	7 (11%)	5	17
24	22	65/67 (97%)	55 (85%)	10 (15%)	2	7
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	10
25	23	50/52 (96%)	44 (88%)	6 (12%)	4	14
26	14	59/63 (94%)	47 (80%)	12 (20%)	1	3
26	24	53/63 (84%)	44 (83%)	9 (17%)	1	5
27	15	50/52 (96%)	44 (88%)	6 (12%)	4	14
27	25	50/52 (96%)	48 (96%)	2 (4%)	27	60
28	16	51/52 (98%)	47 (92%)	4 (8%)	10	31
28	26	50/52 (96%)	40 (80%)	10 (20%)	1	3
29	17	41/42 (98%)	38 (93%)	3 (7%)	11	34
29	27	41/42 (98%)	37 (90%)	4 (10%)	6	21
30	18	54/55 (98%)	50 (93%)	4 (7%)	11	33
30	28	54/55 (98%)	51 (94%)	3 (6%)	17	47
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	71
31	29	34/34 (100%)	31 (91%)	3 (9%)	8	26
33	1b	192/220 (87%)	169 (88%)	23 (12%)	4	14
33	2b	187/220 (85%)	145 (78%)	42 (22%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1c	142/188 (76%)	129 (91%)	13 (9%)	7	24
34	2c	140/188 (74%)	114 (81%)	26 (19%)	1	4
35	1d	169/181 (93%)	147 (87%)	22 (13%)	3	11
35	2d	173/181 (96%)	148 (86%)	25 (14%)	2	8
36	1e	113/123 (92%)	99 (88%)	14 (12%)	4	13
36	2e	114/123 (93%)	99 (87%)	15 (13%)	3	11
37	1f	84/90 (93%)	73 (87%)	11 (13%)	3	11
37	2f	85/90 (94%)	74 (87%)	11 (13%)	3	11
38	1g	119/127 (94%)	101 (85%)	18 (15%)	2	8
38	2g	120/127 (94%)	104 (87%)	16 (13%)	3	10
39	1h	114/119 (96%)	98 (86%)	16 (14%)	3	9
39	2h	114/119 (96%)	100 (88%)	14 (12%)	4	13
40	1i	90/99 (91%)	82 (91%)	8 (9%)	8	25
40	2i	89/99 (90%)	76 (85%)	13 (15%)	2	8
41	1j	66/92 (72%)	58 (88%)	8 (12%)	4	13
41	2j	69/92 (75%)	52 (75%)	17 (25%)	0	2
42	1k	82/99 (83%)	69 (84%)	13 (16%)	2	7
42	2k	83/99 (84%)	74 (89%)	9 (11%)	5	17
43	1l	96/108 (89%)	87 (91%)	9 (9%)	7	23
43	2l	96/108 (89%)	83 (86%)	13 (14%)	3	10
44	1m	93/101 (92%)	83 (89%)	10 (11%)	5	17
44	2m	92/101 (91%)	72 (78%)	20 (22%)	1	2
45	1n	49/50 (98%)	42 (86%)	7 (14%)	2	9
45	2n	49/50 (98%)	40 (82%)	9 (18%)	1	4
46	1o	78/80 (98%)	69 (88%)	9 (12%)	4	15
46	2o	78/80 (98%)	72 (92%)	6 (8%)	10	31
47	1p	69/74 (93%)	61 (88%)	8 (12%)	4	15
47	2p	68/74 (92%)	60 (88%)	8 (12%)	4	14
48	1q	94/97 (97%)	84 (89%)	10 (11%)	5	18
48	2q	94/97 (97%)	74 (79%)	20 (21%)	1	3
49	1r	59/77 (77%)	56 (95%)	3 (5%)	20	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	2r	59/77 (77%)	49 (83%)	10 (17%)	1	5
50	1s	69/80 (86%)	58 (84%)	11 (16%)	2	7
50	2s	67/80 (84%)	54 (81%)	13 (19%)	1	4
51	1t	70/82 (85%)	65 (93%)	5 (7%)	12	35
51	2t	70/82 (85%)	64 (91%)	6 (9%)	8	27
52	1u	18/22 (82%)	17 (94%)	1 (6%)	17	47
52	2u	18/22 (82%)	17 (94%)	1 (6%)	17	47
56	1z	2/2 (100%)	1 (50%)	1 (50%)	0	0
56	2z	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	9307/10068 (92%)	8193 (88%)	1114 (12%)	4	14

5 of 1114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	2e	150	ARG
38	2g	113	GLU
36	2e	120	THR
45	2n	3	ARG
39	1h	23	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	116	GLN
51	2t	16	HIS
36	2e	127	ASN
41	2j	13	HIS
38	1g	28	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	527 (18%)	24 (0%)
1	2A	2791/2915 (95%)	532 (19%)	24 (0%)
2	1B	119/121 (98%)	15 (12%)	0
2	2B	118/121 (97%)	28 (23%)	0
32	1a	1497/1521 (98%)	281 (18%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	2a	1501/1521 (98%)	364 (24%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	5 (41%)	0
54	1w	71/76 (93%)	33 (46%)	0
54	2w	71/76 (93%)	34 (47%)	0
55	1x	75/77 (97%)	17 (22%)	0
55	2x	75/77 (97%)	17 (22%)	0
57	1y	72/76 (94%)	34 (47%)	0
57	2y	72/76 (94%)	38 (52%)	0
All	All	9350/9620 (97%)	1927 (20%)	48 (0%)

5 of 1927 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	15	G
1	1A	29	U
1	1A	34	C

5 of 48 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	277	C
1	2A	1210	A
1	2A	528	A
1	2A	856	C
1	2A	1442	G

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

86 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
54	G7M	2w	46	54	20,26,27	1.19	1 (5%)	16,39,42	0.82	0
1	5MU	2A	1939	1,58	19,22,23	1.39	4 (21%)	27,32,35	2.24	6 (22%)
32	4OC	1a	1402	32	20,23,24	0.73	0	25,32,35	1.04	2 (8%)
1	PSU	2A	1911	1	18,21,22	1.42	3 (16%)	21,30,33	2.06	3 (14%)
43	0TD	2l	92	43	8,9,10	4.49	2 (25%)	6,11,13	7.26	2 (33%)
55	PSU	2x	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.13	4 (19%)
55	5MC	2x	32	55	19,22,23	1.56	3 (15%)	26,32,35	1.18	3 (11%)
54	PSU	1w	39	54	18,21,22	1.37	2 (11%)	21,30,33	2.04	4 (19%)
57	PSU	1y	55	57	18,21,22	1.44	2 (11%)	21,30,33	1.89	3 (14%)
55	5MC	1x	32	55	19,22,23	1.81	3 (15%)	26,32,35	1.19	2 (7%)
32	G7M	2a	527	58,32	20,26,27	1.21	2 (10%)	16,39,42	0.53	0
32	UR3	2a	1498	58,32	19,22,23	0.98	0	26,32,35	1.77	4 (15%)
32	PSU	2a	516	58,32	18,21,22	1.39	3 (16%)	21,30,33	2.17	6 (28%)
32	M2G	1a	966	32	20,27,28	1.31	3 (15%)	19,40,43	1.02	2 (10%)
55	8AN	2x	76	58,55	17,24,25	1.26	3 (17%)	13,35,38	3.30	3 (23%)
57	PSU	1y	39	57	18,21,22	1.50	3 (16%)	21,30,33	1.73	3 (14%)
57	T6A	1y	37	57	17,24,35	0.82	1 (5%)	16,35,52	1.22	2 (12%)
57	PSU	2y	39	57	18,21,22	1.37	2 (11%)	21,30,33	1.85	4 (19%)
32	5MC	1a	1407	32	19,22,23	1.63	3 (15%)	26,32,35	1.17	2 (7%)
32	PSU	1a	516	58,32	18,21,22	1.38	2 (11%)	21,30,33	2.05	4 (19%)
57	T6A	2y	37	57,32	17,24,35	0.80	0	16,35,52	1.24	2 (12%)
1	2MA	2A	2503	1,58	18,25,26	0.65	0	20,37,40	1.87	4 (20%)
32	5MC	1a	1404	32	19,22,23	1.74	3 (15%)	26,32,35	1.15	3 (11%)
54	PSU	2w	39	54	18,21,22	1.43	2 (11%)	21,30,33	1.70	3 (14%)
1	5MU	2A	1915	1	19,22,23	1.47	5 (26%)	27,32,35	2.02	5 (18%)
54	T6A	2w	37	53,54	26,34,35	1.03	1 (3%)	28,49,52	1.94	5 (17%)
54	5MU	1w	54	54	19,22,23	1.43	4 (21%)	27,32,35	2.24	6 (22%)
32	2MG	1a	1207	32	18,26,27	0.98	1 (5%)	16,38,41	1.51	4 (25%)
54	U8U	2w	34	53,54	20,24,25	1.40	3 (15%)	22,34,37	1.37	4 (18%)
55	4SU	2x	8	55	18,21,22	2.20	6 (33%)	25,30,33	1.50	7 (28%)
54	PSU	2w	55	58,54	18,21,22	1.35	2 (11%)	21,30,33	1.99	4 (19%)
32	MA6	1a	1519	32	19,26,27	1.01	2 (10%)	18,38,41	2.06	3 (16%)
57	5MU	1y	54	57	19,22,23	1.41	5 (26%)	27,32,35	2.25	7 (25%)
54	U8U	1w	34	53,54	20,24,25	1.40	3 (15%)	22,34,37	1.71	4 (18%)
56	FME	1z	1	56	8,9,10	1.04	0	8,9,11	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	2a	1518	32	19,26,27	1.00	2 (10%)	18,38,41	1.89	3 (16%)
57	U8U	1y	34	57	17,21,25	1.50	3 (17%)	21,30,37	1.45	3 (14%)
54	G7M	1w	46	54	20,26,27	1.23	1 (5%)	16,39,42	0.66	0
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	21,30,33	2.11	4 (19%)
32	UR3	1a	1498	32	19,22,23	1.07	1 (5%)	26,32,35	1.82	5 (19%)
56	FME	2z	1	56	8,9,10	1.00	0	8,9,11	0.78	0
1	5MU	1A	1915	1	19,22,23	1.42	6 (31%)	27,32,35	2.16	7 (25%)
1	5MC	1A	1942	1	19,22,23	1.63	3 (15%)	26,32,35	1.10	2 (7%)
57	5MU	2y	54	57	19,22,23	1.43	5 (26%)	27,32,35	2.12	7 (25%)
32	MA6	2a	1519	32	19,26,27	0.99	1 (5%)	18,38,41	1.85	3 (16%)
57	G7M	1y	46	57	20,26,27	1.36	2 (10%)	16,39,42	0.59	0
1	OMU	2A	2552	1,58	19,22,23	1.22	3 (15%)	25,31,34	1.69	5 (20%)
1	OMG	2A	2251	1,55	19,26,27	0.87	1 (5%)	21,38,41	1.16	2 (9%)
32	M2G	2a	966	32	20,27,28	1.44	3 (15%)	19,40,43	0.98	2 (10%)
57	G7M	2y	46	57	20,26,27	1.32	1 (5%)	16,39,42	0.74	0
1	5MC	2A	1942	1	19,22,23	1.74	3 (15%)	26,32,35	1.18	2 (7%)
32	5MC	1a	1400	32	19,22,23	1.76	3 (15%)	26,32,35	1.19	3 (11%)
1	5MC	2A	1962	1,58	19,22,23	1.54	3 (15%)	26,32,35	1.15	2 (7%)
1	2MA	1A	2503	1,58	18,25,26	0.66	0	20,37,40	2.12	4 (20%)
1	OMC	2A	1920	1	19,22,23	0.77	0	25,31,34	0.86	1 (4%)
1	PSU	1A	1917	1	18,21,22	1.39	3 (16%)	21,30,33	2.08	3 (14%)
1	PSU	1A	2605	1,58	18,21,22	1.31	4 (22%)	21,30,33	1.92	4 (19%)
32	MA6	1a	1518	32	19,26,27	1.02	2 (10%)	18,38,41	1.86	3 (16%)
1	PSU	1A	1911	1	18,21,22	1.41	3 (16%)	21,30,33	2.01	4 (19%)
32	5MC	1a	967	32	19,22,23	1.44	3 (15%)	26,32,35	1.11	2 (7%)
55	5MU	2x	54	55	19,22,23	1.42	6 (31%)	27,32,35	2.25	7 (25%)
32	G7M	1a	527	58,32	20,26,27	1.20	1 (5%)	16,39,42	0.64	0
32	5MC	2a	1400	32	19,22,23	1.72	3 (15%)	26,32,35	1.21	4 (15%)
54	A1B8A	1w	76	54	26,33,34	1.24	3 (11%)	23,46,49	1.74	3 (13%)
55	5MU	1x	54	55	19,22,23	1.48	5 (26%)	27,32,35	1.74	5 (18%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	21,30,33	1.98	3 (14%)
32	4OC	2a	1402	58,32	20,23,24	0.76	0	25,32,35	1.06	2 (8%)
55	4SU	1x	8	55	18,21,22	2.34	5 (27%)	25,30,33	1.59	5 (20%)
1	OMU	1A	2552	1,58	19,22,23	1.22	3 (15%)	25,31,34	1.89	5 (20%)
54	PSU	1w	55	54	18,21,22	1.35	2 (11%)	21,30,33	1.94	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2A	2605	1	18,21,22	1.39	3 (16%)	21,30,33	2.01	3 (14%)
32	5MC	2a	1404	32	19,22,23	1.70	3 (15%)	26,32,35	1.15	2 (7%)
54	A1B8A	2w	76	54	26,33,34	1.19	3 (11%)	23,46,49	1.66	2 (8%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	0.97	0
1	5MC	1A	1962	1,58	19,22,23	1.64	3 (15%)	26,32,35	1.19	3 (11%)
54	5MU	2w	54	54	19,22,23	1.52	5 (26%)	27,32,35	1.60	7 (25%)
1	OMG	1A	2251	1,58,55	19,26,27	0.94	1 (5%)	21,38,41	1.17	2 (9%)
32	2MG	2a	1207	32	18,26,27	0.95	1 (5%)	16,38,41	1.26	2 (12%)
1	5MU	1A	1939	1,58	19,22,23	1.41	4 (21%)	27,32,35	2.26	6 (22%)
57	U8U	2y	34	57,53	17,21,25	1.64	3 (17%)	21,30,37	1.47	3 (14%)
43	0TD	1l	92	43	8,9,10	4.68	1 (12%)	6,11,13	1.85	2 (33%)
32	5MC	2a	967	58,32	19,22,23	1.71	3 (15%)	26,32,35	1.19	3 (11%)
57	PSU	2y	55	57	18,21,22	1.32	2 (11%)	21,30,33	2.21	4 (19%)
54	T6A	1w	37	54	26,34,35	0.97	1 (3%)	28,49,52	1.79	5 (17%)
55	8AN	1x	76	55	17,24,25	1.24	1 (5%)	13,35,38	4.29	3 (23%)
32	5MC	2a	1407	32	19,22,23	1.65	3 (15%)	26,32,35	1.11	2 (7%)

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
54	G7M	2w	46	54	-	3/3/25/26	0/3/3/3
1	5MU	2A	1939	1,58	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	PSU	2A	1911	1	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	2/7/25/26	0/2/2/2
57	PSU	1y	55	57	-	2/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	58,32	-	2/3/25/26	0/3/3/3
32	UR3	2a	1498	58,32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	58,32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
55	8AN	2x	76	58,55	-	3/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PSU	1y	39	57	-	0/7/25/26	0/2/2/2
57	T6A	1y	37	57	-	1/3/25/42	0/3/3/3
57	PSU	2y	39	57	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	58,32	-	0/7/25/26	0/2/2/2
57	T6A	2y	37	57,32	-	0/3/25/42	0/3/3/3
1	2MA	2A	2503	1,58	-	2/3/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	1/7/25/26	0/2/2/2
54	T6A	2w	37	53,54	-	7/19/41/42	0/3/3/3
54	5MU	1w	54	54	-	2/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
54	U8U	2w	34	53,54	-	3/10/28/29	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	58,54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
54	U8U	1w	34	53,54	-	2/10/28/29	0/2/2/2
56	FME	1z	1	56	-	5/7/9/11	-
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
57	U8U	1y	34	57	-	0/7/25/29	0/2/2/2
54	G7M	1w	46	54	-	2/3/25/26	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
56	FME	2z	1	56	-	3/7/9/11	-
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
57	5MU	2y	54	57	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
57	G7M	1y	46	57	-	1/3/25/26	0/3/3/3
1	OMU	2A	2552	1,58	-	0/9/27/28	0/2/2/2
1	OMG	2A	2251	1,55	-	1/5/27/28	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
57	G7M	2y	46	57	-	0/3/25/26	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	5MC	2A	1962	1,58	-	1/7/25/26	0/2/2/2
1	2MA	1A	2503	1,58	-	3/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,58	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	58,32	-	2/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	A1B8A	1w	76	54	-	3/16/38/39	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	58,32	-	2/9/29/30	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,58	-	0/9/27/28	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
54	A1B8A	2w	76	54	-	3/16/38/39	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	5MC	1A	1962	1,58	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	1/7/25/26	0/2/2/2
1	OMG	1A	2251	1,58,55	-	0/5/27/28	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	5MU	1A	1939	1,58	-	0/7/25/26	0/2/2/2
57	U8U	2y	34	57,53	-	0/7/25/29	0/2/2/2
43	0TD	1l	92	43	-	4/7/12/14	-
32	5MC	2a	967	58,32	-	0/7/25/26	0/2/2/2
57	PSU	2y	55	57	-	0/7/25/26	0/2/2/2
54	T6A	1w	37	54	-	6/19/41/42	0/3/3/3
55	8AN	1x	76	55	-	3/3/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2

The worst 5 of 206 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.80	1.69	1.82
43	2l	92	0TD	CB-SB	-12.16	1.70	1.82
55	1x	32	5MC	C5-C4	6.59	1.49	1.44
32	1a	1400	5MC	C5-C4	6.51	1.49	1.44
32	1a	1404	5MC	C5-C4	6.43	1.49	1.44

The worst 5 of 278 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-17.58	70.76	102.36
55	1x	76	8AN	O4'-C1'-N9	10.95	123.27	108.75
55	1x	76	8AN	C4'-O4'-C1'	-8.54	102.10	109.92
55	2x	76	8AN	C4'-O4'-C1'	-7.60	102.97	109.92
1	1A	2503	2MA	C2-N3-C4	7.47	121.49	115.46

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CG-CB-SB-CSB

There are no ring outliers.

48 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1939	5MU	2	0
32	1a	1402	4OC	3	0
1	2A	1911	PSU	2	0
43	2l	92	0TD	1	0
54	1w	39	PSU	1	0
57	1y	55	PSU	2	0
32	2a	1498	UR3	1	0
32	2a	516	PSU	1	0
55	2x	76	8AN	1	0
57	1y	39	PSU	1	0
57	1y	37	T6A	1	0
57	2y	39	PSU	1	0
32	1a	516	PSU	1	0
57	2y	37	T6A	1	0
1	2A	2503	2MA	2	0
54	2w	39	PSU	1	0
32	1a	1207	2MG	1	0
54	2w	34	U8U	1	0
55	2x	8	4SU	1	0
54	2w	55	PSU	2	0
32	1a	1519	MA6	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	1w	34	U8U	4	0
56	1z	1	FME	1	0
32	2a	1518	MA6	2	0
32	1a	1498	UR3	1	0
56	2z	1	FME	1	0
32	2a	1519	MA6	3	0
57	1y	46	G7M	1	0
1	2A	2552	OMU	1	0
57	2y	46	G7M	5	0
1	2A	1942	5MC	1	0
32	1a	1400	5MC	1	0
1	1A	2503	2MA	1	0
1	1A	1917	PSU	1	0
32	1a	1518	MA6	3	0
32	1a	527	G7M	1	0
32	2a	1400	5MC	2	0
54	1w	76	A1B8A	2	0
32	2a	1402	4OC	2	0
55	1x	8	4SU	1	0
1	1A	2552	OMU	1	0
32	2a	1404	5MC	2	0
54	2w	76	A1B8A	2	0
32	2a	1207	2MG	3	0
1	1A	1939	5MU	1	0
57	2y	34	U8U	2	0
43	1l	92	0TD	1	0
55	1x	76	8AN	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2677 ligands modelled in this entry, 2673 are monoatomic - leaving 4 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	$\# Z > 2$
62	SF4	2d	303	35	0,12,12	-	-	-		
62	SF4	1d	302	35	0,12,12	-	-	-		
60	TEL	2A	3826	-	58,62,62	1.30	4 (6%)	74,92,92	1.88	14 (18%)
60	TEL	1A	4082	-	58,62,62	1.36	5 (8%)	74,92,92	1.54	8 (10%)

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
62	SF4	2d	303	35	-	-	0/6/5/5
62	SF4	1d	302	35	-	-	0/6/5/5
60	TEL	2A	3826	-	-	9/73/108/108	0/4/5/5
60	TEL	1A	4082	-	-	10/73/108/108	0/4/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	1A	4082	TEL	O5-C10	5.74	1.44	1.35
60	2A	3826	TEL	O5-C10	5.43	1.44	1.35
60	1A	4082	TEL	O9-C15	5.08	1.45	1.34
60	2A	3826	TEL	O9-C15	5.01	1.45	1.34
60	1A	4082	TEL	O5-C2	-3.43	1.42	1.47

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	2A	3826	TEL	O9-C15-C21	9.28	120.09	110.93
60	1A	4082	TEL	O9-C15-C21	6.60	117.44	110.93
60	1A	4082	TEL	C17-C11-N6	-5.90	104.31	113.25
60	2A	3826	TEL	C17-C11-N6	-5.71	104.59	113.25
60	2A	3826	TEL	C4-O9-C15	-3.81	111.55	118.20

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

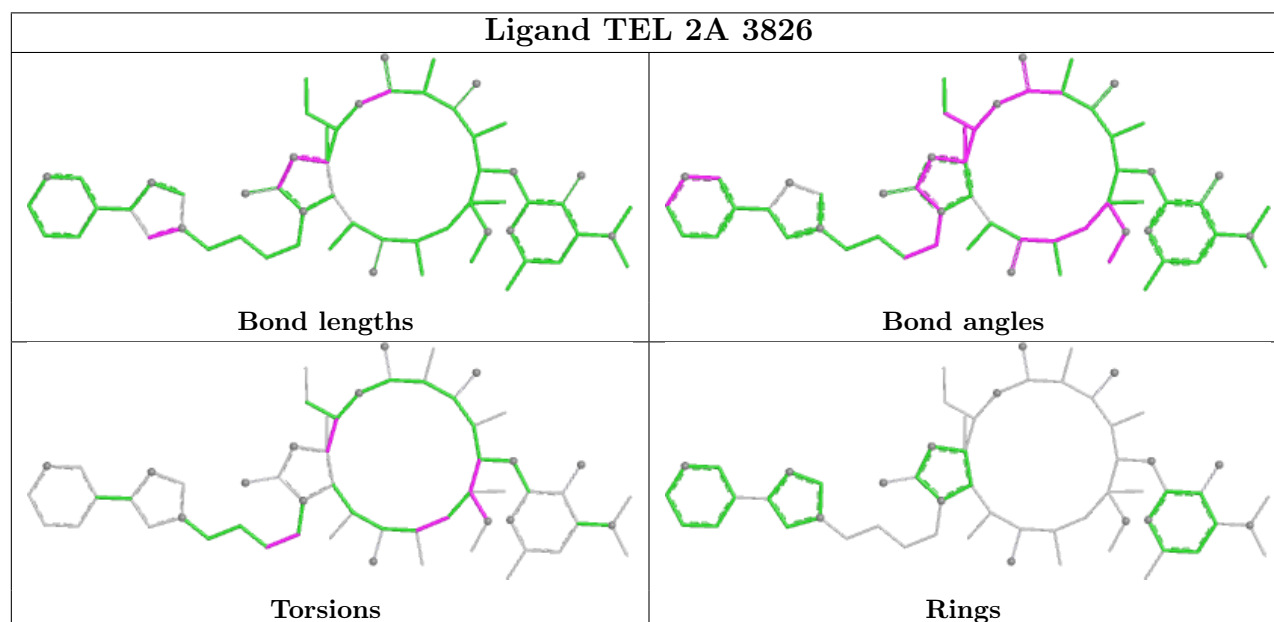
Mol	Chain	Res	Type	Atoms
60	1A	4082	TEL	C1-C2-C4-C8
60	1A	4082	TEL	O5-C2-C4-C8
60	1A	4082	TEL	O5-C2-C4-O9
60	1A	4082	TEL	C24-C28-O32-C38
60	1A	4082	TEL	C33-C28-O32-C38

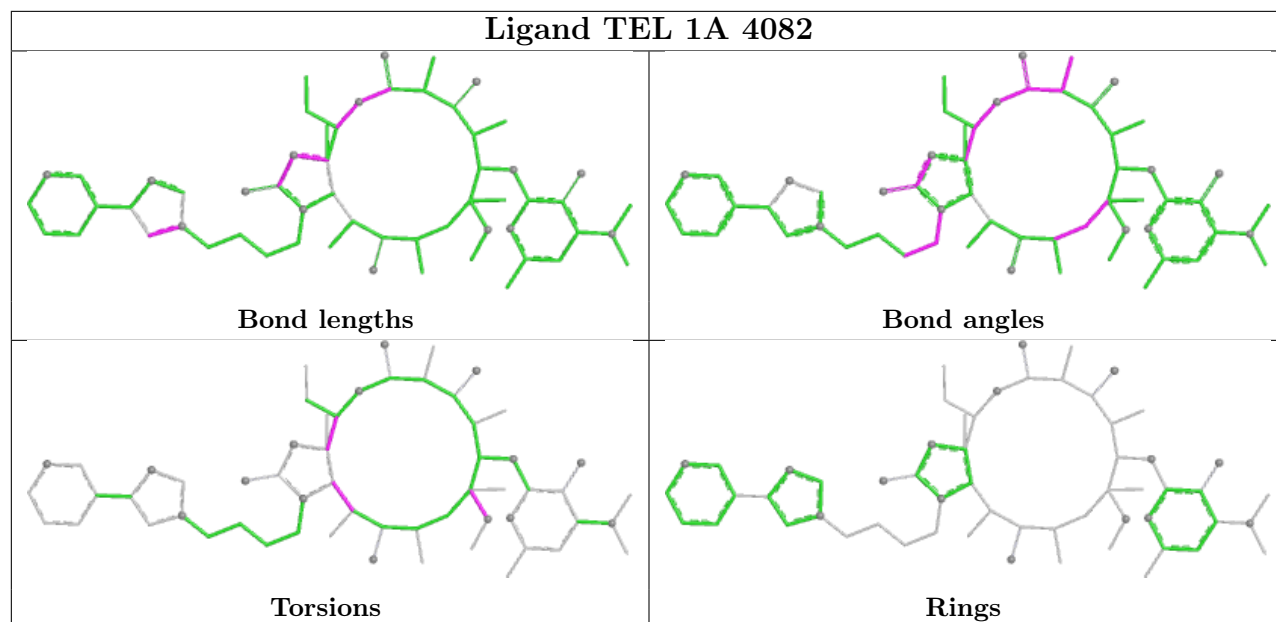
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	2d	303	SF4	2	0
62	1d	302	SF4	1	0
60	2A	3826	TEL	4	0
60	1A	4082	TEL	4	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.10	110 (3%) 44 36	17, 35, 97, 108	0
1	2A	2789/2915 (95%)	0.35	96 (3%) 48 40	30, 58, 93, 107	0
2	1B	120/121 (99%)	-0.06	1 (0%) 82 77	28, 50, 62, 85	0
2	2B	120/121 (99%)	1.27	21 (17%) 5 4	58, 82, 91, 99	0
3	1D	275/276 (99%)	-0.07	3 (1%) 77 71	17, 34, 49, 76	0
3	2D	275/276 (99%)	0.34	5 (1%) 67 60	30, 51, 65, 86	0
4	1E	204/206 (99%)	-0.01	0 100 100	18, 42, 62, 80	0
4	2E	204/206 (99%)	0.38	5 (2%) 58 49	29, 56, 70, 83	0
5	1F	203/210 (96%)	0.01	0 100 100	19, 43, 69, 82	0
5	2F	203/210 (96%)	0.46	2 (0%) 79 73	32, 66, 79, 88	0
6	1G	181/182 (99%)	0.42	7 (3%) 44 36	39, 56, 73, 85	0
6	2G	181/182 (99%)	1.35	36 (19%) 3 3	71, 81, 89, 95	0
7	1H	174/180 (96%)	0.16	2 (1%) 77 71	35, 52, 64, 75	0
7	2H	174/180 (96%)	0.91	11 (6%) 27 21	68, 81, 89, 95	0
8	1I	146/148 (98%)	0.75	5 (3%) 48 40	42, 72, 82, 89	0
8	2I	146/148 (98%)	0.90	15 (10%) 13 10	55, 73, 84, 87	0
9	1N	140/140 (100%)	0.02	0 100 100	25, 40, 60, 75	0
9	2N	140/140 (100%)	0.89	10 (7%) 23 18	43, 65, 76, 81	0
10	1O	122/122 (100%)	-0.06	0 100 100	25, 40, 55, 60	0
10	2O	122/122 (100%)	0.29	0 100 100	41, 53, 67, 75	0
11	1P	149/150 (99%)	0.28	1 (0%) 84 79	20, 45, 67, 77	0
11	2P	149/150 (99%)	0.63	7 (4%) 37 30	38, 67, 79, 87	0
12	1Q	141/141 (100%)	0.02	2 (1%) 73 66	25, 40, 54, 68	0
12	2Q	141/141 (100%)	1.13	14 (9%) 14 11	47, 66, 77, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.06	0 100 100	21, 35, 51, 66	0
13	2R	118/118 (100%)	0.29	0 100 100	35, 49, 62, 68	0
14	1S	110/112 (98%)	0.17	0 100 100	36, 48, 60, 63	0
14	2S	110/112 (98%)	1.21	21 (19%) 4 4	63, 74, 83, 86	0
15	1T	131/146 (89%)	0.29	2 (1%) 71 64	34, 46, 68, 79	0
15	2T	131/146 (89%)	0.36	2 (1%) 71 64	44, 57, 71, 81	0
16	1U	116/118 (98%)	-0.09	1 (0%) 81 75	22, 32, 49, 66	0
16	2U	116/118 (98%)	0.63	2 (1%) 69 61	45, 64, 75, 83	0
17	1V	101/101 (100%)	-0.07	0 100 100	22, 43, 60, 70	0
17	2V	101/101 (100%)	0.76	3 (2%) 52 44	43, 73, 81, 85	0
18	1W	112/113 (99%)	-0.26	0 100 100	25, 33, 49, 73	0
18	2W	112/113 (99%)	0.47	2 (1%) 67 60	36, 50, 67, 85	0
19	1X	95/96 (98%)	-0.07	1 (1%) 77 71	26, 37, 58, 74	0
19	2X	95/96 (98%)	0.90	8 (8%) 18 14	48, 59, 73, 79	0
20	1Y	107/110 (97%)	0.21	3 (2%) 55 46	36, 48, 67, 77	0
20	2Y	107/110 (97%)	1.25	15 (14%) 7 7	61, 71, 79, 82	0
21	1Z	154/206 (74%)	0.49	7 (4%) 39 31	42, 60, 83, 88	0
21	2Z	160/206 (77%)	1.08	18 (11%) 11 9	70, 80, 89, 95	0
22	10	83/85 (97%)	0.35	8 (9%) 15 11	26, 36, 62, 78	0
22	20	83/85 (97%)	1.18	11 (13%) 8 7	51, 65, 75, 91	0
23	11	97/98 (98%)	0.15	1 (1%) 79 73	25, 42, 65, 70	0
23	21	97/98 (98%)	0.53	3 (3%) 51 43	36, 56, 74, 78	0
24	12	70/72 (97%)	-0.05	0 100 100	35, 47, 59, 68	0
24	22	70/72 (97%)	0.67	0 100 100	56, 69, 75, 77	0
25	13	59/60 (98%)	-0.04	0 100 100	28, 38, 56, 63	0
25	23	59/60 (98%)	0.59	0 100 100	54, 67, 77, 82	0
26	14	69/71 (97%)	0.63	4 (5%) 30 23	52, 74, 88, 94	0
26	24	69/71 (97%)	1.01	6 (8%) 17 13	74, 87, 93, 99	0
27	15	59/60 (98%)	-0.20	0 100 100	20, 36, 50, 62	0
27	25	59/60 (98%)	0.26	0 100 100	34, 51, 64, 74	0
28	16	53/54 (98%)	-0.01	1 (1%) 66 58	30, 40, 57, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.87	4 (7%) 22 16	46, 60, 69, 76	0
29	17	48/49 (97%)	-0.12	1 (2%) 63 55	21, 28, 53, 58	0
29	27	48/49 (97%)	0.20	3 (6%) 27 21	31, 41, 59, 66	0
30	18	64/65 (98%)	-0.01	1 (1%) 70 63	24, 33, 40, 49	0
30	28	64/65 (98%)	0.66	1 (1%) 70 63	47, 55, 62, 66	0
31	19	37/37 (100%)	-0.05	1 (2%) 56 47	28, 37, 56, 59	0
31	29	37/37 (100%)	1.29	4 (10%) 12 9	59, 69, 77, 87	0
32	1a	1488/1521 (97%)	0.44	31 (2%) 63 55	31, 65, 92, 106	0
32	2a	1491/1521 (98%)	0.91	124 (8%) 19 14	50, 80, 97, 106	0
33	1b	231/256 (90%)	0.73	21 (9%) 16 12	62, 76, 84, 91	0
33	2b	231/256 (90%)	1.46	55 (23%) 2 3	74, 86, 92, 95	0
34	1c	206/239 (86%)	0.39	5 (2%) 59 51	52, 69, 80, 90	0
34	2c	206/239 (86%)	1.48	61 (29%) 1 2	74, 85, 90, 94	0
35	1d	208/209 (99%)	0.54	8 (3%) 44 36	55, 67, 77, 80	0
35	2d	208/209 (99%)	1.18	33 (15%) 6 5	65, 75, 83, 91	0
36	1e	148/162 (91%)	0.54	1 (0%) 84 79	50, 62, 71, 83	0
36	2e	148/162 (91%)	1.03	20 (13%) 8 7	69, 79, 85, 89	0
37	1f	100/101 (99%)	0.35	0 100 100	49, 64, 75, 79	0
37	2f	100/101 (99%)	0.72	4 (4%) 43 35	60, 72, 80, 83	0
38	1g	155/156 (99%)	0.83	14 (9%) 17 12	57, 70, 84, 99	0
38	2g	155/156 (99%)	1.32	35 (22%) 3 3	73, 82, 88, 94	0
39	1h	137/138 (99%)	0.55	4 (2%) 54 45	55, 65, 72, 78	0
39	2h	137/138 (99%)	1.16	20 (14%) 7 6	69, 79, 84, 89	0
40	1i	127/128 (99%)	1.03	14 (11%) 12 9	50, 75, 84, 88	0
40	2i	127/128 (99%)	1.94	57 (44%) 1 1	74, 86, 91, 93	0
41	1j	97/105 (92%)	1.14	11 (11%) 11 9	51, 74, 85, 90	0
41	2j	96/105 (91%)	1.74	27 (28%) 2 2	75, 86, 92, 94	0
42	1k	114/129 (88%)	0.62	6 (5%) 33 26	39, 64, 77, 84	0
42	2k	114/129 (88%)	0.90	12 (10%) 13 10	63, 75, 83, 86	0
43	1l	121/132 (91%)	0.57	8 (6%) 26 19	45, 55, 66, 76	0
43	2l	121/132 (91%)	1.16	14 (11%) 11 9	53, 71, 78, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.84	11 (8%) 17 13	54, 68, 78, 92	0
44	2m	122/126 (96%)	1.60	36 (29%) 1 2	71, 84, 89, 91	0
45	1n	60/61 (98%)	0.76	5 (8%) 19 14	56, 65, 75, 81	0
45	2n	60/61 (98%)	2.35	33 (55%) 0 0	77, 85, 89, 94	0
46	1o	88/89 (98%)	0.45	2 (2%) 61 52	50, 61, 73, 84	0
46	2o	88/89 (98%)	0.87	4 (4%) 39 31	62, 75, 82, 86	0
47	1p	82/88 (93%)	1.38	12 (14%) 7 6	57, 71, 78, 83	0
47	2p	82/88 (93%)	1.05	4 (4%) 36 28	57, 68, 76, 85	0
48	1q	99/105 (94%)	0.89	7 (7%) 23 18	53, 67, 75, 80	0
48	2q	99/105 (94%)	0.98	13 (13%) 8 7	63, 74, 81, 86	0
49	1r	68/88 (77%)	0.37	2 (2%) 54 45	53, 64, 73, 79	0
49	2r	68/88 (77%)	0.54	0 100 100	67, 76, 84, 87	0
50	1s	83/93 (89%)	0.70	4 (4%) 36 29	59, 70, 82, 93	0
50	2s	83/93 (89%)	1.76	24 (28%) 1 2	79, 86, 92, 93	0
51	1t	96/106 (90%)	0.81	11 (11%) 11 9	59, 70, 78, 86	0
51	2t	96/106 (90%)	0.89	10 (10%) 13 10	54, 69, 82, 84	0
52	1u	23/27 (85%)	1.23	3 (13%) 9 7	58, 64, 69, 76	0
52	2u	23/27 (85%)	2.21	11 (47%) 0 1	76, 81, 84, 89	0
53	1v	13/24 (54%)	1.34	3 (23%) 2 3	41, 77, 94, 95	0
53	2v	13/24 (54%)	1.68	4 (30%) 1 1	78, 91, 95, 97	0
54	1w	67/76 (88%)	1.29	12 (17%) 4 4	58, 96, 102, 104	0
54	2w	67/76 (88%)	1.52	14 (20%) 3 3	78, 99, 105, 106	0
55	1x	72/77 (93%)	0.44	2 (2%) 55 46	41, 65, 83, 84	0
55	2x	72/77 (93%)	1.10	7 (9%) 15 11	52, 82, 91, 97	0
56	1z	2/3 (66%)	0.69	0 100 100	43, 43, 43, 46	0
56	2z	2/3 (66%)	1.57	1 (50%) 0 1	53, 53, 53, 69	0
57	1y	68/76 (89%)	1.24	7 (10%) 13 10	54, 99, 105, 107	0
57	2y	68/76 (89%)	1.64	16 (23%) 2 3	69, 101, 106, 107	0
All	All	20884/21754 (96%)	0.52	1330 (6%) 27 20	17, 63, 91, 108	0

The worst 5 of 1330 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	8.8
45	1n	2	ALA	8.5
38	1g	81	GLY	8.3
44	1m	123	ALA	7.3
44	1m	122	LYS	7.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	PSU	2w	55	20/21	0.41	0.17	94,101,114,114	0
54	5MU	2w	54	21/22	0.43	0.18	86,98,102,109	0
57	G7M	2y	46	24/25	0.44	0.15	93,102,110,121	0
57	PSU	2y	55	20/21	0.51	0.16	94,102,106,116	0
57	U8U	1y	34	20/24	0.55	0.19	88,96,101,112	0
57	G7M	1y	46	24/25	0.56	0.12	91,100,105,115	0
54	PSU	1w	55	20/21	0.57	0.18	85,97,105,106	0
54	G7M	2w	46	24/25	0.58	0.14	92,100,105,110	0
57	T6A	1y	37	22/33	0.61	0.16	79,92,98,108	0
57	PSU	1y	39	20/21	0.64	0.13	91,97,105,111	0
57	T6A	2y	37	22/33	0.64	0.14	86,93,102,117	0
54	G7M	1w	46	24/25	0.65	0.13	86,95,103,104	0
54	T6A	2w	37	32/33	0.66	0.20	76,92,97,98	0
57	U8U	2y	34	20/24	0.68	0.17	96,104,112,115	0
57	PSU	2y	39	20/21	0.68	0.16	89,94,105,106	0
54	PSU	2w	39	20/21	0.69	0.17	85,93,99,104	0
57	5MU	2y	54	21/22	0.71	0.13	87,100,112,125	0
57	5MU	1y	54	21/22	0.71	0.12	92,100,102,113	0
57	PSU	1y	55	20/21	0.71	0.12	95,101,109,118	0
54	U8U	1w	34	23/24	0.72	0.22	76,83,91,105	0
55	5MU	2x	54	21/22	0.72	0.16	84,87,92,107	0
1	5MU	2A	1915	21/22	0.73	0.15	79,86,88,93	0
54	U8U	2w	34	23/24	0.73	0.20	80,92,99,108	0
54	5MU	1w	54	21/22	0.73	0.13	78,89,96,98	0
55	4SU	2x	8	20/21	0.77	0.15	79,85,90,96	0
55	PSU	2x	55	20/21	0.78	0.13	77,81,88,100	0
32	2MG	2a	1207	24/25	0.82	0.15	80,87,94,99	0
32	5MC	2a	1400	21/22	0.83	0.20	74,81,85,86	0
32	PSU	2a	516	20/21	0.83	0.12	80,87,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	M2G	2a	966	25/26	0.85	0.17	61,70,90,94	0
32	5MC	2a	967	21/22	0.85	0.16	71,77,87,89	0
32	G7M	2a	527	24/25	0.85	0.15	58,69,76,78	0
54	T6A	1w	37	32/33	0.85	0.14	67,76,83,84	0
1	PSU	2A	1911	20/21	0.86	0.12	62,70,80,83	0
54	A1B8A	2w	76	31/32	0.86	0.16	48,67,78,84	0
55	PSU	1x	55	20/21	0.87	0.11	57,66,75,81	0
1	OMC	2A	1920	21/22	0.87	0.14	54,71,78,78	0
43	0TD	2l	92	10/11	0.87	0.14	63,68,72,89	0
56	FME	2z	1	10/11	0.87	0.23	62,66,74,74	0
32	4OC	2a	1402	22/23	0.88	0.15	63,74,79,81	0
1	PSU	2A	1917	20/21	0.89	0.11	57,78,83,83	0
55	5MC	2x	32	21/22	0.89	0.14	70,74,79,83	0
54	PSU	1w	39	20/21	0.89	0.10	74,85,90,91	0
1	5MU	1A	1915	21/22	0.89	0.12	53,61,71,73	0
32	5MC	2a	1404	21/22	0.90	0.14	57,65,72,78	0
43	0TD	1l	92	10/11	0.90	0.12	50,54,57,66	0
32	PSU	1a	516	20/21	0.91	0.10	57,64,69,71	0
54	A1B8A	1w	76	31/32	0.91	0.13	31,48,58,65	0
55	8AN	1x	76	22/23	0.91	0.13	31,43,54,60	0
55	5MU	1x	54	21/22	0.91	0.11	65,72,79,85	0
1	5MC	2A	1962	21/22	0.92	0.13	40,53,60,70	0
1	PSU	1A	1917	20/21	0.92	0.11	41,54,63,66	0
56	FME	1z	1	10/11	0.92	0.20	41,52,67,68	0
55	8AN	2x	76	22/23	0.92	0.11	49,55,63,72	0
32	M2G	1a	966	25/26	0.93	0.14	37,48,57,61	0
1	5MC	2A	1942	21/22	0.93	0.12	39,62,73,78	0
55	4SU	1x	8	20/21	0.93	0.10	49,56,61,62	0
55	5MC	1x	32	21/22	0.93	0.13	41,52,57,66	0
32	2MG	1a	1207	24/25	0.93	0.10	59,65,73,76	0
32	5MC	2a	1407	21/22	0.93	0.12	59,64,69,72	0
32	MA6	2a	1518	24/25	0.93	0.13	58,68,72,77	0
32	MA6	2a	1519	24/25	0.93	0.15	60,69,76,78	0
32	MA6	1a	1519	24/25	0.93	0.13	36,39,42,51	0
1	5MC	1A	1942	21/22	0.94	0.10	36,46,53,55	0
32	UR3	2a	1498	21/22	0.94	0.11	55,65,71,74	0
32	G7M	1a	527	24/25	0.94	0.11	48,52,59,60	0
32	4OC	1a	1402	22/23	0.94	0.11	41,47,54,60	0
1	OMU	2A	2552	21/22	0.95	0.09	36,43,50,51	0
1	PSU	2A	2605	20/21	0.95	0.09	33,38,40,43	0
32	5MC	1a	1404	21/22	0.95	0.11	26,39,42,49	0
32	UR3	1a	1498	21/22	0.95	0.10	29,38,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	5MC	1a	967	21/22	0.95	0.11	45,52,57,59	0
1	OMG	2A	2251	24/25	0.95	0.10	34,39,44,45	0
1	PSU	1A	1911	20/21	0.96	0.08	38,48,53,56	0
1	OMC	1A	1920	21/22	0.96	0.10	29,48,53,54	0
1	5MU	2A	1939	21/22	0.96	0.09	32,36,40,43	0
32	MA6	1a	1518	24/25	0.97	0.09	27,37,42,46	0
32	5MC	1a	1400	21/22	0.97	0.10	41,47,52,58	0
1	2MA	2A	2503	23/24	0.97	0.08	27,31,35,36	0
32	5MC	1a	1407	21/22	0.97	0.09	26,38,41,42	0
1	5MC	1A	1962	21/22	0.97	0.07	23,36,41,46	0
1	5MU	1A	1939	21/22	0.98	0.06	23,27,32,36	0
1	OMG	1A	2251	24/25	0.98	0.07	19,24,29,34	0
1	2MA	1A	2503	23/24	0.98	0.07	16,20,25,26	0
1	OMU	1A	2552	21/22	0.98	0.07	21,29,33,37	0
1	PSU	1A	2605	20/21	0.98	0.06	17,28,30,31	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3787	1/1	0.59	0.18	71,71,71,71	0
58	MG	2A	3797	1/1	0.60	0.25	81,81,81,81	0
58	MG	2a	3185	1/1	0.60	0.20	89,89,89,89	0
58	MG	2a	3133	1/1	0.61	0.37	83,83,83,83	0
58	MG	2A	3758	1/1	0.61	0.15	76,76,76,76	0
58	MG	1a	1712	1/1	0.62	0.21	78,78,78,78	0
58	MG	2A	3546	1/1	0.62	0.22	53,53,53,53	0
58	MG	2a	3146	1/1	0.62	0.10	102,102,102,102	0
58	MG	1a	1695	1/1	0.62	0.18	73,73,73,73	0
58	MG	2A	3050	1/1	0.63	0.25	67,67,67,67	0
58	MG	2a	3190	1/1	0.63	0.16	89,89,89,89	0
58	MG	2A	3081	1/1	0.65	0.31	59,59,59,59	0
58	MG	2a	3036	1/1	0.65	0.24	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	3194	1/1	0.65	0.33	81,81,81,81	0
58	MG	1A	3882	1/1	0.66	0.25	26,26,26,26	0
58	MG	1A	3758	1/1	0.66	0.16	24,24,24,24	0
58	MG	1A	4066	1/1	0.67	0.22	78,78,78,78	0
58	MG	2A	3749	1/1	0.67	0.17	77,77,77,77	0
58	MG	2A	3567	1/1	0.68	0.21	82,82,82,82	0
58	MG	2A	3295	1/1	0.68	0.15	67,67,67,67	0
58	MG	2A	3458	1/1	0.69	0.25	61,61,61,61	0
58	MG	2A	3770	1/1	0.69	0.24	48,48,48,48	0
58	MG	1A	3436	1/1	0.69	0.19	60,60,60,60	0
58	MG	2a	3173	1/1	0.70	0.25	72,72,72,72	0
58	MG	2A	3541	1/1	0.70	0.15	59,59,59,59	0
58	MG	2A	3715	1/1	0.70	0.45	48,48,48,48	0
58	MG	1W	207	1/1	0.70	0.17	42,42,42,42	0
58	MG	2I	101	1/1	0.71	0.17	76,76,76,76	0
58	MG	1A	3097	1/1	0.71	0.19	67,67,67,67	0
58	MG	1A	3515	1/1	0.71	0.13	63,63,63,63	0
58	MG	2A	3307	1/1	0.71	0.15	75,75,75,75	0
58	MG	2a	3098	1/1	0.72	0.18	87,87,87,87	0
58	MG	2a	3109	1/1	0.72	0.17	71,71,71,71	0
58	MG	2A	3323	1/1	0.72	0.29	81,81,81,81	0
58	MG	2A	3029	1/1	0.72	0.23	63,63,63,63	0
58	MG	2a	3163	1/1	0.72	0.19	75,75,75,75	0
58	MG	2A	3205	1/1	0.72	0.14	66,66,66,66	0
58	MG	2A	3274	1/1	0.72	0.18	63,63,63,63	0
58	MG	1A	3456	1/1	0.72	0.16	63,63,63,63	0
58	MG	2A	3065	1/1	0.72	0.17	50,50,50,50	0
58	MG	2A	3246	1/1	0.73	0.26	76,76,76,76	0
58	MG	2A	3649	1/1	0.73	0.19	76,76,76,76	0
58	MG	2A	3415	1/1	0.73	0.11	61,61,61,61	0
58	MG	1A	3935	1/1	0.73	0.13	74,74,74,74	0
58	MG	1a	1751	1/1	0.73	0.16	73,73,73,73	0
58	MG	2A	3058	1/1	0.73	0.19	54,54,54,54	0
58	MG	1W	202	1/1	0.74	0.19	53,53,53,53	0
58	MG	2A	3728	1/1	0.74	0.19	60,60,60,60	0
58	MG	1A	3613	1/1	0.74	0.18	44,44,44,44	0
58	MG	1t	201	1/1	0.74	0.32	66,66,66,66	0
58	MG	2A	3296	1/1	0.74	0.28	70,70,70,70	0
58	MG	2A	3010	1/1	0.74	0.16	63,63,63,63	0
58	MG	2a	3181	1/1	0.74	0.23	70,70,70,70	0
58	MG	1B	205	1/1	0.74	0.30	68,68,68,68	0
58	MG	2a	3005	1/1	0.74	0.32	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3653	1/1	0.74	0.32	85,85,85,85	0
58	MG	2l	202	1/1	0.74	0.26	71,71,71,71	0
58	MG	1A	3204	1/1	0.75	0.10	48,48,48,48	0
58	MG	2A	3220	1/1	0.75	0.24	59,59,59,59	0
58	MG	2A	3233	1/1	0.75	0.16	69,69,69,69	0
58	MG	1A	3812	1/1	0.75	0.14	29,29,29,29	0
58	MG	2A	3266	1/1	0.75	0.30	76,76,76,76	0
58	MG	1x	110	1/1	0.75	0.19	69,69,69,69	0
58	MG	2A	3719	1/1	0.75	0.13	61,61,61,61	0
58	MG	1A	4003	1/1	0.75	0.15	70,70,70,70	0
58	MG	1a	1643	1/1	0.75	0.25	70,70,70,70	0
58	MG	1a	1667	1/1	0.75	0.27	68,68,68,68	0
58	MG	1a	1692	1/1	0.75	0.20	63,63,63,63	0
58	MG	1A	4019	1/1	0.75	0.14	27,27,27,27	0
58	MG	2a	3210	1/1	0.75	0.21	80,80,80,80	0
58	MG	1A	3820	1/1	0.75	0.15	72,72,72,72	0
58	MG	2w	101	1/1	0.75	0.24	85,85,85,85	0
58	MG	1A	3815	1/1	0.76	0.14	46,46,46,46	0
58	MG	2a	3139	1/1	0.76	0.29	78,78,78,78	0
58	MG	2A	3252	1/1	0.76	0.15	61,61,61,61	0
58	MG	1B	213	1/1	0.76	0.19	56,56,56,56	0
58	MG	2a	3007	1/1	0.76	0.24	69,69,69,69	0
58	MG	2A	3647	1/1	0.76	0.19	62,62,62,62	0
58	MG	2a	3037	1/1	0.76	0.18	71,71,71,71	0
58	MG	2a	3064	1/1	0.76	0.35	60,60,60,60	0
58	MG	1a	1704	1/1	0.76	0.29	72,72,72,72	0
58	MG	1A	4077	1/1	0.76	0.16	39,39,39,39	0
58	MG	2a	3130	1/1	0.76	0.17	70,70,70,70	0
58	MG	2a	3132	1/1	0.76	0.09	73,73,73,73	0
58	MG	2A	3203	1/1	0.77	0.18	67,67,67,67	0
58	MG	2B	212	1/1	0.77	0.25	71,71,71,71	0
58	MG	1A	3424	1/1	0.77	0.31	44,44,44,44	0
58	MG	1A	3923	1/1	0.77	0.15	62,62,62,62	0
58	MG	2a	3160	1/1	0.77	0.16	74,74,74,74	0
58	MG	1A	3599	1/1	0.77	0.23	53,53,53,53	0
58	MG	2A	3408	1/1	0.77	0.33	79,79,79,79	0
58	MG	2a	3177	1/1	0.77	0.15	68,68,68,68	0
58	MG	1n	102	1/1	0.77	0.21	60,60,60,60	0
58	MG	2A	3440	1/1	0.77	0.10	58,58,58,58	0
58	MG	1A	3035	1/1	0.77	0.10	43,43,43,43	0
58	MG	1A	3371	1/1	0.77	0.13	42,42,42,42	0
58	MG	2a	3121	1/1	0.77	0.22	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	3124	1/1	0.77	0.25	71,71,71,71	0
58	MG	2A	3088	1/1	0.77	0.22	61,61,61,61	0
58	MG	2A	3279	1/1	0.78	0.23	69,69,69,69	0
58	MG	2A	3450	1/1	0.78	0.31	75,75,75,75	0
58	MG	2A	3281	1/1	0.78	0.26	66,66,66,66	0
58	MG	2A	3227	1/1	0.78	0.14	66,66,66,66	0
58	MG	2a	3175	1/1	0.78	0.16	84,84,84,84	0
58	MG	1A	3946	1/1	0.78	0.21	64,64,64,64	0
58	MG	1Y	201	1/1	0.78	0.09	73,73,73,73	0
58	MG	2A	3637	1/1	0.78	0.14	57,57,57,57	0
58	MG	2A	3812	1/1	0.78	0.15	64,64,64,64	0
58	MG	2a	3193	1/1	0.78	0.14	75,75,75,75	0
58	MG	1x	108	1/1	0.78	0.13	66,66,66,66	0
58	MG	20	101	1/1	0.78	0.15	70,70,70,70	0
58	MG	1x	109	1/1	0.78	0.17	61,61,61,61	0
58	MG	1A	3164	1/1	0.78	0.34	59,59,59,59	0
58	MG	2x	102	1/1	0.78	0.27	77,77,77,77	0
58	MG	1A	3130	1/1	0.79	0.11	71,71,71,71	0
58	MG	2A	3095	1/1	0.79	0.11	46,46,46,46	0
58	MG	1A	3425	1/1	0.79	0.24	55,55,55,55	0
58	MG	1a	1608	1/1	0.79	0.19	68,68,68,68	0
58	MG	1A	3321	1/1	0.79	0.11	52,52,52,52	0
58	MG	2A	3346	1/1	0.79	0.20	70,70,70,70	0
58	MG	2a	3092	1/1	0.79	0.10	82,82,82,82	0
58	MG	1a	1656	1/1	0.79	0.17	61,61,61,61	0
58	MG	1A	3693	1/1	0.79	0.17	30,30,30,30	0
58	MG	2A	3244	1/1	0.79	0.15	53,53,53,53	0
58	MG	1A	3868	1/1	0.79	0.11	32,32,32,32	0
58	MG	1A	3702	1/1	0.79	0.12	20,20,20,20	0
58	MG	1A	3188	1/1	0.79	0.31	40,40,40,40	0
58	MG	1S	201	1/1	0.79	0.09	59,59,59,59	0
58	MG	1A	3777	1/1	0.79	0.19	65,65,65,65	0
58	MG	2A	3324	1/1	0.80	0.21	65,65,65,65	0
58	MG	1a	1615	1/1	0.80	0.22	47,47,47,47	0
58	MG	1a	1697	1/1	0.80	0.35	70,70,70,70	0
58	MG	1A	3358	1/1	0.80	0.29	43,43,43,43	0
58	MG	2A	3710	1/1	0.80	0.20	50,50,50,50	0
58	MG	2a	3170	1/1	0.80	0.32	78,78,78,78	0
58	MG	1A	3673	1/1	0.80	0.16	67,67,67,67	0
58	MG	1B	229	1/1	0.80	0.25	73,73,73,73	0
58	MG	1A	3721	1/1	0.80	0.24	63,63,63,63	0
58	MG	2A	3489	1/1	0.80	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	3094	1/1	0.80	0.25	78,78,78,78	0
58	MG	2A	3302	1/1	0.80	0.15	64,64,64,64	0
58	MG	2a	3100	1/1	0.80	0.16	60,60,60,60	0
58	MG	2A	3101	1/1	0.80	0.11	66,66,66,66	0
58	MG	2A	3126	1/1	0.80	0.12	57,57,57,57	0
58	MG	2j	201	1/1	0.80	0.30	73,73,73,73	0
58	MG	2A	3802	1/1	0.80	0.17	58,58,58,58	0
58	MG	2A	3625	1/1	0.80	0.30	79,79,79,79	0
58	MG	2B	204	1/1	0.80	0.23	69,69,69,69	0
58	MG	2a	3097	1/1	0.81	0.35	67,67,67,67	0
58	MG	1a	1660	1/1	0.81	0.20	75,75,75,75	0
58	MG	1A	3569	1/1	0.81	0.14	35,35,35,35	0
58	MG	2A	3260	1/1	0.81	0.23	55,55,55,55	0
58	MG	1A	3883	1/1	0.81	0.20	78,78,78,78	0
58	MG	2A	3754	1/1	0.81	0.17	56,56,56,56	0
58	MG	1A	3543	1/1	0.81	0.15	62,62,62,62	0
58	MG	2A	3466	1/1	0.81	0.18	63,63,63,63	0
58	MG	2A	3777	1/1	0.81	0.13	48,48,48,48	0
58	MG	1A	3687	1/1	0.81	0.14	48,48,48,48	0
58	MG	2A	3192	1/1	0.81	0.20	65,65,65,65	0
58	MG	2A	3804	1/1	0.81	0.19	60,60,60,60	0
58	MG	2A	3195	1/1	0.81	0.10	66,66,66,66	0
58	MG	2A	3559	1/1	0.81	0.17	65,65,65,65	0
58	MG	1A	3795	1/1	0.81	0.17	61,61,61,61	0
58	MG	2A	3583	1/1	0.81	0.17	59,59,59,59	0
58	MG	20	102	1/1	0.81	0.19	73,73,73,73	0
58	MG	2A	3609	1/1	0.81	0.08	56,56,56,56	0
58	MG	2A	3299	1/1	0.81	0.23	72,72,72,72	0
58	MG	2A	3030	1/1	0.81	0.16	51,51,51,51	0
58	MG	2a	3010	1/1	0.81	0.17	63,63,63,63	0
58	MG	2A	3035	1/1	0.81	0.16	51,51,51,51	0
58	MG	1a	1634	1/1	0.81	0.12	62,62,62,62	0
58	MG	1A	3954	1/1	0.81	0.21	68,68,68,68	0
58	MG	2l	201	1/1	0.81	0.16	62,62,62,62	0
58	MG	2a	3080	1/1	0.81	0.27	71,71,71,71	0
58	MG	2A	3696	1/1	0.81	0.19	73,73,73,73	0
58	MG	1A	3870	1/1	0.81	0.14	50,50,50,50	0
58	MG	2A	3534	1/1	0.82	0.20	42,42,42,42	0
58	MG	1A	3796	1/1	0.82	0.17	47,47,47,47	0
58	MG	1A	4014	1/1	0.82	0.10	46,46,46,46	0
58	MG	2a	3034	1/1	0.82	0.34	77,77,77,77	0
58	MG	2A	3553	1/1	0.82	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3459	1/1	0.82	0.27	43,43,43,43	0
58	MG	2A	3040	1/1	0.82	0.37	73,73,73,73	0
58	MG	2a	3071	1/1	0.82	0.33	68,68,68,68	0
58	MG	1A	4065	1/1	0.82	0.19	81,81,81,81	0
58	MG	2A	3584	1/1	0.82	0.18	64,64,64,64	0
58	MG	1A	3473	1/1	0.82	0.22	56,56,56,56	0
58	MG	2A	3062	1/1	0.82	0.13	69,69,69,69	0
58	MG	1A	3691	1/1	0.82	0.12	40,40,40,40	0
58	MG	1A	3495	1/1	0.82	0.11	40,40,40,40	0
58	MG	2A	3083	1/1	0.82	0.14	65,65,65,65	0
58	MG	1A	3701	1/1	0.82	0.16	50,50,50,50	0
58	MG	1B	218	1/1	0.82	0.11	57,57,57,57	0
58	MG	2a	3129	1/1	0.82	0.20	65,65,65,65	0
58	MG	2A	3096	1/1	0.82	0.11	61,61,61,61	0
58	MG	2A	3309	1/1	0.82	0.22	69,69,69,69	0
58	MG	1A	3317	1/1	0.82	0.20	53,53,53,53	0
58	MG	1a	1735	1/1	0.82	0.14	66,66,66,66	0
58	MG	2A	3182	1/1	0.82	0.17	61,61,61,61	0
58	MG	2A	3750	1/1	0.82	0.18	71,71,71,71	0
58	MG	2A	3388	1/1	0.82	0.11	50,50,50,50	0
58	MG	2A	3389	1/1	0.82	0.19	64,64,64,64	0
58	MG	2A	3391	1/1	0.82	0.21	56,56,56,56	0
58	MG	2A	3406	1/1	0.82	0.16	49,49,49,49	0
58	MG	1A	3158	1/1	0.82	0.11	55,55,55,55	0
58	MG	2a	3179	1/1	0.82	0.17	76,76,76,76	0
58	MG	1A	3027	1/1	0.82	0.29	74,74,74,74	0
58	MG	2a	3183	1/1	0.82	0.16	62,62,62,62	0
58	MG	1A	3595	1/1	0.82	0.13	47,47,47,47	0
58	MG	2a	3186	1/1	0.82	0.20	67,67,67,67	0
58	MG	2A	3811	1/1	0.82	0.13	74,74,74,74	0
58	MG	1A	3438	1/1	0.82	0.10	51,51,51,51	0
58	MG	2A	3817	1/1	0.82	0.13	67,67,67,67	0
58	MG	2a	3197	1/1	0.82	0.23	72,72,72,72	0
58	MG	2a	3204	1/1	0.82	0.35	72,72,72,72	0
58	MG	14	101	1/1	0.82	0.13	63,63,63,63	0
58	MG	2B	205	1/1	0.82	0.09	63,63,63,63	0
58	MG	1A	3293	1/1	0.82	0.27	71,71,71,71	0
58	MG	2A	3474	1/1	0.82	0.28	73,73,73,73	0
58	MG	1A	3980	1/1	0.82	0.13	23,23,23,23	0
58	MG	2A	3505	1/1	0.82	0.17	66,66,66,66	0
58	MG	2A	3721	1/1	0.83	0.20	65,65,65,65	0
58	MG	1a	1677	1/1	0.83	0.24	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	3096	1/1	0.83	0.19	62,62,62,62	0
58	MG	1A	3002	1/1	0.83	0.16	54,54,54,54	0
58	MG	2A	3008	1/1	0.83	0.18	51,51,51,51	0
58	MG	1A	3912	1/1	0.83	0.17	40,40,40,40	0
58	MG	2A	3287	1/1	0.83	0.23	66,66,66,66	0
58	MG	2a	3120	1/1	0.83	0.19	69,69,69,69	0
58	MG	1B	216	1/1	0.83	0.18	70,70,70,70	0
58	MG	2A	3526	1/1	0.83	0.13	60,60,60,60	0
58	MG	2A	3784	1/1	0.83	0.16	76,76,76,76	0
58	MG	2A	3149	1/1	0.83	0.18	57,57,57,57	0
58	MG	1a	1613	1/1	0.83	0.18	61,61,61,61	0
58	MG	2A	3185	1/1	0.83	0.40	73,73,73,73	0
58	MG	2A	3810	1/1	0.83	0.11	55,55,55,55	0
58	MG	2a	3141	1/1	0.83	0.18	62,62,62,62	0
58	MG	1A	3666	1/1	0.83	0.14	58,58,58,58	0
58	MG	1A	3060	1/1	0.83	0.20	50,50,50,50	0
58	MG	2A	3046	1/1	0.83	0.21	65,65,65,65	0
58	MG	2A	3047	1/1	0.83	0.13	59,59,59,59	0
58	MG	1a	1744	1/1	0.83	0.13	48,48,48,48	0
58	MG	2A	3384	1/1	0.83	0.11	46,46,46,46	0
58	MG	2W	201	1/1	0.83	0.15	57,57,57,57	0
58	MG	1B	232	1/1	0.83	0.11	86,86,86,86	0
58	MG	2A	3231	1/1	0.83	0.32	66,66,66,66	0
58	MG	1a	1768	1/1	0.83	0.20	43,43,43,43	0
58	MG	2A	3648	1/1	0.83	0.17	72,72,72,72	0
58	MG	2A	3399	1/1	0.83	0.20	51,51,51,51	0
58	MG	2A	3651	1/1	0.83	0.10	57,57,57,57	0
58	MG	2a	3027	1/1	0.83	0.28	70,70,70,70	0
58	MG	1A	3368	1/1	0.83	0.20	53,53,53,53	0
58	MG	2A	3066	1/1	0.83	0.12	61,61,61,61	0
58	MG	1A	3457	1/1	0.83	0.11	57,57,57,57	0
58	MG	2a	3051	1/1	0.83	0.10	66,66,66,66	0
58	MG	2a	3052	1/1	0.83	0.22	83,83,83,83	0
58	MG	2A	3712	1/1	0.83	0.15	52,52,52,52	0
58	MG	1A	3955	1/1	0.83	0.12	60,60,60,60	0
58	MG	2A	3448	1/1	0.83	0.16	59,59,59,59	0
58	MG	2w	102	1/1	0.83	0.19	77,77,77,77	0
58	MG	2a	3090	1/1	0.83	0.12	63,63,63,63	0
58	MG	2A	3285	1/1	0.84	0.20	59,59,59,59	0
58	MG	1A	3810	1/1	0.84	0.14	32,32,32,32	0
58	MG	1A	3573	1/1	0.84	0.23	57,57,57,57	0
58	MG	2a	3040	1/1	0.84	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	3048	1/1	0.84	0.15	62,62,62,62	0
58	MG	1Q	204	1/1	0.84	0.07	47,47,47,47	0
58	MG	1A	3970	1/1	0.84	0.12	31,31,31,31	0
58	MG	2a	3060	1/1	0.84	0.21	68,68,68,68	0
58	MG	2A	3071	1/1	0.84	0.22	60,60,60,60	0
58	MG	2a	3065	1/1	0.84	0.15	61,61,61,61	0
58	MG	1A	3700	1/1	0.84	0.12	50,50,50,50	0
58	MG	1a	1731	1/1	0.84	0.13	81,81,81,81	0
58	MG	2a	3084	1/1	0.84	0.18	61,61,61,61	0
58	MG	2a	3085	1/1	0.84	0.18	77,77,77,77	0
58	MG	2A	3313	1/1	0.84	0.10	76,76,76,76	0
58	MG	1A	3323	1/1	0.84	0.18	44,44,44,44	0
58	MG	1A	3332	1/1	0.84	0.10	42,42,42,42	0
58	MG	1A	3496	1/1	0.84	0.13	48,48,48,48	0
58	MG	2A	3360	1/1	0.84	0.18	68,68,68,68	0
58	MG	1a	1757	1/1	0.84	0.15	59,59,59,59	0
58	MG	1a	1760	1/1	0.84	0.21	61,61,61,61	0
58	MG	2a	3105	1/1	0.84	0.24	75,75,75,75	0
58	MG	1A	3420	1/1	0.84	0.14	46,46,46,46	0
58	MG	1a	1776	1/1	0.84	0.16	56,56,56,56	0
58	MG	2A	3730	1/1	0.84	0.11	67,67,67,67	0
58	MG	1a	1795	1/1	0.84	0.21	66,66,66,66	0
58	MG	1A	3671	1/1	0.84	0.17	45,45,45,45	0
58	MG	1A	4068	1/1	0.84	0.14	79,79,79,79	0
58	MG	1w	101	1/1	0.84	0.10	69,69,69,69	0
58	MG	2A	3428	1/1	0.84	0.18	69,69,69,69	0
58	MG	2A	3775	1/1	0.84	0.18	39,39,39,39	0
58	MG	1a	1623	1/1	0.84	0.22	65,65,65,65	0
58	MG	2a	3145	1/1	0.84	0.11	82,82,82,82	0
58	MG	2A	3446	1/1	0.84	0.20	69,69,69,69	0
58	MG	1A	3270	1/1	0.84	0.21	59,59,59,59	0
58	MG	1a	1639	1/1	0.84	0.21	60,60,60,60	0
58	MG	1A	3561	1/1	0.84	0.10	54,54,54,54	0
58	MG	2a	3172	1/1	0.84	0.18	71,71,71,71	0
58	MG	1a	1648	1/1	0.84	0.31	64,64,64,64	0
58	MG	2a	3174	1/1	0.84	0.21	70,70,70,70	0
58	MG	1a	1649	1/1	0.84	0.26	57,57,57,57	0
58	MG	2A	3481	1/1	0.84	0.11	52,52,52,52	0
58	MG	1B	209	1/1	0.84	0.30	64,64,64,64	0
58	MG	2A	3819	1/1	0.84	0.14	66,66,66,66	0
58	MG	2A	3824	1/1	0.84	0.15	58,58,58,58	0
58	MG	2A	3502	1/1	0.84	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3365	1/1	0.84	0.24	41,41,41,41	0
58	MG	2A	3513	1/1	0.84	0.13	54,54,54,54	0
58	MG	2B	215	1/1	0.84	0.23	75,75,75,75	0
58	MG	1A	3797	1/1	0.84	0.11	35,35,35,35	0
58	MG	1a	1675	1/1	0.84	0.17	66,66,66,66	0
58	MG	2A	3272	1/1	0.84	0.12	78,78,78,78	0
58	MG	1A	3947	1/1	0.84	0.15	17,17,17,17	0
58	MG	1a	1682	1/1	0.84	0.08	61,61,61,61	0
58	MG	2A	3052	1/1	0.84	0.16	76,76,76,76	0
58	MG	2A	3282	1/1	0.84	0.14	62,62,62,62	0
58	MG	2v	101	1/1	0.84	0.09	60,60,60,60	0
58	MG	2a	3017	1/1	0.84	0.18	63,63,63,63	0
58	MG	2A	3570	1/1	0.84	0.11	52,52,52,52	0
58	MG	2a	3032	1/1	0.84	0.19	80,80,80,80	0
58	MG	2x	104	1/1	0.84	0.27	74,74,74,74	0
58	MG	1a	1631	1/1	0.85	0.27	59,59,59,59	0
58	MG	1A	3189	1/1	0.85	0.17	57,57,57,57	0
58	MG	1A	3062	1/1	0.85	0.16	50,50,50,50	0
58	MG	2A	3581	1/1	0.85	0.16	57,57,57,57	0
58	MG	2a	3041	1/1	0.85	0.16	67,67,67,67	0
58	MG	2a	3046	1/1	0.85	0.18	81,81,81,81	0
58	MG	1a	1764	1/1	0.85	0.21	66,66,66,66	0
58	MG	1A	3871	1/1	0.85	0.12	23,23,23,23	0
58	MG	2A	3085	1/1	0.85	0.13	47,47,47,47	0
58	MG	1a	1773	1/1	0.85	0.16	63,63,63,63	0
58	MG	1A	3878	1/1	0.85	0.12	22,22,22,22	0
58	MG	2A	3639	1/1	0.85	0.16	55,55,55,55	0
58	MG	1B	226	1/1	0.85	0.17	59,59,59,59	0
58	MG	2A	3098	1/1	0.85	0.14	58,58,58,58	0
58	MG	2A	3310	1/1	0.85	0.18	65,65,65,65	0
58	MG	2A	3311	1/1	0.85	0.17	78,78,78,78	0
58	MG	2A	3312	1/1	0.85	0.09	63,63,63,63	0
58	MG	1a	1797	1/1	0.85	0.13	66,66,66,66	0
58	MG	2A	3707	1/1	0.85	0.14	64,64,64,64	0
58	MG	2A	3318	1/1	0.85	0.13	57,57,57,57	0
58	MG	2A	3711	1/1	0.85	0.19	63,63,63,63	0
58	MG	2A	3319	1/1	0.85	0.26	72,72,72,72	0
58	MG	1A	3986	1/1	0.85	0.09	74,74,74,74	0
58	MG	2A	3142	1/1	0.85	0.26	67,67,67,67	0
58	MG	2A	3340	1/1	0.85	0.17	66,66,66,66	0
58	MG	2a	3115	1/1	0.85	0.26	69,69,69,69	0
58	MG	1A	3210	1/1	0.85	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3158	1/1	0.85	0.19	68,68,68,68	0
58	MG	2A	3364	1/1	0.85	0.15	62,62,62,62	0
58	MG	2A	3383	1/1	0.85	0.16	51,51,51,51	0
58	MG	2A	3170	1/1	0.85	0.11	50,50,50,50	0
58	MG	2a	3131	1/1	0.85	0.34	76,76,76,76	0
58	MG	1A	3040	1/1	0.85	0.18	58,58,58,58	0
58	MG	1A	3894	1/1	0.85	0.12	52,52,52,52	0
58	MG	1V	201	1/1	0.85	0.30	30,30,30,30	0
58	MG	1A	4020	1/1	0.85	0.38	62,62,62,62	0
58	MG	2A	3400	1/1	0.85	0.21	43,43,43,43	0
58	MG	2A	3007	1/1	0.85	0.19	54,54,54,54	0
58	MG	1A	4025	1/1	0.85	0.12	28,28,28,28	0
58	MG	1A	4031	1/1	0.85	0.12	46,46,46,46	0
58	MG	2A	3223	1/1	0.85	0.15	59,59,59,59	0
58	MG	1A	3353	1/1	0.85	0.11	40,40,40,40	0
58	MG	2A	3444	1/1	0.85	0.30	59,59,59,59	0
58	MG	19	101	1/1	0.85	0.12	55,55,55,55	0
58	MG	1A	3669	1/1	0.85	0.15	47,47,47,47	0
58	MG	2A	3242	1/1	0.85	0.11	57,57,57,57	0
58	MG	2B	202	1/1	0.85	0.11	70,70,70,70	0
58	MG	2A	3037	1/1	0.85	0.15	39,39,39,39	0
58	MG	1a	1714	1/1	0.85	0.15	57,57,57,57	0
58	MG	2A	3251	1/1	0.85	0.23	60,60,60,60	0
58	MG	1a	1716	1/1	0.85	0.09	47,47,47,47	0
58	MG	2a	3189	1/1	0.85	0.26	61,61,61,61	0
58	MG	2D	302	1/1	0.85	0.14	51,51,51,51	0
58	MG	2A	3258	1/1	0.85	0.08	40,40,40,40	0
58	MG	1a	1729	1/1	0.85	0.16	57,57,57,57	0
58	MG	1A	3026	1/1	0.85	0.24	49,49,49,49	0
58	MG	2a	3201	1/1	0.85	0.26	54,54,54,54	0
58	MG	2A	3268	1/1	0.85	0.23	70,70,70,70	0
58	MG	2a	3206	1/1	0.85	0.17	69,69,69,69	0
58	MG	2I	103	1/1	0.85	0.23	65,65,65,65	0
58	MG	2A	3269	1/1	0.85	0.32	63,63,63,63	0
58	MG	2a	3006	1/1	0.85	0.28	72,72,72,72	0
58	MG	1A	3753	1/1	0.85	0.10	19,19,19,19	0
58	MG	1a	1739	1/1	0.85	0.11	63,63,63,63	0
58	MG	1A	3570	1/1	0.85	0.11	32,32,32,32	0
58	MG	2a	3023	1/1	0.85	0.14	65,65,65,65	0
58	MG	2A	3552	1/1	0.85	0.17	65,65,65,65	0
58	MG	2A	3280	1/1	0.85	0.22	57,57,57,57	0
58	MG	2A	3375	1/1	0.86	0.21	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	3038	1/1	0.86	0.23	75,75,75,75	0
58	MG	1W	201	1/1	0.86	0.27	51,51,51,51	0
58	MG	1A	3462	1/1	0.86	0.12	50,50,50,50	0
58	MG	1A	3629	1/1	0.86	0.17	62,62,62,62	0
58	MG	2A	3663	1/1	0.86	0.14	46,46,46,46	0
58	MG	2A	3666	1/1	0.86	0.10	57,57,57,57	0
58	MG	1a	1779	1/1	0.86	0.22	56,56,56,56	0
58	MG	1A	3635	1/1	0.86	0.10	37,37,37,37	0
58	MG	2A	3074	1/1	0.86	0.17	65,65,65,65	0
58	MG	1Z	302	1/1	0.86	0.07	57,57,57,57	0
58	MG	2a	3070	1/1	0.86	0.30	73,73,73,73	0
58	MG	1A	3823	1/1	0.86	0.15	63,63,63,63	0
58	MG	1A	3207	1/1	0.86	0.22	57,57,57,57	0
58	MG	2A	3716	1/1	0.86	0.11	47,47,47,47	0
58	MG	2A	3267	1/1	0.86	0.14	67,67,67,67	0
58	MG	2a	3086	1/1	0.86	0.26	54,54,54,54	0
58	MG	2A	3417	1/1	0.86	0.14	65,65,65,65	0
58	MG	1a	1603	1/1	0.86	0.17	57,57,57,57	0
58	MG	1w	104	1/1	0.86	0.26	71,71,71,71	0
58	MG	2A	3735	1/1	0.86	0.28	66,66,66,66	0
58	MG	2A	3741	1/1	0.86	0.18	56,56,56,56	0
58	MG	1a	1701	1/1	0.86	0.12	58,58,58,58	0
58	MG	1A	3474	1/1	0.86	0.11	54,54,54,54	0
58	MG	2A	3275	1/1	0.86	0.23	52,52,52,52	0
58	MG	2A	3449	1/1	0.86	0.28	53,53,53,53	0
58	MG	2A	3100	1/1	0.86	0.13	47,47,47,47	0
58	MG	1A	3482	1/1	0.86	0.30	54,54,54,54	0
58	MG	2A	3107	1/1	0.86	0.16	55,55,55,55	0
58	MG	2A	3120	1/1	0.86	0.24	66,66,66,66	0
58	MG	2A	3788	1/1	0.86	0.13	43,43,43,43	0
58	MG	2A	3004	1/1	0.86	0.28	58,58,58,58	0
58	MG	2A	3482	1/1	0.86	0.10	66,66,66,66	0
58	MG	2A	3486	1/1	0.86	0.23	75,75,75,75	0
58	MG	2A	3805	1/1	0.86	0.23	52,52,52,52	0
58	MG	1A	3377	1/1	0.86	0.13	55,55,55,55	0
58	MG	2A	3291	1/1	0.86	0.12	54,54,54,54	0
58	MG	1a	1617	1/1	0.86	0.10	55,55,55,55	0
58	MG	2A	3815	1/1	0.86	0.24	67,67,67,67	0
58	MG	2A	3508	1/1	0.86	0.17	62,62,62,62	0
58	MG	2A	3150	1/1	0.86	0.13	69,69,69,69	0
58	MG	2A	3821	1/1	0.86	0.15	65,65,65,65	0
58	MG	1a	1728	1/1	0.86	0.11	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2B	201	1/1	0.86	0.12	71,71,71,71	0
58	MG	2A	3022	1/1	0.86	0.21	54,54,54,54	0
58	MG	2B	203	1/1	0.86	0.15	66,66,66,66	0
58	MG	2A	3305	1/1	0.86	0.25	68,68,68,68	0
58	MG	2A	3543	1/1	0.86	0.15	61,61,61,61	0
58	MG	2A	3181	1/1	0.86	0.29	73,73,73,73	0
58	MG	2A	3550	1/1	0.86	0.16	65,65,65,65	0
58	MG	1B	225	1/1	0.86	0.20	45,45,45,45	0
58	MG	2E	305	1/1	0.86	0.10	26,26,26,26	0
58	MG	2P	202	1/1	0.86	0.18	62,62,62,62	0
58	MG	1A	3675	1/1	0.86	0.14	32,32,32,32	0
58	MG	1A	3686	1/1	0.86	0.09	25,25,25,25	0
58	MG	1a	1637	1/1	0.86	0.24	70,70,70,70	0
58	MG	2a	3195	1/1	0.86	0.11	65,65,65,65	0
58	MG	2A	3039	1/1	0.86	0.16	57,57,57,57	0
58	MG	1A	3574	1/1	0.86	0.21	38,38,38,38	0
58	MG	2A	3209	1/1	0.86	0.21	64,64,64,64	0
58	MG	2a	3205	1/1	0.86	0.21	69,69,69,69	0
58	MG	2A	3219	1/1	0.86	0.10	46,46,46,46	0
58	MG	2A	3590	1/1	0.86	0.12	19,19,19,19	0
58	MG	1E	308	1/1	0.86	0.11	29,29,29,29	0
58	MG	2A	3619	1/1	0.86	0.14	41,41,41,41	0
58	MG	2a	3018	1/1	0.86	0.20	62,62,62,62	0
58	MG	2l	204	1/1	0.86	0.12	69,69,69,69	0
58	MG	1A	3431	1/1	0.86	0.20	46,46,46,46	0
58	MG	1A	3806	1/1	0.86	0.09	46,46,46,46	0
58	MG	2A	3229	1/1	0.86	0.13	67,67,67,67	0
58	MG	2A	3646	1/1	0.86	0.15	67,67,67,67	0
58	MG	1A	3170	1/1	0.86	0.13	45,45,45,45	0
58	MG	1a	1808	1/1	0.87	0.16	57,57,57,57	0
58	MG	1a	1809	1/1	0.87	0.23	70,70,70,70	0
58	MG	1B	203	1/1	0.87	0.14	47,47,47,47	0
58	MG	2A	3599	1/1	0.87	0.26	66,66,66,66	0
58	MG	2A	3604	1/1	0.87	0.14	60,60,60,60	0
58	MG	2a	3021	1/1	0.87	0.42	73,73,73,73	0
58	MG	2a	3022	1/1	0.87	0.15	68,68,68,68	0
58	MG	2A	3155	1/1	0.87	0.12	43,43,43,43	0
58	MG	2a	3025	1/1	0.87	0.26	72,72,72,72	0
58	MG	2a	3026	1/1	0.87	0.13	77,77,77,77	0
58	MG	1A	3578	1/1	0.87	0.12	41,41,41,41	0
58	MG	1A	3010	1/1	0.87	0.08	40,40,40,40	0
58	MG	2A	3634	1/1	0.87	0.28	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	3035	1/1	0.87	0.22	71,71,71,71	0
58	MG	2A	3636	1/1	0.87	0.18	69,69,69,69	0
58	MG	1A	3597	1/1	0.87	0.16	59,59,59,59	0
58	MG	1A	3485	1/1	0.87	0.15	55,55,55,55	0
58	MG	2A	3641	1/1	0.87	0.12	60,60,60,60	0
58	MG	2A	3184	1/1	0.87	0.17	57,57,57,57	0
58	MG	2a	3042	1/1	0.87	0.10	57,57,57,57	0
58	MG	2a	3044	1/1	0.87	0.11	52,52,52,52	0
58	MG	1A	3248	1/1	0.87	0.13	56,56,56,56	0
58	MG	1A	3929	1/1	0.87	0.14	30,30,30,30	0
58	MG	2a	3050	1/1	0.87	0.18	75,75,75,75	0
58	MG	1A	3931	1/1	0.87	0.18	61,61,61,61	0
58	MG	1a	1670	1/1	0.87	0.18	62,62,62,62	0
58	MG	2A	3357	1/1	0.87	0.27	70,70,70,70	0
58	MG	2A	3656	1/1	0.87	0.20	63,63,63,63	0
58	MG	1a	1673	1/1	0.87	0.21	60,60,60,60	0
58	MG	1A	3320	1/1	0.87	0.08	42,42,42,42	0
58	MG	2A	3368	1/1	0.87	0.13	58,58,58,58	0
58	MG	2A	3706	1/1	0.87	0.13	48,48,48,48	0
58	MG	2A	3371	1/1	0.87	0.16	46,46,46,46	0
58	MG	1A	3508	1/1	0.87	0.16	76,76,76,76	0
58	MG	1A	3639	1/1	0.87	0.12	48,48,48,48	0
58	MG	2A	3222	1/1	0.87	0.10	36,36,36,36	0
58	MG	2A	3713	1/1	0.87	0.14	43,43,43,43	0
58	MG	1a	1686	1/1	0.87	0.24	59,59,59,59	0
58	MG	2A	3225	1/1	0.87	0.12	57,57,57,57	0
58	MG	1N	204	1/1	0.87	0.11	43,43,43,43	0
58	MG	1P	207	1/1	0.87	0.14	48,48,48,48	0
58	MG	2A	3230	1/1	0.87	0.18	78,78,78,78	0
58	MG	2a	3102	1/1	0.87	0.10	61,61,61,61	0
58	MG	2A	3729	1/1	0.87	0.15	61,61,61,61	0
58	MG	2A	3405	1/1	0.87	0.20	51,51,51,51	0
58	MG	2a	3114	1/1	0.87	0.15	62,62,62,62	0
58	MG	1A	3644	1/1	0.87	0.19	41,41,41,41	0
58	MG	1A	3653	1/1	0.87	0.13	25,25,25,25	0
58	MG	2A	3742	1/1	0.87	0.12	46,46,46,46	0
58	MG	2A	3743	1/1	0.87	0.11	65,65,65,65	0
58	MG	2a	3128	1/1	0.87	0.18	69,69,69,69	0
58	MG	2A	3409	1/1	0.87	0.20	46,46,46,46	0
58	MG	2A	3413	1/1	0.87	0.11	60,60,60,60	0
58	MG	2A	3234	1/1	0.87	0.07	56,56,56,56	0
58	MG	2A	3239	1/1	0.87	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3760	1/1	0.87	0.11	64,64,64,64	0
58	MG	1A	3966	1/1	0.87	0.17	62,62,62,62	0
58	MG	2a	3140	1/1	0.87	0.18	59,59,59,59	0
58	MG	1A	3968	1/1	0.87	0.11	34,34,34,34	0
58	MG	1A	3800	1/1	0.87	0.13	54,54,54,54	0
58	MG	2A	3248	1/1	0.87	0.15	75,75,75,75	0
58	MG	2A	3249	1/1	0.87	0.15	44,44,44,44	0
58	MG	2A	3792	1/1	0.87	0.09	60,60,60,60	0
58	MG	2a	3164	1/1	0.87	0.22	63,63,63,63	0
58	MG	1A	3258	1/1	0.87	0.15	51,51,51,51	0
58	MG	1A	3261	1/1	0.87	0.08	44,44,44,44	0
58	MG	2A	3255	1/1	0.87	0.16	67,67,67,67	0
58	MG	1A	3544	1/1	0.87	0.12	36,36,36,36	0
58	MG	2A	3809	1/1	0.87	0.11	74,74,74,74	0
58	MG	2A	3468	1/1	0.87	0.09	54,54,54,54	0
58	MG	2A	3471	1/1	0.87	0.16	72,72,72,72	0
58	MG	10	108	1/1	0.87	0.12	49,49,49,49	0
58	MG	2A	3265	1/1	0.87	0.21	68,68,68,68	0
58	MG	2a	3184	1/1	0.87	0.24	70,70,70,70	0
58	MG	1A	3547	1/1	0.87	0.15	44,44,44,44	0
58	MG	15	107	1/1	0.87	0.22	33,33,33,33	0
58	MG	1A	3324	1/1	0.87	0.17	45,45,45,45	0
58	MG	1a	1602	1/1	0.87	0.21	58,58,58,58	0
58	MG	1a	1756	1/1	0.87	0.09	72,72,72,72	0
58	MG	1A	3383	1/1	0.87	0.39	41,41,41,41	0
58	MG	1A	3854	1/1	0.87	0.10	31,31,31,31	0
58	MG	2a	3196	1/1	0.87	0.09	73,73,73,73	0
58	MG	2A	3516	1/1	0.87	0.23	65,65,65,65	0
58	MG	1A	3387	1/1	0.87	0.14	71,71,71,71	0
58	MG	1A	4060	1/1	0.87	0.18	54,54,54,54	0
58	MG	1A	3105	1/1	0.87	0.13	37,37,37,37	0
58	MG	1A	3333	1/1	0.87	0.18	67,67,67,67	0
58	MG	2a	3209	1/1	0.87	0.23	70,70,70,70	0
58	MG	1a	1627	1/1	0.87	0.18	66,66,66,66	0
58	MG	2F	303	1/1	0.87	0.14	67,67,67,67	0
58	MG	2A	3104	1/1	0.87	0.12	57,57,57,57	0
58	MG	2A	3289	1/1	0.87	0.11	48,48,48,48	0
58	MG	1A	3875	1/1	0.87	0.10	42,42,42,42	0
58	MG	1A	3577	1/1	0.87	0.20	53,53,53,53	0
58	MG	2A	3124	1/1	0.87	0.18	72,72,72,72	0
58	MG	1a	1806	1/1	0.87	0.31	54,54,54,54	0
58	MG	28	102	1/1	0.87	0.23	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3141	1/1	0.87	0.13	51,51,51,51	0
58	MG	1A	3451	1/1	0.88	0.23	43,43,43,43	0
58	MG	1a	1661	1/1	0.88	0.16	69,69,69,69	0
58	MG	2A	3042	1/1	0.88	0.20	53,53,53,53	0
58	MG	1A	3874	1/1	0.88	0.09	23,23,23,23	0
58	MG	1A	3571	1/1	0.88	0.10	40,40,40,40	0
58	MG	2A	3049	1/1	0.88	0.15	63,63,63,63	0
58	MG	1A	3339	1/1	0.88	0.15	60,60,60,60	0
58	MG	1A	3024	1/1	0.88	0.24	55,55,55,55	0
58	MG	2A	3571	1/1	0.88	0.19	66,66,66,66	0
58	MG	2a	3019	1/1	0.88	0.13	59,59,59,59	0
58	MG	1A	3277	1/1	0.88	0.17	61,61,61,61	0
58	MG	2A	3061	1/1	0.88	0.17	52,52,52,52	0
58	MG	1a	1681	1/1	0.88	0.17	63,63,63,63	0
58	MG	1A	3891	1/1	0.88	0.17	51,51,51,51	0
58	MG	1A	3703	1/1	0.88	0.11	45,45,45,45	0
58	MG	1A	3911	1/1	0.88	0.14	68,68,68,68	0
58	MG	1a	1693	1/1	0.88	0.22	57,57,57,57	0
58	MG	1A	3713	1/1	0.88	0.10	72,72,72,72	0
58	MG	2A	3623	1/1	0.88	0.21	61,61,61,61	0
58	MG	1D	302	1/1	0.88	0.36	54,54,54,54	0
58	MG	2A	3630	1/1	0.88	0.16	56,56,56,56	0
58	MG	2A	3631	1/1	0.88	0.19	69,69,69,69	0
58	MG	2A	3297	1/1	0.88	0.18	64,64,64,64	0
58	MG	1D	306	1/1	0.88	0.10	35,35,35,35	0
58	MG	1A	3154	1/1	0.88	0.14	43,43,43,43	0
58	MG	2A	3304	1/1	0.88	0.15	63,63,63,63	0
58	MG	1F	308	1/1	0.88	0.09	44,44,44,44	0
58	MG	1F	311	1/1	0.88	0.11	47,47,47,47	0
58	MG	1A	3928	1/1	0.88	0.16	24,24,24,24	0
58	MG	1A	3463	1/1	0.88	0.15	46,46,46,46	0
58	MG	1A	3469	1/1	0.88	0.17	48,48,48,48	0
58	MG	1A	3598	1/1	0.88	0.10	17,17,17,17	0
58	MG	2A	3652	1/1	0.88	0.18	56,56,56,56	0
58	MG	1A	3302	1/1	0.88	0.14	37,37,37,37	0
58	MG	2a	3069	1/1	0.88	0.20	69,69,69,69	0
58	MG	2A	3109	1/1	0.88	0.17	48,48,48,48	0
58	MG	1V	203	1/1	0.88	0.75	36,36,36,36	0
58	MG	2a	3072	1/1	0.88	0.12	50,50,50,50	0
58	MG	1A	3311	1/1	0.88	0.12	39,39,39,39	0
58	MG	2a	3083	1/1	0.88	0.24	61,61,61,61	0
58	MG	2A	3671	1/1	0.88	0.08	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3692	1/1	0.88	0.15	53,53,53,53	0
58	MG	1a	1750	1/1	0.88	0.18	65,65,65,65	0
58	MG	2A	3698	1/1	0.88	0.17	60,60,60,60	0
58	MG	1A	3315	1/1	0.88	0.11	53,53,53,53	0
58	MG	1A	3222	1/1	0.88	0.16	37,37,37,37	0
58	MG	2A	3348	1/1	0.88	0.16	65,65,65,65	0
58	MG	1A	3959	1/1	0.88	0.12	42,42,42,42	0
58	MG	2A	3358	1/1	0.88	0.10	66,66,66,66	0
58	MG	2a	3099	1/1	0.88	0.13	75,75,75,75	0
58	MG	1A	3075	1/1	0.88	0.14	57,57,57,57	0
58	MG	2A	3362	1/1	0.88	0.10	58,58,58,58	0
58	MG	1A	3399	1/1	0.88	0.14	55,55,55,55	0
58	MG	2A	3156	1/1	0.88	0.11	52,52,52,52	0
58	MG	13	104	1/1	0.88	0.16	58,58,58,58	0
58	MG	2A	3159	1/1	0.88	0.15	74,74,74,74	0
58	MG	2A	3161	1/1	0.88	0.18	76,76,76,76	0
58	MG	1A	3249	1/1	0.88	0.11	51,51,51,51	0
58	MG	2a	3123	1/1	0.88	0.27	56,56,56,56	0
58	MG	2A	3175	1/1	0.88	0.23	60,60,60,60	0
58	MG	2A	3740	1/1	0.88	0.10	72,72,72,72	0
58	MG	2A	3179	1/1	0.88	0.10	51,51,51,51	0
58	MG	1A	3979	1/1	0.88	0.10	20,20,20,20	0
58	MG	18	102	1/1	0.88	0.08	36,36,36,36	0
58	MG	2A	3183	1/1	0.88	0.14	66,66,66,66	0
58	MG	1a	1793	1/1	0.88	0.18	55,55,55,55	0
58	MG	1a	1794	1/1	0.88	0.18	53,53,53,53	0
58	MG	2A	3757	1/1	0.88	0.16	72,72,72,72	0
58	MG	1A	3322	1/1	0.88	0.13	53,53,53,53	0
58	MG	1A	3981	1/1	0.88	0.13	39,39,39,39	0
58	MG	2A	3767	1/1	0.88	0.16	67,67,67,67	0
58	MG	2a	3158	1/1	0.88	0.28	77,77,77,77	0
58	MG	2A	3412	1/1	0.88	0.24	46,46,46,46	0
58	MG	1A	3533	1/1	0.88	0.10	55,55,55,55	0
58	MG	1A	3251	1/1	0.88	0.15	49,49,49,49	0
58	MG	2a	3169	1/1	0.88	0.27	57,57,57,57	0
58	MG	1A	4010	1/1	0.88	0.16	42,42,42,42	0
58	MG	2A	3211	1/1	0.88	0.22	57,57,57,57	0
58	MG	1n	101	1/1	0.88	0.31	57,57,57,57	0
58	MG	1A	3197	1/1	0.88	0.21	50,50,50,50	0
58	MG	2A	3445	1/1	0.88	0.21	55,55,55,55	0
58	MG	1A	3840	1/1	0.88	0.14	63,63,63,63	0
58	MG	1A	3846	1/1	0.88	0.26	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1w	102	1/1	0.88	0.10	78,78,78,78	0
58	MG	1A	3852	1/1	0.88	0.11	43,43,43,43	0
58	MG	1x	105	1/1	0.88	0.25	63,63,63,63	0
58	MG	2A	3463	1/1	0.88	0.26	60,60,60,60	0
58	MG	2A	3813	1/1	0.88	0.09	53,53,53,53	0
58	MG	2a	3187	1/1	0.88	0.29	68,68,68,68	0
58	MG	2a	3188	1/1	0.88	0.26	61,61,61,61	0
58	MG	1a	1628	1/1	0.88	0.13	64,64,64,64	0
58	MG	1a	1630	1/1	0.88	0.11	45,45,45,45	0
58	MG	1A	4029	1/1	0.88	0.16	46,46,46,46	0
58	MG	2A	3001	1/1	0.88	0.30	53,53,53,53	0
58	MG	1A	3853	1/1	0.88	0.09	49,49,49,49	0
58	MG	2A	3005	1/1	0.88	0.16	56,56,56,56	0
58	MG	2A	3006	1/1	0.88	0.16	39,39,39,39	0
58	MG	1A	3112	1/1	0.88	0.10	32,32,32,32	0
58	MG	2A	3490	1/1	0.88	0.18	59,59,59,59	0
58	MG	2A	3498	1/1	0.88	0.11	49,49,49,49	0
58	MG	1A	3864	1/1	0.88	0.14	45,45,45,45	0
58	MG	1a	1641	1/1	0.88	0.14	51,51,51,51	0
58	MG	2B	219	1/1	0.88	0.13	65,65,65,65	0
58	MG	1A	3866	1/1	0.88	0.12	30,30,30,30	0
58	MG	2A	3027	1/1	0.88	0.12	45,45,45,45	0
58	MG	1a	1644	1/1	0.88	0.24	66,66,66,66	0
58	MG	2O	201	1/1	0.88	0.22	72,72,72,72	0
58	MG	1A	3267	1/1	0.88	0.23	62,62,62,62	0
58	MG	2T	202	1/1	0.88	0.23	70,70,70,70	0
58	MG	1A	3449	1/1	0.88	0.27	55,55,55,55	0
58	MG	2x	101	1/1	0.88	0.24	66,66,66,66	0
58	MG	2A	3539	1/1	0.88	0.16	46,46,46,46	0
58	MG	1A	4080	1/1	0.88	0.16	41,41,41,41	0
58	MG	2a	3031	1/1	0.89	0.30	58,58,58,58	0
58	MG	2A	3664	1/1	0.89	0.20	67,67,67,67	0
58	MG	1A	3129	1/1	0.89	0.15	33,33,33,33	0
58	MG	2A	3404	1/1	0.89	0.18	52,52,52,52	0
58	MG	2A	3683	1/1	0.89	0.09	65,65,65,65	0
58	MG	2A	3689	1/1	0.89	0.10	59,59,59,59	0
58	MG	11	102	1/1	0.89	0.14	56,56,56,56	0
58	MG	2a	3039	1/1	0.89	0.24	61,61,61,61	0
58	MG	1A	3181	1/1	0.89	0.22	34,34,34,34	0
58	MG	1A	3089	1/1	0.89	0.23	37,37,37,37	0
58	MG	2A	3701	1/1	0.89	0.24	45,45,45,45	0
58	MG	2a	3043	1/1	0.89	0.30	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3702	1/1	0.89	0.15	62,62,62,62	0
58	MG	1A	3134	1/1	0.89	0.11	44,44,44,44	0
58	MG	1A	3592	1/1	0.89	0.12	39,39,39,39	0
58	MG	1A	4035	1/1	0.89	0.10	48,48,48,48	0
58	MG	2A	3055	1/1	0.89	0.17	54,54,54,54	0
58	MG	2A	3416	1/1	0.89	0.28	46,46,46,46	0
58	MG	2a	3056	1/1	0.89	0.17	51,51,51,51	0
58	MG	1A	4038	1/1	0.89	0.10	34,34,34,34	0
58	MG	2a	3061	1/1	0.89	0.15	63,63,63,63	0
58	MG	2A	3423	1/1	0.89	0.22	40,40,40,40	0
58	MG	2A	3426	1/1	0.89	0.25	57,57,57,57	0
58	MG	2a	3066	1/1	0.89	0.25	69,69,69,69	0
58	MG	2a	3068	1/1	0.89	0.11	76,76,76,76	0
58	MG	1A	3877	1/1	0.89	0.13	52,52,52,52	0
58	MG	1A	3259	1/1	0.89	0.14	54,54,54,54	0
58	MG	2A	3442	1/1	0.89	0.11	41,41,41,41	0
58	MG	2A	3063	1/1	0.89	0.18	49,49,49,49	0
58	MG	2a	3078	1/1	0.89	0.22	65,65,65,65	0
58	MG	1a	1609	1/1	0.89	0.15	57,57,57,57	0
58	MG	1A	3733	1/1	0.89	0.16	59,59,59,59	0
58	MG	1A	3059	1/1	0.89	0.12	39,39,39,39	0
58	MG	2A	3073	1/1	0.89	0.12	42,42,42,42	0
58	MG	1a	1759	1/1	0.89	0.08	58,58,58,58	0
58	MG	1A	4074	1/1	0.89	0.19	67,67,67,67	0
58	MG	2A	3747	1/1	0.89	0.10	56,56,56,56	0
58	MG	2A	3082	1/1	0.89	0.18	75,75,75,75	0
58	MG	1A	3887	1/1	0.89	0.13	48,48,48,48	0
58	MG	2A	3753	1/1	0.89	0.13	57,57,57,57	0
58	MG	1a	1624	1/1	0.89	0.23	52,52,52,52	0
58	MG	1A	3263	1/1	0.89	0.19	56,56,56,56	0
58	MG	2A	3091	1/1	0.89	0.14	60,60,60,60	0
58	MG	2A	3759	1/1	0.89	0.13	65,65,65,65	0
58	MG	2a	3103	1/1	0.89	0.17	68,68,68,68	0
58	MG	2a	3104	1/1	0.89	0.11	60,60,60,60	0
58	MG	2A	3478	1/1	0.89	0.07	61,61,61,61	0
58	MG	1A	3418	1/1	0.89	0.21	55,55,55,55	0
58	MG	2a	3112	1/1	0.89	0.25	53,53,53,53	0
58	MG	1a	1629	1/1	0.89	0.22	52,52,52,52	0
58	MG	1a	1783	1/1	0.89	0.12	66,66,66,66	0
58	MG	2a	3119	1/1	0.89	0.40	71,71,71,71	0
58	MG	2A	3099	1/1	0.89	0.16	44,44,44,44	0
58	MG	1a	1787	1/1	0.89	0.17	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3607	1/1	0.89	0.09	39,39,39,39	0
58	MG	1A	3054	1/1	0.89	0.11	52,52,52,52	0
58	MG	2a	3125	1/1	0.89	0.21	61,61,61,61	0
58	MG	2a	3126	1/1	0.89	0.20	47,47,47,47	0
58	MG	1B	211	1/1	0.89	0.15	58,58,58,58	0
58	MG	2A	3286	1/1	0.89	0.17	70,70,70,70	0
58	MG	1A	3625	1/1	0.89	0.12	48,48,48,48	0
58	MG	2A	3515	1/1	0.89	0.10	40,40,40,40	0
58	MG	2A	3113	1/1	0.89	0.11	68,68,68,68	0
58	MG	1B	215	1/1	0.89	0.16	67,67,67,67	0
58	MG	2a	3134	1/1	0.89	0.23	69,69,69,69	0
58	MG	1A	3626	1/1	0.89	0.12	59,59,59,59	0
58	MG	1A	3798	1/1	0.89	0.12	25,25,25,25	0
58	MG	1A	3325	1/1	0.89	0.26	48,48,48,48	0
58	MG	2a	3144	1/1	0.89	0.11	58,58,58,58	0
58	MG	1A	3934	1/1	0.89	0.09	56,56,56,56	0
58	MG	1A	3803	1/1	0.89	0.11	49,49,49,49	0
58	MG	2a	3154	1/1	0.89	0.21	75,75,75,75	0
58	MG	1A	3329	1/1	0.89	0.20	51,51,51,51	0
58	MG	1A	3509	1/1	0.89	0.08	49,49,49,49	0
58	MG	1A	3948	1/1	0.89	0.09	48,48,48,48	0
58	MG	2A	3558	1/1	0.89	0.20	63,63,63,63	0
58	MG	2a	3166	1/1	0.89	0.13	61,61,61,61	0
58	MG	1x	101	1/1	0.89	0.27	65,65,65,65	0
58	MG	1x	103	1/1	0.89	0.15	56,56,56,56	0
58	MG	1a	1663	1/1	0.89	0.13	66,66,66,66	0
58	MG	2A	3163	1/1	0.89	0.07	43,43,43,43	0
58	MG	2B	210	1/1	0.89	0.14	63,63,63,63	0
58	MG	2A	3164	1/1	0.89	0.13	68,68,68,68	0
58	MG	2B	214	1/1	0.89	0.26	66,66,66,66	0
58	MG	2A	3314	1/1	0.89	0.10	58,58,58,58	0
58	MG	1a	1664	1/1	0.89	0.16	58,58,58,58	0
58	MG	1A	3426	1/1	0.89	0.10	55,55,55,55	0
58	MG	2D	308	1/1	0.89	0.20	53,53,53,53	0
58	MG	2A	3592	1/1	0.89	0.15	56,56,56,56	0
58	MG	1a	1668	1/1	0.89	0.14	52,52,52,52	0
58	MG	2F	306	1/1	0.89	0.14	64,64,64,64	0
58	MG	2G	201	1/1	0.89	0.26	67,67,67,67	0
58	MG	1A	3522	1/1	0.89	0.29	64,64,64,64	0
58	MG	2A	3338	1/1	0.89	0.09	58,58,58,58	0
58	MG	1A	3162	1/1	0.89	0.44	31,31,31,31	0
58	MG	2A	3345	1/1	0.89	0.27	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3542	1/1	0.89	0.15	37,37,37,37	0
58	MG	1A	3829	1/1	0.89	0.11	54,54,54,54	0
58	MG	1A	3084	1/1	0.89	0.17	36,36,36,36	0
58	MG	2A	3187	1/1	0.89	0.21	54,54,54,54	0
58	MG	2a	3203	1/1	0.89	0.19	62,62,62,62	0
58	MG	2A	3188	1/1	0.89	0.20	56,56,56,56	0
58	MG	1A	3335	1/1	0.89	0.15	38,38,38,38	0
58	MG	1A	3169	1/1	0.89	0.17	56,56,56,56	0
58	MG	1A	3450	1/1	0.89	0.11	37,37,37,37	0
58	MG	2a	3008	1/1	0.89	0.25	64,64,64,64	0
58	MG	2a	3211	1/1	0.89	0.18	68,68,68,68	0
58	MG	2A	3204	1/1	0.89	0.25	56,56,56,56	0
58	MG	1A	3985	1/1	0.89	0.12	63,63,63,63	0
58	MG	1A	3300	1/1	0.89	0.10	33,33,33,33	0
58	MG	1A	3861	1/1	0.89	0.30	40,40,40,40	0
58	MG	2t	201	1/1	0.89	0.19	49,49,49,49	0
58	MG	2A	3650	1/1	0.89	0.10	45,45,45,45	0
58	MG	1A	3356	1/1	0.89	0.11	48,48,48,48	0
58	MG	1a	1703	1/1	0.89	0.09	57,57,57,57	0
58	MG	2A	3038	1/1	0.89	0.14	61,61,61,61	0
58	MG	2A	3398	1/1	0.89	0.21	51,51,51,51	0
58	MG	1A	3228	1/1	0.89	0.08	38,38,38,38	0
58	MG	2a	3016	1/1	0.90	0.12	61,61,61,61	0
58	MG	1A	3099	1/1	0.90	0.20	43,43,43,43	0
58	MG	1A	3621	1/1	0.90	0.13	53,53,53,53	0
58	MG	1X	105	1/1	0.90	0.08	43,43,43,43	0
58	MG	1A	3807	1/1	0.90	0.09	23,23,23,23	0
58	MG	2A	3608	1/1	0.90	0.14	37,37,37,37	0
58	MG	2A	3306	1/1	0.90	0.12	55,55,55,55	0
58	MG	1A	3489	1/1	0.90	0.08	58,58,58,58	0
58	MG	2A	3110	1/1	0.90	0.29	62,62,62,62	0
58	MG	1A	3491	1/1	0.90	0.16	52,52,52,52	0
58	MG	2a	3029	1/1	0.90	0.18	73,73,73,73	0
58	MG	2A	3117	1/1	0.90	0.10	67,67,67,67	0
58	MG	1a	1771	1/1	0.90	0.20	75,75,75,75	0
58	MG	2a	3033	1/1	0.90	0.18	75,75,75,75	0
58	MG	1A	3400	1/1	0.90	0.15	56,56,56,56	0
58	MG	1A	3001	1/1	0.90	0.08	30,30,30,30	0
58	MG	2A	3138	1/1	0.90	0.24	52,52,52,52	0
58	MG	1A	3132	1/1	0.90	0.10	33,33,33,33	0
58	MG	1A	3827	1/1	0.90	0.09	36,36,36,36	0
58	MG	2A	3644	1/1	0.90	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3146	1/1	0.90	0.22	54,54,54,54	0
58	MG	2A	3335	1/1	0.90	0.11	46,46,46,46	0
58	MG	1a	1785	1/1	0.90	0.20	61,61,61,61	0
58	MG	1A	3107	1/1	0.90	0.14	52,52,52,52	0
58	MG	1A	3990	1/1	0.90	0.11	26,26,26,26	0
58	MG	1A	3995	1/1	0.90	0.11	40,40,40,40	0
58	MG	2a	3047	1/1	0.90	0.14	64,64,64,64	0
58	MG	1A	3830	1/1	0.90	0.10	72,72,72,72	0
58	MG	2A	3351	1/1	0.90	0.18	60,60,60,60	0
58	MG	2A	3353	1/1	0.90	0.16	56,56,56,56	0
58	MG	1A	3832	1/1	0.90	0.09	53,53,53,53	0
58	MG	1a	1800	1/1	0.90	0.31	66,66,66,66	0
58	MG	1a	1801	1/1	0.90	0.16	73,73,73,73	0
58	MG	2A	3667	1/1	0.90	0.08	71,71,71,71	0
58	MG	2A	3668	1/1	0.90	0.14	63,63,63,63	0
58	MG	1A	3647	1/1	0.90	0.09	22,22,22,22	0
58	MG	2A	3681	1/1	0.90	0.17	64,64,64,64	0
58	MG	2A	3363	1/1	0.90	0.12	71,71,71,71	0
58	MG	2A	3684	1/1	0.90	0.07	71,71,71,71	0
58	MG	2A	3168	1/1	0.90	0.09	64,64,64,64	0
58	MG	1A	3264	1/1	0.90	0.12	64,64,64,64	0
58	MG	2A	3173	1/1	0.90	0.09	31,31,31,31	0
58	MG	2a	3077	1/1	0.90	0.18	65,65,65,65	0
58	MG	1A	3657	1/1	0.90	0.07	36,36,36,36	0
58	MG	1A	4022	1/1	0.90	0.17	46,46,46,46	0
58	MG	1a	1622	1/1	0.90	0.08	56,56,56,56	0
58	MG	2A	3385	1/1	0.90	0.12	62,62,62,62	0
58	MG	1A	3227	1/1	0.90	0.17	51,51,51,51	0
58	MG	1A	3524	1/1	0.90	0.12	41,41,41,41	0
58	MG	2a	3088	1/1	0.90	0.09	45,45,45,45	0
58	MG	1A	3856	1/1	0.90	0.09	39,39,39,39	0
58	MG	2a	3091	1/1	0.90	0.11	62,62,62,62	0
58	MG	2A	3393	1/1	0.90	0.21	46,46,46,46	0
58	MG	1A	3141	1/1	0.90	0.11	18,18,18,18	0
58	MG	1w	105	1/1	0.90	0.14	80,80,80,80	0
58	MG	1A	3432	1/1	0.90	0.26	38,38,38,38	0
58	MG	1A	4046	1/1	0.90	0.08	41,41,41,41	0
58	MG	2A	3720	1/1	0.90	0.23	50,50,50,50	0
58	MG	2A	3193	1/1	0.90	0.22	63,63,63,63	0
58	MG	2A	3194	1/1	0.90	0.10	55,55,55,55	0
58	MG	1A	4048	1/1	0.90	0.14	50,50,50,50	0
58	MG	2A	3196	1/1	0.90	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3411	1/1	0.90	0.11	45,45,45,45	0
58	MG	2A	3199	1/1	0.90	0.16	69,69,69,69	0
58	MG	2a	3111	1/1	0.90	0.07	79,79,79,79	0
58	MG	1A	3271	1/1	0.90	0.14	45,45,45,45	0
58	MG	1A	4064	1/1	0.90	0.09	48,48,48,48	0
58	MG	1A	3867	1/1	0.90	0.13	68,68,68,68	0
58	MG	2A	3745	1/1	0.90	0.09	55,55,55,55	0
58	MG	1A	3235	1/1	0.90	0.10	54,54,54,54	0
58	MG	1A	3288	1/1	0.90	0.11	37,37,37,37	0
58	MG	1A	3552	1/1	0.90	0.07	44,44,44,44	0
58	MG	1A	3237	1/1	0.90	0.14	55,55,55,55	0
58	MG	2A	3430	1/1	0.90	0.13	56,56,56,56	0
58	MG	2A	3435	1/1	0.90	0.07	57,57,57,57	0
58	MG	1A	4079	1/1	0.90	0.11	40,40,40,40	0
58	MG	1A	3297	1/1	0.90	0.26	46,46,46,46	0
58	MG	1A	3452	1/1	0.90	0.14	40,40,40,40	0
58	MG	2A	3764	1/1	0.90	0.12	62,62,62,62	0
58	MG	1A	3454	1/1	0.90	0.14	58,58,58,58	0
58	MG	2A	3023	1/1	0.90	0.16	50,50,50,50	0
58	MG	1A	3149	1/1	0.90	0.27	28,28,28,28	0
58	MG	1A	3098	1/1	0.90	0.11	39,39,39,39	0
58	MG	1A	3714	1/1	0.90	0.13	55,55,55,55	0
58	MG	2A	3456	1/1	0.90	0.13	51,51,51,51	0
58	MG	1A	3888	1/1	0.90	0.09	51,51,51,51	0
58	MG	2A	3793	1/1	0.90	0.12	68,68,68,68	0
58	MG	1A	3575	1/1	0.90	0.26	63,63,63,63	0
58	MG	2a	3152	1/1	0.90	0.10	60,60,60,60	0
58	MG	1A	3892	1/1	0.90	0.35	36,36,36,36	0
58	MG	2a	3155	1/1	0.90	0.12	61,61,61,61	0
58	MG	2a	3156	1/1	0.90	0.10	67,67,67,67	0
58	MG	2A	3467	1/1	0.90	0.07	60,60,60,60	0
58	MG	1a	1674	1/1	0.90	0.12	50,50,50,50	0
58	MG	1A	3250	1/1	0.90	0.21	35,35,35,35	0
58	MG	2A	3472	1/1	0.90	0.17	54,54,54,54	0
58	MG	2A	3247	1/1	0.90	0.08	70,70,70,70	0
58	MG	1A	3749	1/1	0.90	0.08	16,16,16,16	0
58	MG	1A	3460	1/1	0.90	0.16	45,45,45,45	0
58	MG	2A	3814	1/1	0.90	0.14	61,61,61,61	0
58	MG	1A	3918	1/1	0.90	0.08	42,42,42,42	0
58	MG	1a	1685	1/1	0.90	0.26	39,39,39,39	0
58	MG	1B	234	1/1	0.90	0.12	58,58,58,58	0
58	MG	2A	3256	1/1	0.90	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3493	1/1	0.90	0.13	65,65,65,65	0
58	MG	1a	1689	1/1	0.90	0.28	53,53,53,53	0
58	MG	2A	3501	1/1	0.90	0.13	53,53,53,53	0
58	MG	1B	235	1/1	0.90	0.10	50,50,50,50	0
58	MG	2A	3263	1/1	0.90	0.08	51,51,51,51	0
58	MG	1A	3582	1/1	0.90	0.24	60,60,60,60	0
58	MG	1a	1694	1/1	0.90	0.41	67,67,67,67	0
58	MG	1A	3768	1/1	0.90	0.15	54,54,54,54	0
58	MG	1E	301	1/1	0.90	0.20	43,43,43,43	0
58	MG	1E	305	1/1	0.90	0.10	59,59,59,59	0
58	MG	1A	3590	1/1	0.90	0.20	47,47,47,47	0
58	MG	2A	3536	1/1	0.90	0.15	38,38,38,38	0
58	MG	1E	312	1/1	0.90	0.07	51,51,51,51	0
58	MG	2A	3072	1/1	0.90	0.39	63,63,63,63	0
58	MG	1F	306	1/1	0.90	0.15	27,27,27,27	0
58	MG	2a	3200	1/1	0.90	0.17	61,61,61,61	0
58	MG	1A	3124	1/1	0.90	0.28	33,33,33,33	0
58	MG	1A	3788	1/1	0.90	0.10	53,53,53,53	0
58	MG	1a	1719	1/1	0.90	0.13	41,41,41,41	0
58	MG	1A	3253	1/1	0.90	0.09	69,69,69,69	0
58	MG	1A	3319	1/1	0.90	0.13	42,42,42,42	0
58	MG	1A	3385	1/1	0.90	0.08	47,47,47,47	0
58	MG	1A	3254	1/1	0.90	0.11	45,45,45,45	0
58	MG	2A	3568	1/1	0.90	0.15	53,53,53,53	0
58	MG	2g	201	1/1	0.90	0.19	76,76,76,76	0
58	MG	2A	3290	1/1	0.90	0.13	53,53,53,53	0
58	MG	2k	201	1/1	0.90	0.10	73,73,73,73	0
58	MG	1U	205	1/1	0.90	0.25	45,45,45,45	0
58	MG	2A	3579	1/1	0.90	0.10	24,24,24,24	0
58	MG	2l	203	1/1	0.90	0.14	74,74,74,74	0
58	MG	1A	3949	1/1	0.90	0.09	43,43,43,43	0
58	MG	2A	3582	1/1	0.90	0.21	61,61,61,61	0
58	MG	1A	3952	1/1	0.90	0.11	32,32,32,32	0
58	MG	1A	3394	1/1	0.90	0.16	44,44,44,44	0
58	MG	2A	3589	1/1	0.90	0.11	71,71,71,71	0
58	MG	2a	3011	1/1	0.90	0.29	63,63,63,63	0
58	MG	2a	3012	1/1	0.90	0.30	71,71,71,71	0
58	MG	2a	3015	1/1	0.90	0.19	70,70,70,70	0
59	K	2A	3418	1/1	0.90	0.12	74,74,74,74	0
61	ZN	24	501	1/1	0.90	0.14	128,128,128,128	0
58	MG	1A	3600	1/1	0.91	0.07	30,30,30,30	0
58	MG	2A	3600	1/1	0.91	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3602	1/1	0.91	0.11	55,55,55,55	0
58	MG	1A	3256	1/1	0.91	0.14	46,46,46,46	0
58	MG	1A	3715	1/1	0.91	0.09	60,60,60,60	0
58	MG	2A	3320	1/1	0.91	0.19	63,63,63,63	0
58	MG	2A	3322	1/1	0.91	0.16	59,59,59,59	0
58	MG	2A	3620	1/1	0.91	0.18	51,51,51,51	0
58	MG	1A	3608	1/1	0.91	0.14	77,77,77,77	0
58	MG	2A	3152	1/1	0.91	0.10	45,45,45,45	0
58	MG	2A	3332	1/1	0.91	0.15	67,67,67,67	0
58	MG	2A	3333	1/1	0.91	0.10	62,62,62,62	0
58	MG	1A	3967	1/1	0.91	0.10	27,27,27,27	0
58	MG	2A	3336	1/1	0.91	0.07	61,61,61,61	0
58	MG	1A	3859	1/1	0.91	0.17	40,40,40,40	0
58	MG	1B	228	1/1	0.91	0.13	60,60,60,60	0
58	MG	2A	3343	1/1	0.91	0.21	53,53,53,53	0
58	MG	1A	3727	1/1	0.91	0.10	58,58,58,58	0
58	MG	2A	3160	1/1	0.91	0.28	51,51,51,51	0
58	MG	1b	301	1/1	0.91	0.15	71,71,71,71	0
58	MG	1A	3974	1/1	0.91	0.13	53,53,53,53	0
58	MG	1A	3312	1/1	0.91	0.13	54,54,54,54	0
58	MG	1a	1642	1/1	0.91	0.11	73,73,73,73	0
58	MG	1v	101	1/1	0.91	0.11	76,76,76,76	0
58	MG	2A	3359	1/1	0.91	0.09	55,55,55,55	0
58	MG	1A	3738	1/1	0.91	0.08	68,68,68,68	0
58	MG	1A	3011	1/1	0.91	0.09	37,37,37,37	0
58	MG	2A	3662	1/1	0.91	0.15	59,59,59,59	0
58	MG	1a	1645	1/1	0.91	0.19	50,50,50,50	0
58	MG	2A	3180	1/1	0.91	0.26	69,69,69,69	0
58	MG	1A	3623	1/1	0.91	0.10	23,23,23,23	0
58	MG	2a	3055	1/1	0.91	0.26	60,60,60,60	0
58	MG	1D	312	1/1	0.91	0.10	35,35,35,35	0
58	MG	2A	3373	1/1	0.91	0.22	53,53,53,53	0
58	MG	1A	3398	1/1	0.91	0.10	39,39,39,39	0
58	MG	2a	3062	1/1	0.91	0.24	57,57,57,57	0
58	MG	2A	3673	1/1	0.91	0.17	65,65,65,65	0
58	MG	2A	3378	1/1	0.91	0.21	55,55,55,55	0
58	MG	1A	3273	1/1	0.91	0.13	35,35,35,35	0
58	MG	1x	106	1/1	0.91	0.20	49,49,49,49	0
58	MG	1A	3994	1/1	0.91	0.07	34,34,34,34	0
58	MG	1E	310	1/1	0.91	0.14	59,59,59,59	0
58	MG	2A	3693	1/1	0.91	0.12	54,54,54,54	0
58	MG	2A	3189	1/1	0.91	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	3073	1/1	0.91	0.09	64,64,64,64	0
58	MG	2a	3076	1/1	0.91	0.21	62,62,62,62	0
58	MG	2A	3191	1/1	0.91	0.13	57,57,57,57	0
58	MG	1E	311	1/1	0.91	0.20	51,51,51,51	0
58	MG	2A	3395	1/1	0.91	0.35	66,66,66,66	0
58	MG	2A	3705	1/1	0.91	0.09	47,47,47,47	0
58	MG	1A	3776	1/1	0.91	0.10	24,24,24,24	0
58	MG	1A	3343	1/1	0.91	0.14	39,39,39,39	0
58	MG	1A	3409	1/1	0.91	0.15	66,66,66,66	0
58	MG	1a	1671	1/1	0.91	0.26	70,70,70,70	0
58	MG	1A	3410	1/1	0.91	0.09	54,54,54,54	0
58	MG	1A	3643	1/1	0.91	0.17	35,35,35,35	0
58	MG	1P	206	1/1	0.91	0.13	56,56,56,56	0
58	MG	2A	3014	1/1	0.91	0.17	47,47,47,47	0
58	MG	2A	3718	1/1	0.91	0.21	54,54,54,54	0
58	MG	1A	3555	1/1	0.91	0.09	29,29,29,29	0
58	MG	1a	1679	1/1	0.91	0.17	60,60,60,60	0
58	MG	2A	3217	1/1	0.91	0.15	28,28,28,28	0
58	MG	1P	208	1/1	0.91	0.14	37,37,37,37	0
58	MG	2A	3028	1/1	0.91	0.17	78,78,78,78	0
58	MG	1Q	201	1/1	0.91	0.23	38,38,38,38	0
58	MG	1A	3413	1/1	0.91	0.25	54,54,54,54	0
58	MG	2A	3736	1/1	0.91	0.13	47,47,47,47	0
58	MG	1A	3349	1/1	0.91	0.13	39,39,39,39	0
58	MG	1a	1687	1/1	0.91	0.28	51,51,51,51	0
58	MG	2A	3429	1/1	0.91	0.24	49,49,49,49	0
58	MG	1A	4027	1/1	0.91	0.09	47,47,47,47	0
58	MG	2A	3433	1/1	0.91	0.13	65,65,65,65	0
58	MG	2a	3118	1/1	0.91	0.15	57,57,57,57	0
58	MG	1A	3200	1/1	0.91	0.15	41,41,41,41	0
58	MG	2A	3438	1/1	0.91	0.11	60,60,60,60	0
58	MG	2A	3439	1/1	0.91	0.14	45,45,45,45	0
58	MG	1A	3471	1/1	0.91	0.08	44,44,44,44	0
58	MG	2A	3441	1/1	0.91	0.07	50,50,50,50	0
58	MG	1A	4032	1/1	0.91	0.16	51,51,51,51	0
58	MG	1A	3286	1/1	0.91	0.13	47,47,47,47	0
58	MG	2A	3235	1/1	0.91	0.08	55,55,55,55	0
58	MG	2A	3236	1/1	0.91	0.10	57,57,57,57	0
58	MG	2A	3762	1/1	0.91	0.10	41,41,41,41	0
58	MG	1A	3898	1/1	0.91	0.22	28,28,28,28	0
58	MG	2A	3241	1/1	0.91	0.16	62,62,62,62	0
58	MG	1A	3260	1/1	0.91	0.22	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3774	1/1	0.91	0.10	30,30,30,30	0
58	MG	2A	3243	1/1	0.91	0.14	48,48,48,48	0
58	MG	1A	3364	1/1	0.91	0.31	51,51,51,51	0
58	MG	2A	3780	1/1	0.91	0.17	53,53,53,53	0
58	MG	2A	3461	1/1	0.91	0.17	52,52,52,52	0
58	MG	1A	4052	1/1	0.91	0.06	27,27,27,27	0
58	MG	2A	3054	1/1	0.91	0.17	58,58,58,58	0
58	MG	2a	3148	1/1	0.91	0.21	52,52,52,52	0
58	MG	1a	1707	1/1	0.91	0.23	54,54,54,54	0
58	MG	1a	1708	1/1	0.91	0.13	60,60,60,60	0
58	MG	2A	3059	1/1	0.91	0.12	58,58,58,58	0
58	MG	10	104	1/1	0.91	0.24	39,39,39,39	0
58	MG	10	105	1/1	0.91	0.13	44,44,44,44	0
58	MG	1A	3427	1/1	0.91	0.12	66,66,66,66	0
58	MG	10	109	1/1	0.91	0.11	48,48,48,48	0
58	MG	10	110	1/1	0.91	0.12	47,47,47,47	0
58	MG	1A	3684	1/1	0.91	0.07	26,26,26,26	0
58	MG	1A	3819	1/1	0.91	0.08	40,40,40,40	0
58	MG	1A	3488	1/1	0.91	0.05	57,57,57,57	0
58	MG	1a	1736	1/1	0.91	0.23	57,57,57,57	0
58	MG	15	105	1/1	0.91	0.07	56,56,56,56	0
58	MG	15	106	1/1	0.91	0.20	27,27,27,27	0
58	MG	1A	3430	1/1	0.91	0.12	43,43,43,43	0
58	MG	2A	3503	1/1	0.91	0.10	56,56,56,56	0
58	MG	16	101	1/1	0.91	0.11	57,57,57,57	0
58	MG	2a	3180	1/1	0.91	0.17	71,71,71,71	0
58	MG	1a	1752	1/1	0.91	0.08	52,52,52,52	0
58	MG	2A	3089	1/1	0.91	0.12	52,52,52,52	0
58	MG	17	107	1/1	0.91	0.10	40,40,40,40	0
58	MG	1A	4069	1/1	0.91	0.10	56,56,56,56	0
58	MG	2A	3518	1/1	0.91	0.08	43,43,43,43	0
58	MG	2B	211	1/1	0.91	0.20	66,66,66,66	0
58	MG	2A	3521	1/1	0.91	0.16	62,62,62,62	0
58	MG	2A	3522	1/1	0.91	0.12	39,39,39,39	0
58	MG	1A	3115	1/1	0.91	0.11	39,39,39,39	0
58	MG	2A	3528	1/1	0.91	0.12	62,62,62,62	0
58	MG	2A	3284	1/1	0.91	0.09	56,56,56,56	0
58	MG	1A	4075	1/1	0.91	0.20	49,49,49,49	0
58	MG	1A	3295	1/1	0.91	0.15	52,52,52,52	0
58	MG	2E	307	1/1	0.91	0.17	59,59,59,59	0
58	MG	2a	3199	1/1	0.91	0.20	68,68,68,68	0
58	MG	2F	301	1/1	0.91	0.20	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1765	1/1	0.91	0.14	64,64,64,64	0
58	MG	2A	3288	1/1	0.91	0.10	81,81,81,81	0
58	MG	1A	3072	1/1	0.91	0.11	20,20,20,20	0
58	MG	1a	1769	1/1	0.91	0.10	42,42,42,42	0
58	MG	1A	3133	1/1	0.91	0.09	43,43,43,43	0
58	MG	2Q	202	1/1	0.91	0.19	53,53,53,53	0
58	MG	2A	3292	1/1	0.91	0.08	44,44,44,44	0
58	MG	2V	202	1/1	0.91	0.21	55,55,55,55	0
58	MG	1a	1611	1/1	0.91	0.19	68,68,68,68	0
58	MG	1B	201	1/1	0.91	0.14	40,40,40,40	0
58	MG	1a	1777	1/1	0.91	0.13	48,48,48,48	0
58	MG	2A	3114	1/1	0.91	0.15	46,46,46,46	0
58	MG	1A	3837	1/1	0.91	0.13	34,34,34,34	0
58	MG	1A	3447	1/1	0.91	0.22	59,59,59,59	0
58	MG	2a	3003	1/1	0.91	0.07	72,72,72,72	0
58	MG	2a	3004	1/1	0.91	0.23	54,54,54,54	0
58	MG	1a	1619	1/1	0.91	0.20	53,53,53,53	0
58	MG	1A	3246	1/1	0.91	0.13	40,40,40,40	0
58	MG	2A	3127	1/1	0.91	0.14	53,53,53,53	0
58	MG	2A	3130	1/1	0.91	0.19	63,63,63,63	0
58	MG	2A	3132	1/1	0.91	0.15	64,64,64,64	0
58	MG	1a	1791	1/1	0.91	0.08	48,48,48,48	0
58	MG	2A	3139	1/1	0.91	0.10	41,41,41,41	0
58	MG	1A	3953	1/1	0.91	0.14	47,47,47,47	0
58	MG	1A	3962	1/1	0.92	0.09	74,74,74,74	0
58	MG	2B	206	1/1	0.92	0.14	79,79,79,79	0
58	MG	2B	207	1/1	0.92	0.10	61,61,61,61	0
58	MG	2B	209	1/1	0.92	0.12	62,62,62,62	0
58	MG	10	111	1/1	0.92	0.07	44,44,44,44	0
58	MG	1A	3750	1/1	0.92	0.08	30,30,30,30	0
58	MG	11	103	1/1	0.92	0.10	36,36,36,36	0
58	MG	2B	213	1/1	0.92	0.15	64,64,64,64	0
58	MG	1A	3163	1/1	0.92	0.16	47,47,47,47	0
58	MG	2A	3464	1/1	0.92	0.20	51,51,51,51	0
58	MG	2B	216	1/1	0.92	0.12	59,59,59,59	0
58	MG	2B	217	1/1	0.92	0.11	72,72,72,72	0
58	MG	1A	3755	1/1	0.92	0.11	29,29,29,29	0
58	MG	2A	3210	1/1	0.92	0.22	42,42,42,42	0
58	MG	2D	304	1/1	0.92	0.22	48,48,48,48	0
58	MG	2D	305	1/1	0.92	0.24	67,67,67,67	0
58	MG	1f	202	1/1	0.92	0.08	65,65,65,65	0
58	MG	2E	302	1/1	0.92	0.08	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2E	304	1/1	0.92	0.09	50,50,50,50	0
58	MG	2A	3470	1/1	0.92	0.20	66,66,66,66	0
58	MG	2A	3212	1/1	0.92	0.17	59,59,59,59	0
58	MG	15	103	1/1	0.92	0.32	34,34,34,34	0
58	MG	1A	3757	1/1	0.92	0.09	36,36,36,36	0
58	MG	1A	3564	1/1	0.92	0.17	48,48,48,48	0
58	MG	1A	3278	1/1	0.92	0.12	37,37,37,37	0
58	MG	1A	3771	1/1	0.92	0.06	53,53,53,53	0
58	MG	2P	201	1/1	0.92	0.10	54,54,54,54	0
58	MG	16	102	1/1	0.92	0.25	57,57,57,57	0
58	MG	2A	3488	1/1	0.92	0.16	72,72,72,72	0
58	MG	1A	3344	1/1	0.92	0.23	54,54,54,54	0
58	MG	2T	203	1/1	0.92	0.15	56,56,56,56	0
58	MG	2A	3228	1/1	0.92	0.24	69,69,69,69	0
58	MG	2A	3491	1/1	0.92	0.12	46,46,46,46	0
58	MG	2W	202	1/1	0.92	0.11	55,55,55,55	0
58	MG	2A	3492	1/1	0.92	0.20	56,56,56,56	0
58	MG	1A	3441	1/1	0.92	0.09	41,41,41,41	0
58	MG	2A	3497	1/1	0.92	0.16	65,65,65,65	0
58	MG	1A	3783	1/1	0.92	0.11	17,17,17,17	0
58	MG	23	102	1/1	0.92	0.11	65,65,65,65	0
58	MG	1x	102	1/1	0.92	0.10	59,59,59,59	0
58	MG	1A	3346	1/1	0.92	0.08	37,37,37,37	0
58	MG	1x	104	1/1	0.92	0.14	56,56,56,56	0
58	MG	1A	3282	1/1	0.92	0.18	22,22,22,22	0
58	MG	1a	1606	1/1	0.92	0.07	63,63,63,63	0
58	MG	2A	3237	1/1	0.92	0.07	57,57,57,57	0
58	MG	1A	3350	1/1	0.92	0.09	52,52,52,52	0
58	MG	2a	3009	1/1	0.92	0.20	66,66,66,66	0
58	MG	2A	3240	1/1	0.92	0.32	61,61,61,61	0
58	MG	1A	4002	1/1	0.92	0.14	59,59,59,59	0
58	MG	1A	3233	1/1	0.92	0.10	44,44,44,44	0
58	MG	2a	3013	1/1	0.92	0.13	58,58,58,58	0
58	MG	1x	111	1/1	0.92	0.27	58,58,58,58	0
58	MG	1A	3018	1/1	0.92	0.17	34,34,34,34	0
58	MG	1A	3579	1/1	0.92	0.07	54,54,54,54	0
58	MG	2A	3530	1/1	0.92	0.12	51,51,51,51	0
58	MG	1A	4017	1/1	0.92	0.12	40,40,40,40	0
58	MG	2a	3020	1/1	0.92	0.10	69,69,69,69	0
58	MG	1A	3580	1/1	0.92	0.06	39,39,39,39	0
58	MG	1A	3453	1/1	0.92	0.15	40,40,40,40	0
58	MG	1A	3291	1/1	0.92	0.13	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	3024	1/1	0.92	0.15	68,68,68,68	0
58	MG	1A	3361	1/1	0.92	0.26	32,32,32,32	0
58	MG	1A	3594	1/1	0.92	0.11	23,23,23,23	0
58	MG	2A	3018	1/1	0.92	0.13	68,68,68,68	0
58	MG	2A	3020	1/1	0.92	0.17	46,46,46,46	0
58	MG	1A	3168	1/1	0.92	0.08	28,28,28,28	0
58	MG	1A	3458	1/1	0.92	0.15	49,49,49,49	0
58	MG	2A	3026	1/1	0.92	0.07	39,39,39,39	0
58	MG	2A	3563	1/1	0.92	0.13	49,49,49,49	0
58	MG	2A	3566	1/1	0.92	0.15	38,38,38,38	0
58	MG	1A	3817	1/1	0.92	0.21	52,52,52,52	0
58	MG	1A	3818	1/1	0.92	0.19	55,55,55,55	0
58	MG	1a	1633	1/1	0.92	0.36	62,62,62,62	0
58	MG	1A	3238	1/1	0.92	0.23	36,36,36,36	0
58	MG	2A	3578	1/1	0.92	0.07	69,69,69,69	0
58	MG	2A	3270	1/1	0.92	0.15	56,56,56,56	0
58	MG	2A	3580	1/1	0.92	0.16	54,54,54,54	0
58	MG	2A	3034	1/1	0.92	0.15	36,36,36,36	0
58	MG	1A	4039	1/1	0.92	0.12	31,31,31,31	0
58	MG	1A	4041	1/1	0.92	0.10	50,50,50,50	0
58	MG	1A	3036	1/1	0.92	0.10	33,33,33,33	0
58	MG	1A	3370	1/1	0.92	0.10	49,49,49,49	0
58	MG	1A	3602	1/1	0.92	0.11	48,48,48,48	0
58	MG	1A	4056	1/1	0.92	0.13	32,32,32,32	0
58	MG	2A	3044	1/1	0.92	0.14	55,55,55,55	0
58	MG	1A	3017	1/1	0.92	0.18	37,37,37,37	0
58	MG	1A	3374	1/1	0.92	0.09	45,45,45,45	0
58	MG	1A	3609	1/1	0.92	0.13	27,27,27,27	0
58	MG	2A	3605	1/1	0.92	0.16	48,48,48,48	0
58	MG	1a	1651	1/1	0.92	0.13	47,47,47,47	0
58	MG	1A	3470	1/1	0.92	0.09	35,35,35,35	0
58	MG	2A	3613	1/1	0.92	0.24	57,57,57,57	0
58	MG	2A	3615	1/1	0.92	0.11	44,44,44,44	0
58	MG	1A	4067	1/1	0.92	0.11	48,48,48,48	0
58	MG	1A	3839	1/1	0.92	0.22	41,41,41,41	0
58	MG	2A	3057	1/1	0.92	0.17	45,45,45,45	0
58	MG	2A	3293	1/1	0.92	0.17	41,41,41,41	0
58	MG	1A	3173	1/1	0.92	0.12	36,36,36,36	0
58	MG	1A	3472	1/1	0.92	0.15	48,48,48,48	0
58	MG	2a	3074	1/1	0.92	0.29	72,72,72,72	0
58	MG	2A	3632	1/1	0.92	0.13	48,48,48,48	0
58	MG	2A	3060	1/1	0.92	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3298	1/1	0.92	0.45	54,54,54,54	0
58	MG	1A	3847	1/1	0.92	0.30	24,24,24,24	0
58	MG	1A	3849	1/1	0.92	0.08	44,44,44,44	0
58	MG	1A	3381	1/1	0.92	0.13	56,56,56,56	0
58	MG	1A	3174	1/1	0.92	0.14	35,35,35,35	0
58	MG	1A	3480	1/1	0.92	0.13	45,45,45,45	0
58	MG	2A	3067	1/1	0.92	0.31	69,69,69,69	0
58	MG	2A	3068	1/1	0.92	0.10	49,49,49,49	0
58	MG	1A	3041	1/1	0.92	0.11	42,42,42,42	0
58	MG	1A	3313	1/1	0.92	0.12	37,37,37,37	0
58	MG	1A	3047	1/1	0.92	0.06	26,26,26,26	0
58	MG	2a	3095	1/1	0.92	0.11	52,52,52,52	0
58	MG	1A	3862	1/1	0.92	0.15	29,29,29,29	0
58	MG	2A	3077	1/1	0.92	0.11	50,50,50,50	0
58	MG	2A	3654	1/1	0.92	0.18	67,67,67,67	0
58	MG	1A	3316	1/1	0.92	0.07	29,29,29,29	0
58	MG	1A	3108	1/1	0.92	0.13	30,30,30,30	0
58	MG	1A	3649	1/1	0.92	0.07	25,25,25,25	0
58	MG	1A	3650	1/1	0.92	0.09	51,51,51,51	0
58	MG	2A	3086	1/1	0.92	0.11	50,50,50,50	0
58	MG	1A	3492	1/1	0.92	0.09	36,36,36,36	0
58	MG	2A	3328	1/1	0.92	0.08	46,46,46,46	0
58	MG	1A	3191	1/1	0.92	0.11	33,33,33,33	0
58	MG	1A	3662	1/1	0.92	0.13	20,20,20,20	0
58	MG	2A	3677	1/1	0.92	0.10	33,33,33,33	0
58	MG	2A	3679	1/1	0.92	0.13	58,58,58,58	0
58	MG	2a	3116	1/1	0.92	0.22	52,52,52,52	0
58	MG	1A	3664	1/1	0.92	0.09	29,29,29,29	0
58	MG	1A	3405	1/1	0.92	0.14	49,49,49,49	0
58	MG	2A	3337	1/1	0.92	0.28	60,60,60,60	0
58	MG	2A	3685	1/1	0.92	0.11	58,58,58,58	0
58	MG	1A	3497	1/1	0.92	0.12	43,43,43,43	0
58	MG	1A	3881	1/1	0.92	0.08	25,25,25,25	0
58	MG	1A	3498	1/1	0.92	0.09	49,49,49,49	0
58	MG	2A	3344	1/1	0.92	0.27	62,62,62,62	0
58	MG	1A	3503	1/1	0.92	0.07	29,29,29,29	0
58	MG	2A	3103	1/1	0.92	0.15	53,53,53,53	0
58	MG	1A	3408	1/1	0.92	0.13	49,49,49,49	0
58	MG	2A	3703	1/1	0.92	0.11	50,50,50,50	0
58	MG	1A	3677	1/1	0.92	0.09	25,25,25,25	0
58	MG	1A	3680	1/1	0.92	0.10	60,60,60,60	0
58	MG	2A	3354	1/1	0.92	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1710	1/1	0.92	0.22	40,40,40,40	0
58	MG	1a	1711	1/1	0.92	0.11	44,44,44,44	0
58	MG	1A	3030	1/1	0.92	0.11	34,34,34,34	0
58	MG	2A	3116	1/1	0.92	0.21	47,47,47,47	0
58	MG	1A	3685	1/1	0.92	0.12	37,37,37,37	0
58	MG	1A	3152	1/1	0.92	0.13	40,40,40,40	0
58	MG	2A	3717	1/1	0.92	0.20	56,56,56,56	0
58	MG	1A	3899	1/1	0.92	0.23	26,26,26,26	0
58	MG	2A	3366	1/1	0.92	0.09	42,42,42,42	0
58	MG	1A	3904	1/1	0.92	0.12	40,40,40,40	0
58	MG	2A	3370	1/1	0.92	0.14	62,62,62,62	0
58	MG	1A	3910	1/1	0.92	0.09	61,61,61,61	0
58	MG	2A	3372	1/1	0.92	0.23	44,44,44,44	0
58	MG	1a	1730	1/1	0.92	0.13	45,45,45,45	0
58	MG	1F	309	1/1	0.92	0.16	45,45,45,45	0
58	MG	2A	3376	1/1	0.92	0.16	55,55,55,55	0
58	MG	2a	3168	1/1	0.92	0.18	42,42,42,42	0
58	MG	2A	3377	1/1	0.92	0.23	45,45,45,45	0
58	MG	2A	3136	1/1	0.92	0.24	57,57,57,57	0
58	MG	2A	3380	1/1	0.92	0.08	44,44,44,44	0
58	MG	2A	3382	1/1	0.92	0.35	53,53,53,53	0
58	MG	1A	3519	1/1	0.92	0.15	45,45,45,45	0
58	MG	1A	3521	1/1	0.92	0.24	47,47,47,47	0
58	MG	2a	3176	1/1	0.92	0.25	67,67,67,67	0
58	MG	2A	3748	1/1	0.92	0.15	60,60,60,60	0
58	MG	2A	3140	1/1	0.92	0.14	64,64,64,64	0
58	MG	1O	203	1/1	0.92	0.11	51,51,51,51	0
58	MG	2A	3752	1/1	0.92	0.16	45,45,45,45	0
58	MG	2a	3182	1/1	0.92	0.22	53,53,53,53	0
58	MG	1A	3916	1/1	0.92	0.08	45,45,45,45	0
58	MG	1a	1749	1/1	0.92	0.19	59,59,59,59	0
58	MG	1A	3153	1/1	0.92	0.19	41,41,41,41	0
58	MG	1A	3699	1/1	0.92	0.09	35,35,35,35	0
58	MG	1A	3087	1/1	0.92	0.10	25,25,25,25	0
58	MG	2A	3153	1/1	0.92	0.35	63,63,63,63	0
58	MG	1a	1754	1/1	0.92	0.08	59,59,59,59	0
58	MG	2A	3402	1/1	0.92	0.15	50,50,50,50	0
58	MG	1A	3156	1/1	0.92	0.32	43,43,43,43	0
58	MG	1R	205	1/1	0.92	0.20	23,23,23,23	0
58	MG	1A	3930	1/1	0.92	0.08	62,62,62,62	0
58	MG	1U	201	1/1	0.92	0.17	35,35,35,35	0
58	MG	1a	1761	1/1	0.92	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3534	1/1	0.92	0.14	54,54,54,54	0
58	MG	1A	3539	1/1	0.92	0.35	42,42,42,42	0
58	MG	2A	3167	1/1	0.92	0.14	61,61,61,61	0
58	MG	2a	3202	1/1	0.92	0.16	61,61,61,61	0
58	MG	1A	3704	1/1	0.92	0.10	38,38,38,38	0
58	MG	1V	206	1/1	0.92	0.13	48,48,48,48	0
58	MG	1A	3712	1/1	0.92	0.12	42,42,42,42	0
58	MG	2A	3799	1/1	0.92	0.15	35,35,35,35	0
58	MG	2A	3420	1/1	0.92	0.26	45,45,45,45	0
58	MG	1A	3219	1/1	0.92	0.15	53,53,53,53	0
58	MG	1A	3055	1/1	0.92	0.11	43,43,43,43	0
58	MG	2e	201	1/1	0.92	0.06	67,67,67,67	0
58	MG	1X	104	1/1	0.92	0.10	42,42,42,42	0
58	MG	1A	3330	1/1	0.92	0.09	39,39,39,39	0
58	MG	1A	3223	1/1	0.92	0.09	52,52,52,52	0
58	MG	1a	1784	1/1	0.92	0.11	67,67,67,67	0
58	MG	1A	3225	1/1	0.92	0.10	42,42,42,42	0
58	MG	1a	1786	1/1	0.92	0.17	54,54,54,54	0
58	MG	10	103	1/1	0.92	0.08	39,39,39,39	0
58	MG	1a	1790	1/1	0.92	0.14	68,68,68,68	0
58	MG	2A	3818	1/1	0.92	0.13	66,66,66,66	0
58	MG	2v	102	1/1	0.92	0.21	71,71,71,71	0
58	MG	1A	3554	1/1	0.92	0.10	36,36,36,36	0
58	MG	2A	3190	1/1	0.92	0.27	61,61,61,61	0
58	MG	1A	3125	1/1	0.92	0.08	32,32,32,32	0
58	MG	10	107	1/1	0.92	0.09	48,48,48,48	0
58	MG	1A	3956	1/1	0.92	0.11	64,64,64,64	0
58	MG	2x	105	1/1	0.92	0.15	61,61,61,61	0
58	MG	1a	1796	1/1	0.92	0.28	59,59,59,59	0
58	MG	1A	3560	1/1	0.92	0.10	38,38,38,38	0
58	MG	1A	3116	1/1	0.93	0.11	43,43,43,43	0
58	MG	1A	3860	1/1	0.93	0.07	29,29,29,29	0
58	MG	2A	3238	1/1	0.93	0.10	57,57,57,57	0
58	MG	1A	3244	1/1	0.93	0.26	39,39,39,39	0
58	MG	2A	3011	1/1	0.93	0.11	48,48,48,48	0
58	MG	1A	4059	1/1	0.93	0.14	44,44,44,44	0
58	MG	2A	3016	1/1	0.93	0.19	54,54,54,54	0
58	MG	1A	3122	1/1	0.93	0.25	32,32,32,32	0
58	MG	1A	3247	1/1	0.93	0.07	50,50,50,50	0
58	MG	1A	3865	1/1	0.93	0.17	26,26,26,26	0
58	MG	1a	1638	1/1	0.93	0.14	43,43,43,43	0
58	MG	1A	3697	1/1	0.93	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3461	1/1	0.93	0.12	40,40,40,40	0
58	MG	2E	306	1/1	0.93	0.13	44,44,44,44	0
58	MG	1A	3386	1/1	0.93	0.15	54,54,54,54	0
58	MG	1A	3326	1/1	0.93	0.10	51,51,51,51	0
58	MG	2F	302	1/1	0.93	0.09	52,52,52,52	0
58	MG	1A	4071	1/1	0.93	0.15	50,50,50,50	0
58	MG	1A	3467	1/1	0.93	0.08	41,41,41,41	0
58	MG	2A	3514	1/1	0.93	0.12	37,37,37,37	0
58	MG	1a	1647	1/1	0.93	0.06	51,51,51,51	0
58	MG	2A	3259	1/1	0.93	0.12	55,55,55,55	0
58	MG	2A	3036	1/1	0.93	0.18	49,49,49,49	0
58	MG	2Q	201	1/1	0.93	0.20	66,66,66,66	0
58	MG	2A	3519	1/1	0.93	0.12	48,48,48,48	0
58	MG	2R	201	1/1	0.93	0.10	50,50,50,50	0
58	MG	2T	201	1/1	0.93	0.10	52,52,52,52	0
58	MG	2A	3261	1/1	0.93	0.07	44,44,44,44	0
58	MG	2A	3262	1/1	0.93	0.07	72,72,72,72	0
58	MG	2V	201	1/1	0.93	0.28	46,46,46,46	0
58	MG	1A	3328	1/1	0.93	0.15	42,42,42,42	0
58	MG	1A	3093	1/1	0.93	0.13	38,38,38,38	0
58	MG	1A	3705	1/1	0.93	0.11	61,61,61,61	0
58	MG	2X	101	1/1	0.93	0.10	64,64,64,64	0
58	MG	2Z	301	1/1	0.93	0.16	80,80,80,80	0
58	MG	1a	1654	1/1	0.93	0.11	44,44,44,44	0
58	MG	1a	1655	1/1	0.93	0.20	56,56,56,56	0
58	MG	2A	3043	1/1	0.93	0.06	64,64,64,64	0
58	MG	1A	3708	1/1	0.93	0.07	26,26,26,26	0
58	MG	2A	3542	1/1	0.93	0.09	41,41,41,41	0
58	MG	27	101	1/1	0.93	0.27	42,42,42,42	0
58	MG	27	103	1/1	0.93	0.15	41,41,41,41	0
58	MG	1a	1658	1/1	0.93	0.15	59,59,59,59	0
58	MG	2A	3273	1/1	0.93	0.09	45,45,45,45	0
58	MG	1A	4081	1/1	0.93	0.21	52,52,52,52	0
58	MG	2A	3048	1/1	0.93	0.11	67,67,67,67	0
58	MG	2A	3278	1/1	0.93	0.25	39,39,39,39	0
58	MG	2A	3557	1/1	0.93	0.12	33,33,33,33	0
58	MG	1A	3064	1/1	0.93	0.18	33,33,33,33	0
58	MG	1A	3331	1/1	0.93	0.08	46,46,46,46	0
58	MG	2A	3561	1/1	0.93	0.10	64,64,64,64	0
58	MG	2A	3051	1/1	0.93	0.18	55,55,55,55	0
58	MG	1A	3128	1/1	0.93	0.13	46,46,46,46	0
58	MG	1a	1666	1/1	0.93	0.22	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3885	1/1	0.93	0.10	43,43,43,43	0
58	MG	1B	210	1/1	0.93	0.09	53,53,53,53	0
58	MG	1A	3069	1/1	0.93	0.08	42,42,42,42	0
58	MG	2A	3577	1/1	0.93	0.12	58,58,58,58	0
58	MG	1A	3587	1/1	0.93	0.17	52,52,52,52	0
58	MG	1A	3889	1/1	0.93	0.15	54,54,54,54	0
58	MG	1A	3724	1/1	0.93	0.13	48,48,48,48	0
58	MG	1A	3589	1/1	0.93	0.15	55,55,55,55	0
58	MG	1a	1676	1/1	0.93	0.19	47,47,47,47	0
58	MG	1B	221	1/1	0.93	0.08	41,41,41,41	0
58	MG	1A	3893	1/1	0.93	0.17	55,55,55,55	0
58	MG	1a	1680	1/1	0.93	0.23	74,74,74,74	0
58	MG	1A	3477	1/1	0.93	0.13	45,45,45,45	0
58	MG	2A	3591	1/1	0.93	0.16	23,23,23,23	0
58	MG	2a	3030	1/1	0.93	0.25	68,68,68,68	0
58	MG	2A	3070	1/1	0.93	0.14	22,22,22,22	0
58	MG	2A	3596	1/1	0.93	0.11	37,37,37,37	0
58	MG	2A	3597	1/1	0.93	0.15	56,56,56,56	0
58	MG	1A	3209	1/1	0.93	0.07	42,42,42,42	0
58	MG	2A	3300	1/1	0.93	0.13	59,59,59,59	0
58	MG	1A	3746	1/1	0.93	0.10	19,19,19,19	0
58	MG	1A	3747	1/1	0.93	0.15	41,41,41,41	0
58	MG	1A	3481	1/1	0.93	0.21	50,50,50,50	0
58	MG	1A	3336	1/1	0.93	0.07	43,43,43,43	0
58	MG	2A	3080	1/1	0.93	0.09	46,46,46,46	0
58	MG	2A	3612	1/1	0.93	0.14	49,49,49,49	0
58	MG	2A	3308	1/1	0.93	0.10	55,55,55,55	0
58	MG	1a	1690	1/1	0.93	0.28	49,49,49,49	0
58	MG	1B	239	1/1	0.93	0.07	39,39,39,39	0
58	MG	1A	3752	1/1	0.93	0.10	40,40,40,40	0
58	MG	2A	3084	1/1	0.93	0.12	39,39,39,39	0
58	MG	1D	303	1/1	0.93	0.13	33,33,33,33	0
58	MG	2A	3628	1/1	0.93	0.29	60,60,60,60	0
58	MG	2A	3629	1/1	0.93	0.25	52,52,52,52	0
58	MG	1A	3914	1/1	0.93	0.14	53,53,53,53	0
58	MG	1D	310	1/1	0.93	0.08	33,33,33,33	0
58	MG	1a	1698	1/1	0.93	0.11	53,53,53,53	0
58	MG	2a	3057	1/1	0.93	0.07	58,58,58,58	0
58	MG	2a	3059	1/1	0.93	0.21	55,55,55,55	0
58	MG	1a	1700	1/1	0.93	0.08	54,54,54,54	0
58	MG	2A	3321	1/1	0.93	0.12	56,56,56,56	0
58	MG	1A	3046	1/1	0.93	0.06	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3104	1/1	0.93	0.10	47,47,47,47	0
58	MG	2A	3097	1/1	0.93	0.20	55,55,55,55	0
58	MG	2A	3325	1/1	0.93	0.16	56,56,56,56	0
58	MG	2a	3067	1/1	0.93	0.14	59,59,59,59	0
58	MG	2A	3645	1/1	0.93	0.09	46,46,46,46	0
58	MG	2A	3327	1/1	0.93	0.13	54,54,54,54	0
58	MG	1A	3922	1/1	0.93	0.09	42,42,42,42	0
58	MG	2A	3331	1/1	0.93	0.13	47,47,47,47	0
58	MG	1A	3756	1/1	0.93	0.16	23,23,23,23	0
58	MG	1A	3301	1/1	0.93	0.13	37,37,37,37	0
58	MG	1A	3422	1/1	0.93	0.07	38,38,38,38	0
58	MG	1A	3028	1/1	0.93	0.11	19,19,19,19	0
58	MG	1A	3769	1/1	0.93	0.16	57,57,57,57	0
58	MG	2A	3105	1/1	0.93	0.14	45,45,45,45	0
58	MG	2a	3079	1/1	0.93	0.13	64,64,64,64	0
58	MG	2A	3339	1/1	0.93	0.09	47,47,47,47	0
58	MG	2A	3657	1/1	0.93	0.12	42,42,42,42	0
58	MG	2A	3106	1/1	0.93	0.15	54,54,54,54	0
58	MG	1A	3347	1/1	0.93	0.15	64,64,64,64	0
58	MG	1A	3348	1/1	0.93	0.10	51,51,51,51	0
58	MG	1A	3936	1/1	0.93	0.17	58,58,58,58	0
58	MG	1a	1725	1/1	0.93	0.09	40,40,40,40	0
58	MG	1a	1726	1/1	0.93	0.07	35,35,35,35	0
58	MG	1A	3937	1/1	0.93	0.12	46,46,46,46	0
58	MG	1A	3940	1/1	0.93	0.10	52,52,52,52	0
58	MG	1O	204	1/1	0.93	0.09	59,59,59,59	0
58	MG	2A	3356	1/1	0.93	0.46	54,54,54,54	0
58	MG	1A	3305	1/1	0.93	0.10	39,39,39,39	0
58	MG	1A	3310	1/1	0.93	0.09	35,35,35,35	0
58	MG	1A	3784	1/1	0.93	0.10	12,12,12,12	0
58	MG	2A	3128	1/1	0.93	0.39	44,44,44,44	0
58	MG	2A	3687	1/1	0.93	0.10	62,62,62,62	0
58	MG	2A	3688	1/1	0.93	0.08	56,56,56,56	0
58	MG	2A	3129	1/1	0.93	0.08	42,42,42,42	0
58	MG	1A	3050	1/1	0.93	0.23	41,41,41,41	0
58	MG	2a	3106	1/1	0.93	0.20	65,65,65,65	0
58	MG	1Q	202	1/1	0.93	0.11	39,39,39,39	0
58	MG	2a	3110	1/1	0.93	0.26	53,53,53,53	0
58	MG	2A	3694	1/1	0.93	0.12	59,59,59,59	0
58	MG	2A	3365	1/1	0.93	0.06	42,42,42,42	0
58	MG	1a	1745	1/1	0.93	0.08	54,54,54,54	0
58	MG	2A	3700	1/1	0.93	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3950	1/1	0.93	0.12	49,49,49,49	0
58	MG	1Q	207	1/1	0.93	0.10	34,34,34,34	0
58	MG	1A	3504	1/1	0.93	0.11	48,48,48,48	0
58	MG	1A	3624	1/1	0.93	0.07	38,38,38,38	0
58	MG	1A	3505	1/1	0.93	0.12	37,37,37,37	0
58	MG	1A	3506	1/1	0.93	0.10	44,44,44,44	0
58	MG	2A	3147	1/1	0.93	0.15	42,42,42,42	0
58	MG	1U	206	1/1	0.93	0.20	24,24,24,24	0
58	MG	1A	3627	1/1	0.93	0.08	21,21,21,21	0
58	MG	1V	202	1/1	0.93	0.37	39,39,39,39	0
58	MG	2A	3381	1/1	0.93	0.10	40,40,40,40	0
58	MG	1A	3016	1/1	0.93	0.12	43,43,43,43	0
58	MG	1A	3801	1/1	0.93	0.10	68,68,68,68	0
58	MG	1A	3964	1/1	0.93	0.12	69,69,69,69	0
58	MG	1A	3630	1/1	0.93	0.10	64,64,64,64	0
58	MG	2A	3386	1/1	0.93	0.24	51,51,51,51	0
58	MG	2a	3136	1/1	0.93	0.20	58,58,58,58	0
58	MG	1W	203	1/1	0.93	0.11	27,27,27,27	0
58	MG	2A	3723	1/1	0.93	0.08	41,41,41,41	0
58	MG	1A	3433	1/1	0.93	0.29	34,34,34,34	0
58	MG	2a	3142	1/1	0.93	0.11	81,81,81,81	0
58	MG	1A	3636	1/1	0.93	0.07	45,45,45,45	0
58	MG	1A	3638	1/1	0.93	0.13	38,38,38,38	0
58	MG	2A	3733	1/1	0.93	0.16	53,53,53,53	0
58	MG	2A	3734	1/1	0.93	0.07	39,39,39,39	0
58	MG	1A	3971	1/1	0.93	0.07	30,30,30,30	0
58	MG	2A	3396	1/1	0.93	0.15	48,48,48,48	0
58	MG	2A	3738	1/1	0.93	0.09	52,52,52,52	0
58	MG	1a	1778	1/1	0.93	0.21	59,59,59,59	0
58	MG	1Y	202	1/1	0.93	0.27	46,46,46,46	0
58	MG	2a	3159	1/1	0.93	0.06	75,75,75,75	0
58	MG	1A	3973	1/1	0.93	0.11	48,48,48,48	0
58	MG	2a	3161	1/1	0.93	0.11	71,71,71,71	0
58	MG	1A	3143	1/1	0.93	0.08	57,57,57,57	0
58	MG	2A	3403	1/1	0.93	0.18	50,50,50,50	0
58	MG	1A	3360	1/1	0.93	0.08	33,33,33,33	0
58	MG	2A	3176	1/1	0.93	0.09	56,56,56,56	0
58	MG	1A	3439	1/1	0.93	0.12	46,46,46,46	0
58	MG	1A	3440	1/1	0.93	0.11	33,33,33,33	0
58	MG	1A	3314	1/1	0.93	0.08	31,31,31,31	0
58	MG	1A	3525	1/1	0.93	0.09	43,43,43,43	0
58	MG	1A	3988	1/1	0.93	0.06	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3756	1/1	0.93	0.13	60,60,60,60	0
58	MG	1A	3651	1/1	0.93	0.10	42,42,42,42	0
58	MG	1A	3527	1/1	0.93	0.25	55,55,55,55	0
58	MG	1A	3828	1/1	0.93	0.18	48,48,48,48	0
58	MG	1I	105	1/1	0.93	0.11	42,42,42,42	0
58	MG	2A	3419	1/1	0.93	0.20	25,25,25,25	0
58	MG	1A	3656	1/1	0.93	0.12	25,25,25,25	0
58	MG	1A	3530	1/1	0.93	0.09	40,40,40,40	0
58	MG	2A	3768	1/1	0.93	0.12	46,46,46,46	0
58	MG	2A	3424	1/1	0.93	0.13	49,49,49,49	0
58	MG	2A	3425	1/1	0.93	0.08	47,47,47,47	0
58	MG	1a	1802	1/1	0.93	0.22	51,51,51,51	0
58	MG	1A	4004	1/1	0.93	0.11	48,48,48,48	0
58	MG	1A	4006	1/1	0.93	0.10	61,61,61,61	0
58	MG	2A	3781	1/1	0.93	0.17	39,39,39,39	0
58	MG	2a	3191	1/1	0.93	0.18	64,64,64,64	0
58	MG	1A	4009	1/1	0.93	0.10	38,38,38,38	0
58	MG	2A	3431	1/1	0.93	0.13	38,38,38,38	0
58	MG	2A	3791	1/1	0.93	0.19	63,63,63,63	0
58	MG	2A	3432	1/1	0.93	0.14	60,60,60,60	0
58	MG	1A	3442	1/1	0.93	0.10	47,47,47,47	0
58	MG	1A	3833	1/1	0.93	0.10	44,44,44,44	0
58	MG	2A	3798	1/1	0.93	0.10	52,52,52,52	0
58	MG	1A	3834	1/1	0.93	0.14	44,44,44,44	0
58	MG	1A	3446	1/1	0.93	0.46	40,40,40,40	0
58	MG	1A	3063	1/1	0.93	0.26	51,51,51,51	0
58	MG	18	106	1/1	0.93	0.23	66,66,66,66	0
58	MG	1A	4021	1/1	0.93	0.07	50,50,50,50	0
58	MG	1A	3232	1/1	0.93	0.11	51,51,51,51	0
58	MG	1A	4023	1/1	0.93	0.16	27,27,27,27	0
58	MG	1A	3184	1/1	0.93	0.05	53,53,53,53	0
58	MG	2A	3447	1/1	0.93	0.12	52,52,52,52	0
58	MG	2d	301	1/1	0.93	0.28	61,61,61,61	0
58	MG	2d	302	1/1	0.93	0.10	73,73,73,73	0
58	MG	1A	3187	1/1	0.93	0.11	27,27,27,27	0
58	MG	2f	201	1/1	0.93	0.10	58,58,58,58	0
58	MG	2A	3218	1/1	0.93	0.19	41,41,41,41	0
58	MG	1A	3090	1/1	0.93	0.14	42,42,42,42	0
58	MG	2A	3454	1/1	0.93	0.15	57,57,57,57	0
58	MG	1A	3851	1/1	0.93	0.12	47,47,47,47	0
58	MG	2A	3221	1/1	0.93	0.14	53,53,53,53	0
58	MG	1A	3373	1/1	0.93	0.10	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1614	1/1	0.93	0.11	70,70,70,70	0
58	MG	1A	3272	1/1	0.93	0.09	37,37,37,37	0
58	MG	1A	4037	1/1	0.93	0.08	51,51,51,51	0
58	MG	1A	3376	1/1	0.93	0.16	47,47,47,47	0
58	MG	1A	3556	1/1	0.93	0.36	38,38,38,38	0
58	MG	1A	3857	1/1	0.93	0.11	33,33,33,33	0
58	MG	1A	4045	1/1	0.93	0.13	14,14,14,14	0
58	MG	2B	208	1/1	0.93	0.12	57,57,57,57	0
58	MG	1a	1625	1/1	0.93	0.12	52,52,52,52	0
58	MG	1a	1626	1/1	0.93	0.34	51,51,51,51	0
58	MG	1A	3858	1/1	0.93	0.18	40,40,40,40	0
58	MG	2A	3480	1/1	0.93	0.10	57,57,57,57	0
58	MG	1Z	303	1/1	0.94	0.12	52,52,52,52	0
58	MG	10	101	1/1	0.94	0.12	40,40,40,40	0
58	MG	1A	3403	1/1	0.94	0.12	56,56,56,56	0
58	MG	1a	1753	1/1	0.94	0.17	49,49,49,49	0
58	MG	1A	3475	1/1	0.94	0.40	58,58,58,58	0
58	MG	2A	3585	1/1	0.94	0.10	52,52,52,52	0
58	MG	2A	3587	1/1	0.94	0.12	52,52,52,52	0
58	MG	2W	203	1/1	0.94	0.06	35,35,35,35	0
58	MG	2W	204	1/1	0.94	0.10	58,58,58,58	0
58	MG	1a	1755	1/1	0.94	0.12	54,54,54,54	0
58	MG	1A	4026	1/1	0.94	0.07	30,30,30,30	0
58	MG	1A	3020	1/1	0.94	0.08	24,24,24,24	0
58	MG	2A	3123	1/1	0.94	0.07	59,59,59,59	0
58	MG	2A	3593	1/1	0.94	0.09	46,46,46,46	0
58	MG	1a	1758	1/1	0.94	0.12	50,50,50,50	0
58	MG	1A	3478	1/1	0.94	0.19	52,52,52,52	0
58	MG	1A	3479	1/1	0.94	0.06	36,36,36,36	0
58	MG	1A	3032	1/1	0.94	0.09	32,32,32,32	0
58	MG	1A	3720	1/1	0.94	0.10	54,54,54,54	0
58	MG	2a	3002	1/1	0.94	0.20	59,59,59,59	0
58	MG	1A	3081	1/1	0.94	0.07	47,47,47,47	0
58	MG	1A	3340	1/1	0.94	0.08	37,37,37,37	0
58	MG	2A	3606	1/1	0.94	0.10	40,40,40,40	0
58	MG	11	104	1/1	0.94	0.12	57,57,57,57	0
58	MG	1a	1770	1/1	0.94	0.15	58,58,58,58	0
58	MG	2A	3611	1/1	0.94	0.07	36,36,36,36	0
58	MG	1A	3483	1/1	0.94	0.18	29,29,29,29	0
58	MG	1A	3731	1/1	0.94	0.08	41,41,41,41	0
58	MG	1A	3412	1/1	0.94	0.20	60,60,60,60	0
58	MG	2A	3616	1/1	0.94	0.15	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	15	102	1/1	0.94	0.19	40,40,40,40	0
58	MG	2A	3144	1/1	0.94	0.15	53,53,53,53	0
58	MG	2A	3145	1/1	0.94	0.06	42,42,42,42	0
58	MG	2A	3352	1/1	0.94	0.11	55,55,55,55	0
58	MG	1A	3342	1/1	0.94	0.08	39,39,39,39	0
58	MG	1A	3886	1/1	0.94	0.10	37,37,37,37	0
58	MG	1A	3147	1/1	0.94	0.11	36,36,36,36	0
58	MG	1A	3056	1/1	0.94	0.09	30,30,30,30	0
58	MG	15	108	1/1	0.94	0.07	45,45,45,45	0
58	MG	1A	4057	1/1	0.94	0.11	52,52,52,52	0
58	MG	2A	3154	1/1	0.94	0.16	42,42,42,42	0
58	MG	1A	3151	1/1	0.94	0.23	29,29,29,29	0
58	MG	2A	3638	1/1	0.94	0.08	36,36,36,36	0
58	MG	17	101	1/1	0.94	0.14	56,56,56,56	0
58	MG	2A	3157	1/1	0.94	0.07	51,51,51,51	0
58	MG	2A	3643	1/1	0.94	0.11	53,53,53,53	0
58	MG	1A	3890	1/1	0.94	0.07	30,30,30,30	0
58	MG	1A	3192	1/1	0.94	0.47	41,41,41,41	0
58	MG	18	104	1/1	0.94	0.13	53,53,53,53	0
58	MG	1A	3193	1/1	0.94	0.08	44,44,44,44	0
58	MG	1A	3086	1/1	0.94	0.18	42,42,42,42	0
58	MG	1a	1601	1/1	0.94	0.09	51,51,51,51	0
58	MG	2A	3166	1/1	0.94	0.16	45,45,45,45	0
58	MG	1A	3306	1/1	0.94	0.10	52,52,52,52	0
58	MG	1A	3351	1/1	0.94	0.11	39,39,39,39	0
58	MG	1A	3618	1/1	0.94	0.07	20,20,20,20	0
58	MG	1a	1803	1/1	0.94	0.21	58,58,58,58	0
58	MG	2A	3174	1/1	0.94	0.11	57,57,57,57	0
58	MG	1a	1805	1/1	0.94	0.39	54,54,54,54	0
58	MG	1a	1607	1/1	0.94	0.10	59,59,59,59	0
58	MG	2a	3045	1/1	0.94	0.16	76,76,76,76	0
58	MG	2A	3178	1/1	0.94	0.13	56,56,56,56	0
58	MG	1a	1807	1/1	0.94	0.30	63,63,63,63	0
58	MG	1A	3902	1/1	0.94	0.08	22,22,22,22	0
58	MG	2a	3049	1/1	0.94	0.20	50,50,50,50	0
58	MG	1A	3352	1/1	0.94	0.10	42,42,42,42	0
58	MG	1A	3906	1/1	0.94	0.07	32,32,32,32	0
58	MG	1d	301	1/1	0.94	0.25	63,63,63,63	0
58	MG	2a	3054	1/1	0.94	0.08	49,49,49,49	0
58	MG	2A	3390	1/1	0.94	0.18	46,46,46,46	0
58	MG	1a	1612	1/1	0.94	0.15	32,32,32,32	0
58	MG	2A	3678	1/1	0.94	0.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3392	1/1	0.94	0.14	54,54,54,54	0
58	MG	2A	3680	1/1	0.94	0.11	54,54,54,54	0
58	MG	1m	3001	1/1	0.94	0.11	51,51,51,51	0
58	MG	2A	3394	1/1	0.94	0.14	39,39,39,39	0
58	MG	1A	3308	1/1	0.94	0.11	42,42,42,42	0
58	MG	1A	3198	1/1	0.94	0.06	37,37,37,37	0
58	MG	2A	3397	1/1	0.94	0.12	59,59,59,59	0
58	MG	1p	102	1/1	0.94	0.14	49,49,49,49	0
58	MG	1A	3357	1/1	0.94	0.12	32,32,32,32	0
58	MG	2A	3691	1/1	0.94	0.11	65,65,65,65	0
58	MG	1A	3437	1/1	0.94	0.07	28,28,28,28	0
58	MG	1A	3113	1/1	0.94	0.11	42,42,42,42	0
58	MG	1A	3628	1/1	0.94	0.08	13,13,13,13	0
58	MG	1w	103	1/1	0.94	0.06	81,81,81,81	0
58	MG	1A	3359	1/1	0.94	0.29	46,46,46,46	0
58	MG	2a	3075	1/1	0.94	0.12	59,59,59,59	0
58	MG	1B	207	1/1	0.94	0.21	46,46,46,46	0
58	MG	2A	3197	1/1	0.94	0.07	47,47,47,47	0
58	MG	1A	3042	1/1	0.94	0.11	30,30,30,30	0
58	MG	2A	3410	1/1	0.94	0.21	45,45,45,45	0
58	MG	2A	3704	1/1	0.94	0.07	68,68,68,68	0
58	MG	1A	3926	1/1	0.94	0.14	42,42,42,42	0
58	MG	1A	3632	1/1	0.94	0.07	36,36,36,36	0
58	MG	1A	3792	1/1	0.94	0.08	39,39,39,39	0
58	MG	2A	3709	1/1	0.94	0.09	53,53,53,53	0
58	MG	2A	3414	1/1	0.94	0.16	57,57,57,57	0
58	MG	1A	3155	1/1	0.94	0.08	37,37,37,37	0
58	MG	1A	3362	1/1	0.94	0.10	63,63,63,63	0
58	MG	1A	3443	1/1	0.94	0.09	46,46,46,46	0
58	MG	2A	3714	1/1	0.94	0.09	51,51,51,51	0
58	MG	1B	219	1/1	0.94	0.08	36,36,36,36	0
58	MG	1A	3208	1/1	0.94	0.15	34,34,34,34	0
58	MG	1a	1636	1/1	0.94	0.18	43,43,43,43	0
58	MG	1B	222	1/1	0.94	0.10	40,40,40,40	0
58	MG	2A	3002	1/1	0.94	0.29	50,50,50,50	0
58	MG	1A	3642	1/1	0.94	0.10	36,36,36,36	0
58	MG	2a	3101	1/1	0.94	0.25	65,65,65,65	0
58	MG	2A	3427	1/1	0.94	0.24	52,52,52,52	0
58	MG	1A	3529	1/1	0.94	0.24	54,54,54,54	0
58	MG	1A	3034	1/1	0.94	0.33	24,24,24,24	0
58	MG	1A	3941	1/1	0.94	0.11	59,59,59,59	0
58	MG	2A	3226	1/1	0.94	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3731	1/1	0.94	0.28	59,59,59,59	0
58	MG	1B	231	1/1	0.94	0.06	43,43,43,43	0
58	MG	1A	3646	1/1	0.94	0.08	36,36,36,36	0
58	MG	1A	3531	1/1	0.94	0.07	46,46,46,46	0
58	MG	2a	3113	1/1	0.94	0.19	52,52,52,52	0
58	MG	2A	3436	1/1	0.94	0.09	63,63,63,63	0
58	MG	1a	1646	1/1	0.94	0.23	40,40,40,40	0
58	MG	1A	3809	1/1	0.94	0.15	41,41,41,41	0
58	MG	2a	3117	1/1	0.94	0.24	49,49,49,49	0
58	MG	1B	236	1/1	0.94	0.11	55,55,55,55	0
58	MG	1A	3532	1/1	0.94	0.08	67,67,67,67	0
58	MG	1B	240	1/1	0.94	0.13	42,42,42,42	0
58	MG	2A	3744	1/1	0.94	0.08	59,59,59,59	0
58	MG	1A	3366	1/1	0.94	0.23	39,39,39,39	0
58	MG	1A	3021	1/1	0.94	0.07	36,36,36,36	0
58	MG	1A	3816	1/1	0.94	0.16	46,46,46,46	0
58	MG	1D	309	1/1	0.94	0.26	47,47,47,47	0
58	MG	2a	3127	1/1	0.94	0.19	42,42,42,42	0
58	MG	1A	3214	1/1	0.94	0.06	29,29,29,29	0
58	MG	2A	3751	1/1	0.94	0.16	63,63,63,63	0
58	MG	1A	3540	1/1	0.94	0.06	31,31,31,31	0
58	MG	2A	3031	1/1	0.94	0.12	49,49,49,49	0
58	MG	1A	3007	1/1	0.94	0.08	43,43,43,43	0
58	MG	1E	302	1/1	0.94	0.13	31,31,31,31	0
58	MG	2A	3457	1/1	0.94	0.10	55,55,55,55	0
58	MG	1a	1665	1/1	0.94	0.22	48,48,48,48	0
58	MG	1A	3265	1/1	0.94	0.16	62,62,62,62	0
58	MG	2A	3462	1/1	0.94	0.13	60,60,60,60	0
58	MG	1A	3961	1/1	0.94	0.09	65,65,65,65	0
58	MG	1A	3822	1/1	0.94	0.08	38,38,38,38	0
58	MG	2a	3143	1/1	0.94	0.07	75,75,75,75	0
58	MG	2A	3250	1/1	0.94	0.09	54,54,54,54	0
58	MG	1A	3963	1/1	0.94	0.09	43,43,43,43	0
58	MG	2A	3041	1/1	0.94	0.14	57,57,57,57	0
58	MG	1A	3096	1/1	0.94	0.06	47,47,47,47	0
58	MG	2a	3149	1/1	0.94	0.14	66,66,66,66	0
58	MG	2a	3150	1/1	0.94	0.22	61,61,61,61	0
58	MG	1A	3455	1/1	0.94	0.14	50,50,50,50	0
58	MG	1A	3268	1/1	0.94	0.15	41,41,41,41	0
58	MG	2A	3473	1/1	0.94	0.08	55,55,55,55	0
58	MG	1A	3553	1/1	0.94	0.06	21,21,21,21	0
58	MG	2A	3476	1/1	0.94	0.21	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3051	1/1	0.94	0.21	28,28,28,28	0
58	MG	1N	203	1/1	0.94	0.12	47,47,47,47	0
58	MG	1a	1678	1/1	0.94	0.07	56,56,56,56	0
58	MG	2a	3162	1/1	0.94	0.09	75,75,75,75	0
58	MG	1A	3674	1/1	0.94	0.06	32,32,32,32	0
58	MG	2A	3264	1/1	0.94	0.14	55,55,55,55	0
58	MG	1O	201	1/1	0.94	0.08	53,53,53,53	0
58	MG	2a	3167	1/1	0.94	0.21	50,50,50,50	0
58	MG	1A	3972	1/1	0.94	0.08	34,34,34,34	0
58	MG	1A	3380	1/1	0.94	0.27	26,26,26,26	0
58	MG	2A	3803	1/1	0.94	0.13	56,56,56,56	0
58	MG	1P	204	1/1	0.94	0.35	27,27,27,27	0
58	MG	1A	3066	1/1	0.94	0.13	41,41,41,41	0
58	MG	2A	3806	1/1	0.94	0.09	47,47,47,47	0
58	MG	1A	3835	1/1	0.94	0.11	37,37,37,37	0
58	MG	2A	3495	1/1	0.94	0.20	44,44,44,44	0
58	MG	2A	3496	1/1	0.94	0.05	27,27,27,27	0
58	MG	1a	1688	1/1	0.94	0.28	54,54,54,54	0
58	MG	1A	3557	1/1	0.94	0.16	30,30,30,30	0
58	MG	1P	209	1/1	0.94	0.11	46,46,46,46	0
58	MG	1A	3681	1/1	0.94	0.08	19,19,19,19	0
58	MG	1A	3982	1/1	0.94	0.13	16,16,16,16	0
58	MG	1A	3382	1/1	0.94	0.28	41,41,41,41	0
58	MG	1Q	206	1/1	0.94	0.08	34,34,34,34	0
58	MG	1A	3226	1/1	0.94	0.25	52,52,52,52	0
58	MG	2A	3823	1/1	0.94	0.16	58,58,58,58	0
58	MG	1R	202	1/1	0.94	0.07	34,34,34,34	0
58	MG	2A	3283	1/1	0.94	0.13	54,54,54,54	0
58	MG	1A	3562	1/1	0.94	0.09	44,44,44,44	0
58	MG	1A	3053	1/1	0.94	0.14	44,44,44,44	0
58	MG	2a	3192	1/1	0.94	0.12	54,54,54,54	0
58	MG	1A	3690	1/1	0.94	0.08	19,19,19,19	0
58	MG	2A	3520	1/1	0.94	0.07	39,39,39,39	0
58	MG	1U	202	1/1	0.94	0.17	34,34,34,34	0
58	MG	1U	204	1/1	0.94	0.12	28,28,28,28	0
58	MG	1A	3274	1/1	0.94	0.15	48,48,48,48	0
58	MG	2A	3527	1/1	0.94	0.09	31,31,31,31	0
58	MG	2A	3079	1/1	0.94	0.08	47,47,47,47	0
58	MG	1A	4000	1/1	0.94	0.08	56,56,56,56	0
58	MG	1U	207	1/1	0.94	0.38	35,35,35,35	0
58	MG	2A	3535	1/1	0.94	0.11	40,40,40,40	0
58	MG	1U	210	1/1	0.94	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3294	1/1	0.94	0.11	46,46,46,46	0
58	MG	2A	3540	1/1	0.94	0.07	57,57,57,57	0
58	MG	2a	3207	1/1	0.94	0.11	65,65,65,65	0
58	MG	2a	3208	1/1	0.94	0.08	63,63,63,63	0
58	MG	1A	3275	1/1	0.94	0.10	31,31,31,31	0
58	MG	1a	1715	1/1	0.94	0.17	50,50,50,50	0
58	MG	1A	3695	1/1	0.94	0.16	41,41,41,41	0
58	MG	1A	3696	1/1	0.94	0.09	46,46,46,46	0
58	MG	1a	1724	1/1	0.94	0.07	52,52,52,52	0
58	MG	2D	307	1/1	0.94	0.27	42,42,42,42	0
58	MG	1V	205	1/1	0.94	0.29	31,31,31,31	0
58	MG	2E	301	1/1	0.94	0.14	46,46,46,46	0
58	MG	1A	3131	1/1	0.94	0.29	47,47,47,47	0
58	MG	2A	3555	1/1	0.94	0.18	32,32,32,32	0
58	MG	2A	3556	1/1	0.94	0.17	46,46,46,46	0
58	MG	2A	3092	1/1	0.94	0.17	62,62,62,62	0
58	MG	1V	207	1/1	0.94	0.08	39,39,39,39	0
58	MG	1A	3698	1/1	0.94	0.11	54,54,54,54	0
58	MG	2q	202	1/1	0.94	0.07	71,71,71,71	0
58	MG	1A	3572	1/1	0.94	0.11	31,31,31,31	0
58	MG	1A	3102	1/1	0.94	0.08	42,42,42,42	0
58	MG	1A	3103	1/1	0.94	0.09	41,41,41,41	0
58	MG	1A	4018	1/1	0.94	0.07	39,39,39,39	0
58	MG	2N	201	1/1	0.94	0.07	52,52,52,52	0
58	MG	1A	3175	1/1	0.94	0.16	31,31,31,31	0
58	MG	1a	1743	1/1	0.94	0.11	39,39,39,39	0
58	MG	1A	3863	1/1	0.94	0.33	25,25,25,25	0
58	MG	1A	3576	1/1	0.94	0.12	49,49,49,49	0
58	MG	2A	3316	1/1	0.94	0.12	62,62,62,62	0
60	TEL	2A	3826	58/58	0.94	0.14	27,41,47,55	0
58	MG	1A	3401	1/1	0.94	0.12	50,50,50,50	0
58	MG	1a	1717	1/1	0.95	0.17	76,76,76,76	0
58	MG	2A	3554	1/1	0.95	0.07	32,32,32,32	0
58	MG	1A	3136	1/1	0.95	0.12	30,30,30,30	0
58	MG	1a	1721	1/1	0.95	0.10	48,48,48,48	0
58	MG	1a	1722	1/1	0.95	0.06	57,57,57,57	0
58	MG	1A	4049	1/1	0.95	0.06	20,20,20,20	0
58	MG	1A	4051	1/1	0.95	0.09	51,51,51,51	0
58	MG	2A	3560	1/1	0.95	0.11	27,27,27,27	0
58	MG	1A	3138	1/1	0.95	0.07	35,35,35,35	0
58	MG	2A	3562	1/1	0.95	0.21	55,55,55,55	0
58	MG	2R	202	1/1	0.95	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3372	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3444	1/1	0.95	0.12	50,50,50,50	0
58	MG	1A	3224	1/1	0.95	0.17	35,35,35,35	0
58	MG	1A	3905	1/1	0.95	0.15	49,49,49,49	0
58	MG	1a	1732	1/1	0.95	0.13	50,50,50,50	0
58	MG	1a	1733	1/1	0.95	0.12	48,48,48,48	0
58	MG	2A	3573	1/1	0.95	0.15	45,45,45,45	0
58	MG	2A	3574	1/1	0.95	0.07	47,47,47,47	0
58	MG	1A	4063	1/1	0.95	0.18	48,48,48,48	0
58	MG	1A	3139	1/1	0.95	0.09	31,31,31,31	0
58	MG	1a	1738	1/1	0.95	0.19	42,42,42,42	0
58	MG	1A	3778	1/1	0.95	0.07	57,57,57,57	0
58	MG	1a	1740	1/1	0.95	0.09	46,46,46,46	0
58	MG	2A	3315	1/1	0.95	0.08	55,55,55,55	0
58	MG	1a	1741	1/1	0.95	0.14	35,35,35,35	0
58	MG	23	101	1/1	0.95	0.18	52,52,52,52	0
58	MG	2A	3317	1/1	0.95	0.16	36,36,36,36	0
58	MG	25	103	1/1	0.95	0.17	47,47,47,47	0
58	MG	1A	3781	1/1	0.95	0.07	16,16,16,16	0
58	MG	27	102	1/1	0.95	0.16	47,47,47,47	0
58	MG	1A	3633	1/1	0.95	0.10	28,28,28,28	0
58	MG	1A	3913	1/1	0.95	0.06	39,39,39,39	0
58	MG	1a	1748	1/1	0.95	0.15	43,43,43,43	0
58	MG	1A	3528	1/1	0.95	0.07	44,44,44,44	0
58	MG	2A	3108	1/1	0.95	0.06	47,47,47,47	0
58	MG	11	101	1/1	0.95	0.30	33,33,33,33	0
58	MG	2A	3594	1/1	0.95	0.19	36,36,36,36	0
58	MG	1A	3915	1/1	0.95	0.08	51,51,51,51	0
58	MG	2A	3326	1/1	0.95	0.15	49,49,49,49	0
58	MG	2A	3598	1/1	0.95	0.12	41,41,41,41	0
58	MG	2A	3111	1/1	0.95	0.10	41,41,41,41	0
58	MG	1A	3785	1/1	0.95	0.13	37,37,37,37	0
58	MG	2A	3601	1/1	0.95	0.08	45,45,45,45	0
58	MG	2A	3329	1/1	0.95	0.09	58,58,58,58	0
58	MG	2a	3014	1/1	0.95	0.12	50,50,50,50	0
58	MG	2A	3330	1/1	0.95	0.06	63,63,63,63	0
58	MG	1A	3070	1/1	0.95	0.15	36,36,36,36	0
58	MG	2A	3115	1/1	0.95	0.23	58,58,58,58	0
58	MG	1A	3637	1/1	0.95	0.12	60,60,60,60	0
58	MG	12	101	1/1	0.95	0.07	37,37,37,37	0
58	MG	2A	3118	1/1	0.95	0.17	58,58,58,58	0
58	MG	12	102	1/1	0.95	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	13	102	1/1	0.95	0.09	37,37,37,37	0
58	MG	1A	3178	1/1	0.95	0.10	27,27,27,27	0
58	MG	2A	3125	1/1	0.95	0.07	40,40,40,40	0
58	MG	2A	3617	1/1	0.95	0.19	64,64,64,64	0
58	MG	2A	3341	1/1	0.95	0.12	57,57,57,57	0
58	MG	1A	3180	1/1	0.95	0.05	30,30,30,30	0
58	MG	2a	3028	1/1	0.95	0.13	77,77,77,77	0
58	MG	2A	3622	1/1	0.95	0.11	46,46,46,46	0
58	MG	1A	3641	1/1	0.95	0.09	33,33,33,33	0
58	MG	1A	3229	1/1	0.95	0.15	29,29,29,29	0
58	MG	2A	3627	1/1	0.95	0.06	30,30,30,30	0
58	MG	1a	1762	1/1	0.95	0.16	62,62,62,62	0
58	MG	2A	3347	1/1	0.95	0.07	56,56,56,56	0
58	MG	15	104	1/1	0.95	0.21	38,38,38,38	0
58	MG	2A	3349	1/1	0.95	0.15	51,51,51,51	0
58	MG	2A	3350	1/1	0.95	0.09	49,49,49,49	0
58	MG	2A	3633	1/1	0.95	0.10	56,56,56,56	0
58	MG	2A	3131	1/1	0.95	0.12	31,31,31,31	0
58	MG	1A	3276	1/1	0.95	0.11	62,62,62,62	0
58	MG	2A	3135	1/1	0.95	0.13	43,43,43,43	0
58	MG	1a	1766	1/1	0.95	0.15	59,59,59,59	0
58	MG	1a	1767	1/1	0.95	0.09	57,57,57,57	0
58	MG	1A	3142	1/1	0.95	0.06	38,38,38,38	0
58	MG	1B	206	1/1	0.95	0.06	39,39,39,39	0
58	MG	1A	3536	1/1	0.95	0.06	31,31,31,31	0
58	MG	1B	208	1/1	0.95	0.17	52,52,52,52	0
58	MG	2A	3143	1/1	0.95	0.14	59,59,59,59	0
58	MG	1A	3537	1/1	0.95	0.09	53,53,53,53	0
58	MG	1A	3805	1/1	0.95	0.09	33,33,33,33	0
58	MG	17	105	1/1	0.95	0.13	35,35,35,35	0
58	MG	1A	3384	1/1	0.95	0.09	62,62,62,62	0
58	MG	2A	3367	1/1	0.95	0.08	59,59,59,59	0
58	MG	1B	212	1/1	0.95	0.20	52,52,52,52	0
58	MG	1a	1782	1/1	0.95	0.09	75,75,75,75	0
58	MG	2A	3151	1/1	0.95	0.16	55,55,55,55	0
58	MG	2a	3058	1/1	0.95	0.21	60,60,60,60	0
58	MG	1A	3091	1/1	0.95	0.05	28,28,28,28	0
58	MG	18	105	1/1	0.95	0.07	32,32,32,32	0
58	MG	2A	3658	1/1	0.95	0.07	62,62,62,62	0
58	MG	2A	3659	1/1	0.95	0.13	46,46,46,46	0
58	MG	2A	3660	1/1	0.95	0.06	64,64,64,64	0
58	MG	2A	3374	1/1	0.95	0.20	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3005	1/1	0.95	0.10	39,39,39,39	0
58	MG	1A	3944	1/1	0.95	0.06	31,31,31,31	0
58	MG	2A	3665	1/1	0.95	0.07	72,72,72,72	0
58	MG	1B	217	1/1	0.95	0.20	46,46,46,46	0
58	MG	1a	1788	1/1	0.95	0.11	38,38,38,38	0
58	MG	1A	3284	1/1	0.95	0.39	27,27,27,27	0
58	MG	2A	3669	1/1	0.95	0.05	60,60,60,60	0
58	MG	1A	3390	1/1	0.95	0.07	30,30,30,30	0
58	MG	1a	1604	1/1	0.95	0.10	60,60,60,60	0
58	MG	1a	1605	1/1	0.95	0.16	39,39,39,39	0
58	MG	2A	3162	1/1	0.95	0.06	36,36,36,36	0
58	MG	1A	3391	1/1	0.95	0.10	53,53,53,53	0
58	MG	1A	3658	1/1	0.95	0.08	32,32,32,32	0
58	MG	2A	3387	1/1	0.95	0.22	38,38,38,38	0
58	MG	2A	3165	1/1	0.95	0.12	36,36,36,36	0
58	MG	2a	3081	1/1	0.95	0.17	44,44,44,44	0
58	MG	1A	3550	1/1	0.95	0.08	38,38,38,38	0
58	MG	1a	1798	1/1	0.95	0.19	46,46,46,46	0
58	MG	2A	3686	1/1	0.95	0.11	36,36,36,36	0
58	MG	1a	1799	1/1	0.95	0.23	55,55,55,55	0
58	MG	2A	3169	1/1	0.95	0.08	32,32,32,32	0
58	MG	1A	3551	1/1	0.95	0.25	34,34,34,34	0
58	MG	2A	3171	1/1	0.95	0.10	50,50,50,50	0
58	MG	1a	1610	1/1	0.95	0.13	34,34,34,34	0
58	MG	2a	3093	1/1	0.95	0.07	64,64,64,64	0
58	MG	1A	3665	1/1	0.95	0.06	25,25,25,25	0
58	MG	1A	3236	1/1	0.95	0.29	42,42,42,42	0
58	MG	1a	1804	1/1	0.95	0.35	50,50,50,50	0
58	MG	1A	3395	1/1	0.95	0.09	38,38,38,38	0
58	MG	1A	3396	1/1	0.95	0.20	59,59,59,59	0
58	MG	1B	233	1/1	0.95	0.07	57,57,57,57	0
58	MG	1A	3957	1/1	0.95	0.08	57,57,57,57	0
58	MG	1A	3958	1/1	0.95	0.11	54,54,54,54	0
58	MG	1A	3397	1/1	0.95	0.08	44,44,44,44	0
58	MG	1A	3337	1/1	0.95	0.12	37,37,37,37	0
58	MG	1A	3338	1/1	0.95	0.08	35,35,35,35	0
58	MG	2A	3186	1/1	0.95	0.12	44,44,44,44	0
58	MG	2A	3708	1/1	0.95	0.13	45,45,45,45	0
58	MG	1A	3022	1/1	0.95	0.07	18,18,18,18	0
58	MG	1A	3118	1/1	0.95	0.14	39,39,39,39	0
58	MG	1A	3242	1/1	0.95	0.17	38,38,38,38	0
58	MG	1p	101	1/1	0.95	0.07	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3682	1/1	0.95	0.09	35,35,35,35	0
58	MG	1A	3120	1/1	0.95	0.10	29,29,29,29	0
58	MG	1D	311	1/1	0.95	0.16	30,30,30,30	0
58	MG	1A	3078	1/1	0.95	0.07	35,35,35,35	0
58	MG	1A	3476	1/1	0.95	0.21	30,30,30,30	0
58	MG	1A	3079	1/1	0.95	0.05	29,29,29,29	0
58	MG	1E	303	1/1	0.95	0.05	21,21,21,21	0
58	MG	1A	3196	1/1	0.95	0.26	31,31,31,31	0
58	MG	2A	3200	1/1	0.95	0.11	59,59,59,59	0
58	MG	2A	3201	1/1	0.95	0.16	48,48,48,48	0
58	MG	2A	3724	1/1	0.95	0.22	62,62,62,62	0
58	MG	2A	3202	1/1	0.95	0.06	34,34,34,34	0
58	MG	1A	3006	1/1	0.95	0.10	43,43,43,43	0
58	MG	1A	3975	1/1	0.95	0.09	33,33,33,33	0
58	MG	1a	1640	1/1	0.95	0.21	42,42,42,42	0
58	MG	2A	3208	1/1	0.95	0.10	51,51,51,51	0
58	MG	1A	3848	1/1	0.95	0.07	48,48,48,48	0
58	MG	1A	3082	1/1	0.95	0.16	34,34,34,34	0
58	MG	1F	304	1/1	0.95	0.10	43,43,43,43	0
58	MG	1A	3417	1/1	0.95	0.07	36,36,36,36	0
58	MG	2A	3215	1/1	0.95	0.10	37,37,37,37	0
58	MG	1A	3157	1/1	0.95	0.11	24,24,24,24	0
58	MG	2a	3137	1/1	0.95	0.17	53,53,53,53	0
58	MG	1A	3984	1/1	0.95	0.06	56,56,56,56	0
58	MG	1A	3419	1/1	0.95	0.16	54,54,54,54	0
58	MG	1x	112	1/1	0.95	0.20	60,60,60,60	0
58	MG	2A	3443	1/1	0.95	0.22	31,31,31,31	0
58	MG	1G	201	1/1	0.95	0.14	42,42,42,42	0
58	MG	1G	203	1/1	0.95	0.06	53,53,53,53	0
58	MG	2A	3003	1/1	0.95	0.17	48,48,48,48	0
58	MG	2A	3224	1/1	0.95	0.14	40,40,40,40	0
58	MG	1G	204	1/1	0.95	0.09	33,33,33,33	0
58	MG	1G	205	1/1	0.95	0.13	47,47,47,47	0
58	MG	1N	201	1/1	0.95	0.07	28,28,28,28	0
58	MG	1N	202	1/1	0.95	0.07	34,34,34,34	0
58	MG	2A	3455	1/1	0.95	0.13	53,53,53,53	0
58	MG	1a	1657	1/1	0.95	0.06	61,61,61,61	0
58	MG	1A	3307	1/1	0.95	0.19	54,54,54,54	0
58	MG	2a	3157	1/1	0.95	0.10	66,66,66,66	0
58	MG	1A	3486	1/1	0.95	0.28	40,40,40,40	0
58	MG	2A	3459	1/1	0.95	0.13	57,57,57,57	0
58	MG	2A	3013	1/1	0.95	0.22	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1N	205	1/1	0.95	0.10	57,57,57,57	0
58	MG	2A	3015	1/1	0.95	0.11	68,68,68,68	0
58	MG	1a	1662	1/1	0.95	0.13	43,43,43,43	0
58	MG	1A	3487	1/1	0.95	0.15	48,48,48,48	0
58	MG	1A	3581	1/1	0.95	0.10	36,36,36,36	0
58	MG	1A	3421	1/1	0.95	0.09	45,45,45,45	0
58	MG	2A	3776	1/1	0.95	0.13	44,44,44,44	0
58	MG	1P	201	1/1	0.95	0.14	31,31,31,31	0
58	MG	2A	3025	1/1	0.95	0.22	42,42,42,42	0
58	MG	2a	3171	1/1	0.95	0.15	64,64,64,64	0
58	MG	1A	3019	1/1	0.95	0.09	43,43,43,43	0
58	MG	1A	3309	1/1	0.95	0.20	55,55,55,55	0
58	MG	1A	3206	1/1	0.95	0.07	28,28,28,28	0
58	MG	1A	3255	1/1	0.95	0.11	43,43,43,43	0
58	MG	2A	3477	1/1	0.95	0.20	41,41,41,41	0
58	MG	1A	3043	1/1	0.95	0.31	34,34,34,34	0
58	MG	2A	3479	1/1	0.95	0.24	56,56,56,56	0
58	MG	1A	3044	1/1	0.95	0.16	33,33,33,33	0
58	MG	2A	3033	1/1	0.95	0.06	60,60,60,60	0
58	MG	2A	3800	1/1	0.95	0.10	27,27,27,27	0
58	MG	1A	3596	1/1	0.95	0.12	24,24,24,24	0
58	MG	2A	3485	1/1	0.95	0.10	48,48,48,48	0
58	MG	1A	3088	1/1	0.95	0.13	34,34,34,34	0
58	MG	2A	3487	1/1	0.95	0.10	65,65,65,65	0
58	MG	1A	4015	1/1	0.95	0.07	55,55,55,55	0
58	MG	1A	4016	1/1	0.95	0.07	47,47,47,47	0
58	MG	1R	201	1/1	0.95	0.12	37,37,37,37	0
58	MG	2A	3257	1/1	0.95	0.10	46,46,46,46	0
58	MG	1A	3716	1/1	0.95	0.07	42,42,42,42	0
58	MG	1R	203	1/1	0.95	0.06	38,38,38,38	0
58	MG	1R	204	1/1	0.95	0.31	48,48,48,48	0
58	MG	1A	3502	1/1	0.95	0.07	41,41,41,41	0
58	MG	1R	207	1/1	0.95	0.12	38,38,38,38	0
58	MG	1A	3165	1/1	0.95	0.12	40,40,40,40	0
58	MG	1T	202	1/1	0.95	0.10	41,41,41,41	0
58	MG	2a	3198	1/1	0.95	0.11	70,70,70,70	0
58	MG	1A	3872	1/1	0.95	0.08	27,27,27,27	0
58	MG	1A	3211	1/1	0.95	0.08	31,31,31,31	0
58	MG	1a	1691	1/1	0.95	0.14	36,36,36,36	0
58	MG	1A	3004	1/1	0.95	0.06	22,22,22,22	0
58	MG	2A	3509	1/1	0.95	0.07	40,40,40,40	0
58	MG	2A	3512	1/1	0.95	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3604	1/1	0.95	0.10	35,35,35,35	0
58	MG	1A	3732	1/1	0.95	0.08	19,19,19,19	0
58	MG	2A	3271	1/1	0.95	0.15	40,40,40,40	0
58	MG	1A	3318	1/1	0.95	0.14	49,49,49,49	0
58	MG	1a	1696	1/1	0.95	0.24	50,50,50,50	0
58	MG	1U	208	1/1	0.95	0.13	32,32,32,32	0
58	MG	1A	3507	1/1	0.95	0.17	60,60,60,60	0
58	MG	1A	3745	1/1	0.95	0.07	54,54,54,54	0
58	MG	1A	3111	1/1	0.95	0.41	32,32,32,32	0
58	MG	2A	3525	1/1	0.95	0.09	40,40,40,40	0
58	MG	1a	1702	1/1	0.95	0.17	37,37,37,37	0
58	MG	1A	3611	1/1	0.95	0.11	40,40,40,40	0
58	MG	1V	204	1/1	0.95	0.07	27,27,27,27	0
58	MG	1a	1705	1/1	0.95	0.19	44,44,44,44	0
58	MG	1A	3367	1/1	0.95	0.19	50,50,50,50	0
58	MG	2D	301	1/1	0.95	0.18	49,49,49,49	0
58	MG	1A	3616	1/1	0.95	0.05	23,23,23,23	0
58	MG	2D	303	1/1	0.95	0.06	42,42,42,42	0
58	MG	2q	201	1/1	0.95	0.07	57,57,57,57	0
58	MG	1A	3510	1/1	0.95	0.08	42,42,42,42	0
58	MG	2r	101	1/1	0.95	0.14	52,52,52,52	0
58	MG	2A	3537	1/1	0.95	0.11	42,42,42,42	0
58	MG	2A	3069	1/1	0.95	0.09	41,41,41,41	0
58	MG	1A	3513	1/1	0.95	0.16	33,33,33,33	0
58	MG	2v	103	1/1	0.95	0.17	61,61,61,61	0
58	MG	1A	3221	1/1	0.95	0.07	33,33,33,33	0
58	MG	1a	1713	1/1	0.95	0.13	44,44,44,44	0
58	MG	2E	303	1/1	0.95	0.18	52,52,52,52	0
58	MG	1A	3516	1/1	0.95	0.15	38,38,38,38	0
58	MG	1A	3518	1/1	0.95	0.25	45,45,45,45	0
58	MG	2A	3547	1/1	0.95	0.08	46,46,46,46	0
58	MG	2A	3549	1/1	0.95	0.14	50,50,50,50	0
58	MG	2A	3076	1/1	0.95	0.09	48,48,48,48	0
58	MG	1X	102	1/1	0.95	0.08	37,37,37,37	0
58	MG	1A	4072	1/1	0.96	0.10	51,51,51,51	0
58	MG	1A	4073	1/1	0.96	0.06	40,40,40,40	0
58	MG	1A	3740	1/1	0.96	0.09	31,31,31,31	0
58	MG	1a	1772	1/1	0.96	0.10	40,40,40,40	0
58	MG	2A	3355	1/1	0.96	0.08	48,48,48,48	0
58	MG	2A	3603	1/1	0.96	0.21	55,55,55,55	0
58	MG	1A	3744	1/1	0.96	0.18	43,43,43,43	0
58	MG	1a	1774	1/1	0.96	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2Y	201	1/1	0.96	0.16	37,37,37,37	0
58	MG	1A	4076	1/1	0.96	0.19	46,46,46,46	0
58	MG	2A	3607	1/1	0.96	0.10	40,40,40,40	0
58	MG	1A	3517	1/1	0.96	0.09	37,37,37,37	0
58	MG	1A	4078	1/1	0.96	0.06	23,23,23,23	0
58	MG	2I	102	1/1	0.96	0.22	53,53,53,53	0
58	MG	1A	3614	1/1	0.96	0.07	20,20,20,20	0
58	MG	1A	3077	1/1	0.96	0.07	41,41,41,41	0
58	MG	17	106	1/1	0.96	0.07	40,40,40,40	0
58	MG	25	102	1/1	0.96	0.10	49,49,49,49	0
58	MG	2A	3614	1/1	0.96	0.12	43,43,43,43	0
58	MG	1A	3617	1/1	0.96	0.06	30,30,30,30	0
58	MG	18	101	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3901	1/1	0.96	0.12	30,30,30,30	0
58	MG	18	103	1/1	0.96	0.10	32,32,32,32	0
58	MG	2a	3001	1/1	0.96	0.10	57,57,57,57	0
58	MG	1B	202	1/1	0.96	0.12	38,38,38,38	0
58	MG	2A	3621	1/1	0.96	0.06	48,48,48,48	0
58	MG	1A	3378	1/1	0.96	0.18	25,25,25,25	0
58	MG	1A	3903	1/1	0.96	0.09	30,30,30,30	0
58	MG	1A	3327	1/1	0.96	0.05	26,26,26,26	0
58	MG	1A	3622	1/1	0.96	0.06	37,37,37,37	0
58	MG	1A	3754	1/1	0.96	0.12	26,26,26,26	0
58	MG	1A	3094	1/1	0.96	0.10	53,53,53,53	0
58	MG	1A	3031	1/1	0.96	0.17	26,26,26,26	0
58	MG	1A	3177	1/1	0.96	0.10	31,31,31,31	0
58	MG	1A	3526	1/1	0.96	0.17	47,47,47,47	0
58	MG	1A	3760	1/1	0.96	0.07	12,12,12,12	0
58	MG	1B	214	1/1	0.96	0.18	65,65,65,65	0
58	MG	2A	3635	1/1	0.96	0.06	79,79,79,79	0
58	MG	1A	3765	1/1	0.96	0.10	21,21,21,21	0
58	MG	1A	3767	1/1	0.96	0.07	24,24,24,24	0
58	MG	1A	3145	1/1	0.96	0.20	28,28,28,28	0
58	MG	1A	3919	1/1	0.96	0.10	51,51,51,51	0
58	MG	1A	3008	1/1	0.96	0.08	17,17,17,17	0
58	MG	1B	220	1/1	0.96	0.10	34,34,34,34	0
58	MG	1A	3148	1/1	0.96	0.08	39,39,39,39	0
58	MG	1a	1616	1/1	0.96	0.08	63,63,63,63	0
58	MG	1A	3775	1/1	0.96	0.05	34,34,34,34	0
58	MG	1B	224	1/1	0.96	0.09	47,47,47,47	0
58	MG	1e	201	1/1	0.96	0.09	57,57,57,57	0
58	MG	1f	201	1/1	0.96	0.06	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1620	1/1	0.96	0.10	59,59,59,59	0
58	MG	1A	3927	1/1	0.96	0.06	48,48,48,48	0
58	MG	1A	3334	1/1	0.96	0.10	46,46,46,46	0
58	MG	1B	227	1/1	0.96	0.09	55,55,55,55	0
58	MG	1A	3631	1/1	0.96	0.14	30,30,30,30	0
58	MG	2A	3655	1/1	0.96	0.05	42,42,42,42	0
58	MG	1A	3388	1/1	0.96	0.08	28,28,28,28	0
58	MG	1A	3780	1/1	0.96	0.10	54,54,54,54	0
58	MG	1A	3932	1/1	0.96	0.12	49,49,49,49	0
58	MG	1A	3933	1/1	0.96	0.08	52,52,52,52	0
58	MG	1A	3279	1/1	0.96	0.34	24,24,24,24	0
58	MG	1A	3230	1/1	0.96	0.06	29,29,29,29	0
58	MG	1a	1632	1/1	0.96	0.11	40,40,40,40	0
58	MG	1A	3037	1/1	0.96	0.09	21,21,21,21	0
58	MG	1B	237	1/1	0.96	0.07	55,55,55,55	0
58	MG	1a	1635	1/1	0.96	0.07	27,27,27,27	0
58	MG	1A	3535	1/1	0.96	0.27	23,23,23,23	0
58	MG	1A	3938	1/1	0.96	0.06	56,56,56,56	0
58	MG	1A	3786	1/1	0.96	0.05	36,36,36,36	0
58	MG	2A	3670	1/1	0.96	0.12	24,24,24,24	0
58	MG	1A	3185	1/1	0.96	0.06	63,63,63,63	0
58	MG	2A	3672	1/1	0.96	0.12	54,54,54,54	0
58	MG	1x	107	1/1	0.96	0.07	52,52,52,52	0
58	MG	2A	3674	1/1	0.96	0.07	51,51,51,51	0
58	MG	1A	3943	1/1	0.96	0.08	51,51,51,51	0
58	MG	2A	3207	1/1	0.96	0.11	49,49,49,49	0
58	MG	1A	3234	1/1	0.96	0.10	33,33,33,33	0
58	MG	2A	3421	1/1	0.96	0.09	41,41,41,41	0
58	MG	2A	3422	1/1	0.96	0.18	34,34,34,34	0
58	MG	1A	3945	1/1	0.96	0.05	41,41,41,41	0
58	MG	1A	3790	1/1	0.96	0.09	29,29,29,29	0
58	MG	1A	3290	1/1	0.96	0.13	23,23,23,23	0
58	MG	1A	3794	1/1	0.96	0.28	25,25,25,25	0
58	MG	1A	3150	1/1	0.96	0.09	36,36,36,36	0
58	MG	1A	3541	1/1	0.96	0.06	35,35,35,35	0
58	MG	1A	3039	1/1	0.96	0.14	42,42,42,42	0
58	MG	1E	306	1/1	0.96	0.06	32,32,32,32	0
58	MG	1E	307	1/1	0.96	0.27	56,56,56,56	0
58	MG	1a	1652	1/1	0.96	0.14	42,42,42,42	0
58	MG	1a	1653	1/1	0.96	0.20	43,43,43,43	0
58	MG	2A	3695	1/1	0.96	0.09	35,35,35,35	0
58	MG	2A	3434	1/1	0.96	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3645	1/1	0.96	0.15	37,37,37,37	0
58	MG	2A	3699	1/1	0.96	0.06	49,49,49,49	0
58	MG	1A	3100	1/1	0.96	0.15	23,23,23,23	0
58	MG	1A	3465	1/1	0.96	0.10	35,35,35,35	0
58	MG	1A	3545	1/1	0.96	0.21	42,42,42,42	0
58	MG	1F	302	1/1	0.96	0.10	34,34,34,34	0
58	MG	1A	3466	1/1	0.96	0.18	35,35,35,35	0
58	MG	2A	3017	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3548	1/1	0.96	0.10	30,30,30,30	0
58	MG	1A	3345	1/1	0.96	0.12	48,48,48,48	0
58	MG	2A	3232	1/1	0.96	0.10	75,75,75,75	0
58	MG	2A	3021	1/1	0.96	0.11	62,62,62,62	0
58	MG	1A	3808	1/1	0.96	0.05	29,29,29,29	0
58	MG	1A	3468	1/1	0.96	0.04	44,44,44,44	0
58	MG	2a	3087	1/1	0.96	0.16	66,66,66,66	0
58	MG	1A	3402	1/1	0.96	0.12	35,35,35,35	0
58	MG	2a	3089	1/1	0.96	0.12	61,61,61,61	0
58	MG	1G	202	1/1	0.96	0.15	46,46,46,46	0
58	MG	2A	3451	1/1	0.96	0.08	50,50,50,50	0
58	MG	2A	3453	1/1	0.96	0.11	60,60,60,60	0
58	MG	1A	3811	1/1	0.96	0.08	31,31,31,31	0
58	MG	1A	3190	1/1	0.96	0.09	36,36,36,36	0
58	MG	1a	1669	1/1	0.96	0.32	59,59,59,59	0
58	MG	1A	3660	1/1	0.96	0.05	25,25,25,25	0
58	MG	1A	3661	1/1	0.96	0.10	14,14,14,14	0
58	MG	1a	1672	1/1	0.96	0.07	48,48,48,48	0
58	MG	1A	3404	1/1	0.96	0.11	41,41,41,41	0
58	MG	2A	3245	1/1	0.96	0.15	43,43,43,43	0
58	MG	2A	3726	1/1	0.96	0.08	32,32,32,32	0
58	MG	1A	3127	1/1	0.96	0.29	29,29,29,29	0
58	MG	1A	3406	1/1	0.96	0.05	48,48,48,48	0
58	MG	2A	3465	1/1	0.96	0.05	48,48,48,48	0
58	MG	1A	3407	1/1	0.96	0.15	39,39,39,39	0
58	MG	2A	3732	1/1	0.96	0.07	49,49,49,49	0
58	MG	2a	3108	1/1	0.96	0.12	70,70,70,70	0
58	MG	1N	206	1/1	0.96	0.04	39,39,39,39	0
58	MG	1A	3821	1/1	0.96	0.22	35,35,35,35	0
58	MG	1A	3558	1/1	0.96	0.05	36,36,36,36	0
58	MG	1A	3976	1/1	0.96	0.08	38,38,38,38	0
58	MG	2A	3253	1/1	0.96	0.06	39,39,39,39	0
58	MG	1A	3559	1/1	0.96	0.20	29,29,29,29	0
58	MG	1A	3825	1/1	0.96	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1684	1/1	0.96	0.15	30,30,30,30	0
58	MG	2A	3045	1/1	0.96	0.15	31,31,31,31	0
58	MG	1A	3826	1/1	0.96	0.13	36,36,36,36	0
58	MG	1A	3083	1/1	0.96	0.14	26,26,26,26	0
58	MG	1A	3067	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3304	1/1	0.96	0.20	44,44,44,44	0
58	MG	1A	3676	1/1	0.96	0.12	28,28,28,28	0
58	MG	2A	3483	1/1	0.96	0.10	63,63,63,63	0
58	MG	1A	3411	1/1	0.96	0.09	56,56,56,56	0
58	MG	1A	3567	1/1	0.96	0.08	44,44,44,44	0
58	MG	1Q	205	1/1	0.96	0.08	33,33,33,33	0
58	MG	1A	3991	1/1	0.96	0.07	35,35,35,35	0
58	MG	2A	3056	1/1	0.96	0.10	65,65,65,65	0
58	MG	1A	3568	1/1	0.96	0.08	37,37,37,37	0
58	MG	1A	3194	1/1	0.96	0.19	27,27,27,27	0
58	MG	1A	3997	1/1	0.96	0.08	39,39,39,39	0
58	MG	1A	3999	1/1	0.96	0.06	69,69,69,69	0
58	MG	2A	3761	1/1	0.96	0.08	53,53,53,53	0
58	MG	1A	3836	1/1	0.96	0.11	57,57,57,57	0
58	MG	2A	3763	1/1	0.96	0.14	47,47,47,47	0
58	MG	1A	3683	1/1	0.96	0.12	39,39,39,39	0
58	MG	1A	3838	1/1	0.96	0.05	19,19,19,19	0
58	MG	2A	3277	1/1	0.96	0.13	44,44,44,44	0
58	MG	2A	3769	1/1	0.96	0.11	42,42,42,42	0
58	MG	2A	3064	1/1	0.96	0.06	34,34,34,34	0
58	MG	1A	3195	1/1	0.96	0.08	17,17,17,17	0
58	MG	1A	4005	1/1	0.96	0.15	53,53,53,53	0
58	MG	1A	3415	1/1	0.96	0.08	29,29,29,29	0
58	MG	2a	3147	1/1	0.96	0.08	76,76,76,76	0
58	MG	2A	3506	1/1	0.96	0.15	42,42,42,42	0
58	MG	2A	3778	1/1	0.96	0.06	34,34,34,34	0
58	MG	1A	4007	1/1	0.96	0.07	52,52,52,52	0
58	MG	1A	3842	1/1	0.96	0.07	24,24,24,24	0
58	MG	2A	3782	1/1	0.96	0.09	44,44,44,44	0
58	MG	2A	3783	1/1	0.96	0.12	56,56,56,56	0
58	MG	2A	3510	1/1	0.96	0.06	48,48,48,48	0
58	MG	2A	3786	1/1	0.96	0.10	48,48,48,48	0
58	MG	1A	3845	1/1	0.96	0.10	46,46,46,46	0
58	MG	2A	3789	1/1	0.96	0.10	45,45,45,45	0
58	MG	1a	1709	1/1	0.96	0.06	43,43,43,43	0
58	MG	1A	3416	1/1	0.96	0.14	37,37,37,37	0
58	MG	1A	3085	1/1	0.96	0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3795	1/1	0.96	0.08	49,49,49,49	0
58	MG	1A	3688	1/1	0.96	0.07	27,27,27,27	0
58	MG	2a	3165	1/1	0.96	0.10	45,45,45,45	0
58	MG	2A	3517	1/1	0.96	0.16	42,42,42,42	0
58	MG	1U	209	1/1	0.96	0.28	30,30,30,30	0
58	MG	1A	3689	1/1	0.96	0.09	16,16,16,16	0
58	MG	2A	3801	1/1	0.96	0.10	33,33,33,33	0
58	MG	1A	3850	1/1	0.96	0.09	36,36,36,36	0
58	MG	1A	3033	1/1	0.96	0.36	28,28,28,28	0
58	MG	1A	3057	1/1	0.96	0.19	36,36,36,36	0
58	MG	2A	3524	1/1	0.96	0.09	27,27,27,27	0
58	MG	1a	1718	1/1	0.96	0.16	60,60,60,60	0
58	MG	1A	3199	1/1	0.96	0.29	42,42,42,42	0
58	MG	1a	1720	1/1	0.96	0.16	49,49,49,49	0
58	MG	1A	3159	1/1	0.96	0.07	25,25,25,25	0
58	MG	1A	3160	1/1	0.96	0.09	24,24,24,24	0
58	MG	2A	3087	1/1	0.96	0.06	32,32,32,32	0
58	MG	1a	1723	1/1	0.96	0.07	59,59,59,59	0
58	MG	1A	4024	1/1	0.96	0.09	28,28,28,28	0
58	MG	2A	3090	1/1	0.96	0.08	46,46,46,46	0
58	MG	1A	3423	1/1	0.96	0.18	29,29,29,29	0
58	MG	1A	3161	1/1	0.96	0.05	24,24,24,24	0
58	MG	2A	3820	1/1	0.96	0.10	42,42,42,42	0
58	MG	2A	3093	1/1	0.96	0.07	52,52,52,52	0
58	MG	2A	3094	1/1	0.96	0.10	37,37,37,37	0
58	MG	1a	1727	1/1	0.96	0.06	34,34,34,34	0
58	MG	2A	3544	1/1	0.96	0.12	34,34,34,34	0
58	MG	1A	3493	1/1	0.96	0.08	28,28,28,28	0
58	MG	1W	204	1/1	0.96	0.07	40,40,40,40	0
58	MG	2A	3548	1/1	0.96	0.12	34,34,34,34	0
58	MG	1A	3048	1/1	0.96	0.05	24,24,24,24	0
58	MG	1X	101	1/1	0.96	0.06	35,35,35,35	0
58	MG	2A	3551	1/1	0.96	0.10	32,32,32,32	0
58	MG	1A	3110	1/1	0.96	0.06	31,31,31,31	0
58	MG	1A	3588	1/1	0.96	0.10	41,41,41,41	0
58	MG	1A	4033	1/1	0.96	0.06	15,15,15,15	0
58	MG	1A	3135	1/1	0.96	0.06	27,27,27,27	0
58	MG	1A	3429	1/1	0.96	0.16	36,36,36,36	0
58	MG	1Z	301	1/1	0.96	0.07	54,54,54,54	0
58	MG	1A	3500	1/1	0.96	0.13	29,29,29,29	0
58	MG	1A	3593	1/1	0.96	0.10	54,54,54,54	0
58	MG	1a	1742	1/1	0.96	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3711	1/1	0.96	0.08	41,41,41,41	0
58	MG	2B	218	1/1	0.96	0.14	53,53,53,53	0
58	MG	1A	3073	1/1	0.96	0.17	26,26,26,26	0
58	MG	1A	3167	1/1	0.96	0.07	36,36,36,36	0
58	MG	1a	1747	1/1	0.96	0.12	37,37,37,37	0
58	MG	1A	3213	1/1	0.96	0.16	29,29,29,29	0
58	MG	10	106	1/1	0.96	0.10	47,47,47,47	0
58	MG	2A	3569	1/1	0.96	0.07	64,64,64,64	0
58	MG	1A	3015	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3434	1/1	0.96	0.15	31,31,31,31	0
58	MG	2A	3119	1/1	0.96	0.18	46,46,46,46	0
58	MG	1A	3717	1/1	0.96	0.07	34,34,34,34	0
58	MG	2A	3576	1/1	0.96	0.10	43,43,43,43	0
58	MG	1A	4054	1/1	0.96	0.10	48,48,48,48	0
58	MG	2A	3334	1/1	0.96	0.09	58,58,58,58	0
58	MG	1A	4055	1/1	0.96	0.06	33,33,33,33	0
58	MG	1A	3876	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3435	1/1	0.96	0.17	33,33,33,33	0
58	MG	1A	3266	1/1	0.96	0.11	55,55,55,55	0
58	MG	1A	3722	1/1	0.96	0.09	52,52,52,52	0
58	MG	2F	304	1/1	0.96	0.28	45,45,45,45	0
58	MG	1A	3215	1/1	0.96	0.07	39,39,39,39	0
58	MG	1A	3076	1/1	0.96	0.05	23,23,23,23	0
58	MG	2A	3342	1/1	0.96	0.17	40,40,40,40	0
58	MG	2A	3588	1/1	0.96	0.12	56,56,56,56	0
58	MG	1A	3729	1/1	0.96	0.10	16,16,16,16	0
58	MG	1A	3511	1/1	0.96	0.07	30,30,30,30	0
58	MG	2A	3133	1/1	0.96	0.21	43,43,43,43	0
58	MG	13	103	1/1	0.96	0.11	49,49,49,49	0
58	MG	1A	3140	1/1	0.96	0.10	30,30,30,30	0
58	MG	1A	3375	1/1	0.96	0.19	55,55,55,55	0
60	TEL	1A	4082	58/58	0.96	0.10	18,25,33,38	0
58	MG	1A	3735	1/1	0.96	0.16	42,42,42,42	0
58	MG	1A	3171	1/1	0.96	0.07	41,41,41,41	0
58	MG	1A	3252	1/1	0.97	0.14	29,29,29,29	0
58	MG	1A	3292	1/1	0.97	0.07	43,43,43,43	0
58	MG	1A	3220	1/1	0.97	0.11	43,43,43,43	0
58	MG	2a	3053	1/1	0.97	0.13	43,43,43,43	0
58	MG	2A	3765	1/1	0.97	0.04	36,36,36,36	0
58	MG	1A	3694	1/1	0.97	0.08	36,36,36,36	0
58	MG	2A	3586	1/1	0.97	0.09	48,48,48,48	0
58	MG	1W	205	1/1	0.97	0.12	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3873	1/1	0.97	0.11	32,32,32,32	0
58	MG	2A	3773	1/1	0.97	0.08	55,55,55,55	0
58	MG	1A	3106	1/1	0.97	0.11	25,25,25,25	0
58	MG	1A	3058	1/1	0.97	0.04	28,28,28,28	0
58	MG	1X	103	1/1	0.97	0.13	42,42,42,42	0
58	MG	2a	3063	1/1	0.97	0.13	57,57,57,57	0
58	MG	1A	3298	1/1	0.97	0.12	41,41,41,41	0
58	MG	1A	3978	1/1	0.97	0.10	31,31,31,31	0
58	MG	1A	3299	1/1	0.97	0.12	31,31,31,31	0
58	MG	1A	3563	1/1	0.97	0.15	36,36,36,36	0
58	MG	1A	3879	1/1	0.97	0.05	22,22,22,22	0
58	MG	2A	3121	1/1	0.97	0.12	53,53,53,53	0
58	MG	2A	3122	1/1	0.97	0.10	37,37,37,37	0
58	MG	2A	3785	1/1	0.97	0.13	36,36,36,36	0
58	MG	1A	3880	1/1	0.97	0.07	22,22,22,22	0
58	MG	1a	1683	1/1	0.97	0.10	48,48,48,48	0
58	MG	1A	3038	1/1	0.97	0.12	33,33,33,33	0
58	MG	1A	3565	1/1	0.97	0.08	46,46,46,46	0
58	MG	10	102	1/1	0.97	0.29	48,48,48,48	0
58	MG	1A	3566	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3987	1/1	0.97	0.08	46,46,46,46	0
58	MG	1A	3884	1/1	0.97	0.10	29,29,29,29	0
58	MG	1A	3989	1/1	0.97	0.07	22,22,22,22	0
58	MG	1A	3514	1/1	0.97	0.07	32,32,32,32	0
58	MG	2a	3082	1/1	0.97	0.11	50,50,50,50	0
58	MG	1A	3109	1/1	0.97	0.05	22,22,22,22	0
58	MG	2A	3134	1/1	0.97	0.11	44,44,44,44	0
58	MG	1A	3176	1/1	0.97	0.20	33,33,33,33	0
58	MG	1A	3802	1/1	0.97	0.05	22,22,22,22	0
58	MG	2A	3137	1/1	0.97	0.10	38,38,38,38	0
58	MG	1A	3996	1/1	0.97	0.10	28,28,28,28	0
58	MG	1A	3707	1/1	0.97	0.07	46,46,46,46	0
58	MG	1A	3998	1/1	0.97	0.09	39,39,39,39	0
58	MG	1A	3804	1/1	0.97	0.15	30,30,30,30	0
58	MG	1A	3303	1/1	0.97	0.15	42,42,42,42	0
58	MG	1A	4001	1/1	0.97	0.10	56,56,56,56	0
58	MG	1B	238	1/1	0.97	0.06	31,31,31,31	0
58	MG	2A	3624	1/1	0.97	0.10	43,43,43,43	0
58	MG	1A	3710	1/1	0.97	0.07	45,45,45,45	0
58	MG	2A	3816	1/1	0.97	0.09	32,32,32,32	0
58	MG	1A	3003	1/1	0.97	0.09	24,24,24,24	0
58	MG	1D	301	1/1	0.97	0.15	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3148	1/1	0.97	0.10	55,55,55,55	0
58	MG	1a	1706	1/1	0.97	0.14	39,39,39,39	0
58	MG	1A	3144	1/1	0.97	0.05	39,39,39,39	0
58	MG	2A	3822	1/1	0.97	0.18	47,47,47,47	0
58	MG	1A	3896	1/1	0.97	0.08	41,41,41,41	0
58	MG	2A	3301	1/1	0.97	0.20	51,51,51,51	0
58	MG	2A	3825	1/1	0.97	0.10	49,49,49,49	0
58	MG	2a	3107	1/1	0.97	0.28	48,48,48,48	0
58	MG	1D	304	1/1	0.97	0.09	31,31,31,31	0
58	MG	2A	3303	1/1	0.97	0.15	48,48,48,48	0
58	MG	1D	305	1/1	0.97	0.06	17,17,17,17	0
58	MG	2A	3009	1/1	0.97	0.06	47,47,47,47	0
58	MG	1A	3897	1/1	0.97	0.05	31,31,31,31	0
58	MG	1D	308	1/1	0.97	0.13	29,29,29,29	0
58	MG	2A	3012	1/1	0.97	0.07	46,46,46,46	0
58	MG	2A	3642	1/1	0.97	0.08	34,34,34,34	0
58	MG	1A	3061	1/1	0.97	0.06	32,32,32,32	0
58	MG	1A	4008	1/1	0.97	0.13	36,36,36,36	0
58	MG	1A	3201	1/1	0.97	0.08	19,19,19,19	0
58	MG	1A	3428	1/1	0.97	0.13	41,41,41,41	0
58	MG	2A	3469	1/1	0.97	0.07	29,29,29,29	0
58	MG	1A	4013	1/1	0.97	0.09	42,42,42,42	0
58	MG	2a	3122	1/1	0.97	0.09	44,44,44,44	0
58	MG	1A	3202	1/1	0.97	0.06	34,34,34,34	0
58	MG	17	104	1/1	0.97	0.15	34,34,34,34	0
58	MG	1A	3813	1/1	0.97	0.06	37,37,37,37	0
58	MG	1A	3203	1/1	0.97	0.09	40,40,40,40	0
58	MG	2A	3475	1/1	0.97	0.07	36,36,36,36	0
58	MG	1A	3052	1/1	0.97	0.21	39,39,39,39	0
58	MG	2A	3024	1/1	0.97	0.09	50,50,50,50	0
58	MG	1A	3389	1/1	0.97	0.20	29,29,29,29	0
58	MG	1A	3909	1/1	0.97	0.06	29,29,29,29	0
58	MG	1E	309	1/1	0.97	0.08	23,23,23,23	0
58	MG	2D	306	1/1	0.97	0.06	27,27,27,27	0
58	MG	2A	3172	1/1	0.97	0.10	37,37,37,37	0
58	MG	2a	3135	1/1	0.97	0.14	57,57,57,57	0
58	MG	1A	3182	1/1	0.97	0.16	41,41,41,41	0
58	MG	2A	3661	1/1	0.97	0.04	50,50,50,50	0
58	MG	2a	3138	1/1	0.97	0.08	51,51,51,51	0
58	MG	1A	3723	1/1	0.97	0.11	47,47,47,47	0
58	MG	1A	3045	1/1	0.97	0.12	30,30,30,30	0
58	MG	1F	301	1/1	0.97	0.15	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3177	1/1	0.97	0.07	43,43,43,43	0
58	MG	2A	3032	1/1	0.97	0.07	40,40,40,40	0
58	MG	1A	3725	1/1	0.97	0.05	46,46,46,46	0
58	MG	1A	3392	1/1	0.97	0.04	26,26,26,26	0
58	MG	1A	3728	1/1	0.97	0.06	46,46,46,46	0
58	MG	1A	3824	1/1	0.97	0.05	47,47,47,47	0
58	MG	1A	3917	1/1	0.97	0.05	17,17,17,17	0
58	MG	1F	310	1/1	0.97	0.04	47,47,47,47	0
58	MG	1a	1737	1/1	0.97	0.08	51,51,51,51	0
58	MG	2a	3151	1/1	0.97	0.21	52,52,52,52	0
58	MG	1A	4028	1/1	0.97	0.06	35,35,35,35	0
58	MG	2a	3153	1/1	0.97	0.07	83,83,83,83	0
58	MG	2A	3676	1/1	0.97	0.06	32,32,32,32	0
58	MG	1A	3584	1/1	0.97	0.06	26,26,26,26	0
58	MG	1A	3730	1/1	0.97	0.17	29,29,29,29	0
58	MG	1A	3585	1/1	0.97	0.05	34,34,34,34	0
58	MG	1A	3586	1/1	0.97	0.16	56,56,56,56	0
58	MG	1A	4034	1/1	0.97	0.11	38,38,38,38	0
58	MG	1A	3924	1/1	0.97	0.05	45,45,45,45	0
58	MG	2A	3507	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3654	1/1	0.97	0.07	23,23,23,23	0
58	MG	1A	3734	1/1	0.97	0.05	33,33,33,33	0
58	MG	2U	201	1/1	0.97	0.17	47,47,47,47	0
58	MG	1A	3393	1/1	0.97	0.07	39,39,39,39	0
58	MG	2A	3511	1/1	0.97	0.06	34,34,34,34	0
58	MG	1A	3009	1/1	0.97	0.04	23,23,23,23	0
58	MG	1a	1618	1/1	0.97	0.10	66,66,66,66	0
58	MG	2A	3198	1/1	0.97	0.22	61,61,61,61	0
58	MG	1A	4042	1/1	0.97	0.12	57,57,57,57	0
58	MG	1A	4044	1/1	0.97	0.06	38,38,38,38	0
58	MG	1a	1621	1/1	0.97	0.25	54,54,54,54	0
58	MG	1O	202	1/1	0.97	0.12	50,50,50,50	0
58	MG	2A	3697	1/1	0.97	0.11	51,51,51,51	0
58	MG	1A	3186	1/1	0.97	0.07	27,27,27,27	0
58	MG	1A	3741	1/1	0.97	0.09	19,19,19,19	0
58	MG	1A	3013	1/1	0.97	0.17	25,25,25,25	0
58	MG	2a	3178	1/1	0.97	0.13	48,48,48,48	0
58	MG	2A	3206	1/1	0.97	0.15	42,42,42,42	0
58	MG	2I	104	1/1	0.97	0.07	43,43,43,43	0
58	MG	2A	3523	1/1	0.97	0.17	52,52,52,52	0
58	MG	1P	202	1/1	0.97	0.14	36,36,36,36	0
58	MG	25	101	1/1	0.97	0.30	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3591	1/1	0.97	0.07	22,22,22,22	0
58	MG	1P	205	1/1	0.97	0.28	28,28,28,28	0
58	MG	2A	3361	1/1	0.97	0.12	61,61,61,61	0
58	MG	1A	3240	1/1	0.97	0.18	35,35,35,35	0
58	MG	2A	3529	1/1	0.97	0.07	32,32,32,32	0
58	MG	28	101	1/1	0.97	0.10	64,64,64,64	0
58	MG	1A	3355	1/1	0.97	0.07	51,51,51,51	0
58	MG	1a	1763	1/1	0.97	0.08	62,62,62,62	0
58	MG	2A	3214	1/1	0.97	0.21	39,39,39,39	0
58	MG	1A	3538	1/1	0.97	0.19	31,31,31,31	0
58	MG	1A	3841	1/1	0.97	0.04	38,38,38,38	0
58	MG	1A	3166	1/1	0.97	0.06	27,27,27,27	0
58	MG	2A	3369	1/1	0.97	0.13	40,40,40,40	0
58	MG	1A	3843	1/1	0.97	0.12	32,32,32,32	0
58	MG	1Q	203	1/1	0.97	0.18	43,43,43,43	0
58	MG	1A	3667	1/1	0.97	0.06	37,37,37,37	0
58	MG	1A	3668	1/1	0.97	0.05	24,24,24,24	0
58	MG	2A	3545	1/1	0.97	0.09	51,51,51,51	0
58	MG	1A	4062	1/1	0.97	0.10	34,34,34,34	0
58	MG	2A	3722	1/1	0.97	0.08	54,54,54,54	0
58	MG	1A	3243	1/1	0.97	0.18	21,21,21,21	0
58	MG	2A	3075	1/1	0.97	0.11	49,49,49,49	0
58	MG	2A	3725	1/1	0.97	0.06	36,36,36,36	0
58	MG	1A	3490	1/1	0.97	0.04	40,40,40,40	0
58	MG	2A	3727	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3212	1/1	0.97	0.15	36,36,36,36	0
58	MG	1a	1775	1/1	0.97	0.09	49,49,49,49	0
58	MG	1A	3245	1/1	0.97	0.10	56,56,56,56	0
58	MG	1A	3117	1/1	0.97	0.09	37,37,37,37	0
58	MG	1A	3280	1/1	0.97	0.07	30,30,30,30	0
58	MG	1R	206	1/1	0.97	0.13	34,34,34,34	0
58	MG	1A	3762	1/1	0.97	0.07	24,24,24,24	0
58	MG	1A	4070	1/1	0.97	0.11	40,40,40,40	0
58	MG	1A	3014	1/1	0.97	0.07	27,27,27,27	0
58	MG	1A	3855	1/1	0.97	0.12	36,36,36,36	0
58	MG	1A	3605	1/1	0.97	0.20	11,11,11,11	0
58	MG	1U	203	1/1	0.97	0.17	42,42,42,42	0
58	MG	1A	3049	1/1	0.97	0.10	26,26,26,26	0
58	MG	1A	3549	1/1	0.97	0.13	18,18,18,18	0
58	MG	2A	3564	1/1	0.97	0.20	65,65,65,65	0
58	MG	2A	3565	1/1	0.97	0.04	40,40,40,40	0
58	MG	2A	3746	1/1	0.97	0.05	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3770	1/1	0.97	0.11	18,18,18,18	0
58	MG	1A	3285	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3773	1/1	0.97	0.07	39,39,39,39	0
58	MG	1A	3960	1/1	0.97	0.06	60,60,60,60	0
58	MG	1a	1659	1/1	0.97	0.28	64,64,64,64	0
58	MG	1A	3499	1/1	0.97	0.29	20,20,20,20	0
58	MG	1A	3612	1/1	0.97	0.14	42,42,42,42	0
58	MG	1A	3216	1/1	0.97	0.16	42,42,42,42	0
58	MG	1A	3218	1/1	0.97	0.07	33,33,33,33	0
58	MG	1A	3965	1/1	0.97	0.10	48,48,48,48	0
59	K	1A	3546	1/1	0.97	0.08	75,75,75,75	0
58	MG	1B	204	1/1	0.97	0.04	26,26,26,26	0
58	MG	1A	3121	1/1	0.97	0.07	39,39,39,39	0
58	MG	1A	3369	1/1	0.97	0.07	39,39,39,39	0
61	ZN	14	102	1/1	0.97	0.07	110,110,110,110	0
61	ZN	2Y	202	1/1	0.97	0.05	100,100,100,100	0
58	MG	2A	3407	1/1	0.97	0.10	40,40,40,40	0
61	ZN	29	501	1/1	0.97	0.05	79,79,79,79	0
61	ZN	2n	501	1/1	0.97	0.05	84,84,84,84	0
62	SF4	2d	303	8/8	0.97	0.05	72,78,84,91	0
58	MG	2A	3766	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3799	1/1	0.98	0.04	39,39,39,39	0
58	MG	23	103	1/1	0.98	0.06	49,49,49,49	0
58	MG	1A	3678	1/1	0.98	0.05	11,11,11,11	0
58	MG	1A	3679	1/1	0.98	0.06	20,20,20,20	0
58	MG	2A	3112	1/1	0.98	0.05	40,40,40,40	0
58	MG	2A	3771	1/1	0.98	0.08	44,44,44,44	0
58	MG	1A	3281	1/1	0.98	0.09	32,32,32,32	0
58	MG	1A	3241	1/1	0.98	0.20	34,34,34,34	0
58	MG	2A	3532	1/1	0.98	0.08	29,29,29,29	0
58	MG	2A	3213	1/1	0.98	0.13	54,54,54,54	0
58	MG	1A	3283	1/1	0.98	0.21	30,30,30,30	0
58	MG	1P	203	1/1	0.98	0.12	26,26,26,26	0
58	MG	2A	3216	1/1	0.98	0.08	33,33,33,33	0
58	MG	2A	3019	1/1	0.98	0.04	38,38,38,38	0
58	MG	1A	3736	1/1	0.98	0.03	23,23,23,23	0
58	MG	1A	3023	1/1	0.98	0.07	37,37,37,37	0
58	MG	1A	3634	1/1	0.98	0.05	26,26,26,26	0
58	MG	17	102	1/1	0.98	0.04	28,28,28,28	0
58	MG	17	103	1/1	0.98	0.09	23,23,23,23	0
58	MG	2A	3787	1/1	0.98	0.07	40,40,40,40	0
58	MG	1A	4011	1/1	0.98	0.05	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3869	1/1	0.98	0.12	40,40,40,40	0
58	MG	2A	3790	1/1	0.98	0.12	26,26,26,26	0
58	MG	1A	3484	1/1	0.98	0.12	30,30,30,30	0
58	MG	1A	3939	1/1	0.98	0.10	42,42,42,42	0
58	MG	1A	3742	1/1	0.98	0.06	29,29,29,29	0
58	MG	2A	3794	1/1	0.98	0.04	61,61,61,61	0
58	MG	1A	3743	1/1	0.98	0.10	42,42,42,42	0
58	MG	2A	3796	1/1	0.98	0.10	24,24,24,24	0
58	MG	1A	3942	1/1	0.98	0.04	40,40,40,40	0
58	MG	2A	3437	1/1	0.98	0.05	51,51,51,51	0
58	MG	1A	3262	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3068	1/1	0.98	0.10	24,24,24,24	0
58	MG	1A	3523	1/1	0.98	0.10	21,21,21,21	0
58	MG	1A	3012	1/1	0.98	0.04	29,29,29,29	0
58	MG	1a	1781	1/1	0.98	0.08	53,53,53,53	0
58	MG	1B	223	1/1	0.98	0.05	30,30,30,30	0
58	MG	1A	3640	1/1	0.98	0.06	26,26,26,26	0
58	MG	1A	3289	1/1	0.98	0.08	38,38,38,38	0
58	MG	2A	3807	1/1	0.98	0.06	42,42,42,42	0
58	MG	2A	3808	1/1	0.98	0.06	47,47,47,47	0
58	MG	1A	3751	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	3341	1/1	0.98	0.28	29,29,29,29	0
58	MG	1A	3137	1/1	0.98	0.13	34,34,34,34	0
58	MG	1A	3172	1/1	0.98	0.05	40,40,40,40	0
58	MG	1a	1789	1/1	0.98	0.05	45,45,45,45	0
58	MG	1B	230	1/1	0.98	0.05	42,42,42,42	0
58	MG	2A	3452	1/1	0.98	0.05	31,31,31,31	0
58	MG	1A	3114	1/1	0.98	0.04	22,22,22,22	0
58	MG	1a	1792	1/1	0.98	0.19	50,50,50,50	0
58	MG	1A	4030	1/1	0.98	0.04	26,26,26,26	0
58	MG	1A	3603	1/1	0.98	0.06	13,13,13,13	0
58	MG	1A	3095	1/1	0.98	0.14	18,18,18,18	0
58	MG	1A	3648	1/1	0.98	0.06	28,28,28,28	0
58	MG	2A	3575	1/1	0.98	0.08	44,44,44,44	0
58	MG	1A	3294	1/1	0.98	0.11	41,41,41,41	0
58	MG	2A	3460	1/1	0.98	0.04	42,42,42,42	0
58	MG	2A	3053	1/1	0.98	0.06	47,47,47,47	0
58	MG	1A	3269	1/1	0.98	0.04	24,24,24,24	0
58	MG	1A	3764	1/1	0.98	0.05	37,37,37,37	0
58	MG	2A	3254	1/1	0.98	0.07	50,50,50,50	0
58	MG	1A	3464	1/1	0.98	0.17	27,27,27,27	0
58	MG	1A	3766	1/1	0.98	0.04	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3831	1/1	0.98	0.10	50,50,50,50	0
58	MG	1A	3652	1/1	0.98	0.09	37,37,37,37	0
58	MG	1A	4043	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3231	1/1	0.98	0.12	29,29,29,29	0
58	MG	1A	3895	1/1	0.98	0.04	40,40,40,40	0
58	MG	1A	3610	1/1	0.98	0.07	25,25,25,25	0
58	MG	1D	307	1/1	0.98	0.04	28,28,28,28	0
58	MG	1V	208	1/1	0.98	0.04	45,45,45,45	0
58	MG	1A	3706	1/1	0.98	0.15	42,42,42,42	0
58	MG	1A	3969	1/1	0.98	0.06	25,25,25,25	0
58	MG	1A	4050	1/1	0.98	0.04	41,41,41,41	0
58	MG	2A	3595	1/1	0.98	0.06	37,37,37,37	0
58	MG	1A	3655	1/1	0.98	0.07	20,20,20,20	0
58	MG	1A	3772	1/1	0.98	0.06	39,39,39,39	0
58	MG	1I	201	1/1	0.98	0.03	59,59,59,59	0
58	MG	1A	3025	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	3217	1/1	0.98	0.12	31,31,31,31	0
58	MG	1A	3501	1/1	0.98	0.08	31,31,31,31	0
58	MG	2A	3484	1/1	0.98	0.07	65,65,65,65	0
58	MG	1E	304	1/1	0.98	0.11	22,22,22,22	0
58	MG	1A	3659	1/1	0.98	0.07	21,21,21,21	0
58	MG	2A	3276	1/1	0.98	0.13	45,45,45,45	0
58	MG	1A	4058	1/1	0.98	0.10	37,37,37,37	0
58	MG	2A	3078	1/1	0.98	0.04	38,38,38,38	0
58	MG	1A	3379	1/1	0.98	0.14	22,22,22,22	0
58	MG	1A	3977	1/1	0.98	0.04	30,30,30,30	0
58	MG	2A	3610	1/1	0.98	0.07	51,51,51,51	0
58	MG	1A	4061	1/1	0.98	0.05	36,36,36,36	0
58	MG	1A	3615	1/1	0.98	0.07	38,38,38,38	0
58	MG	1A	3907	1/1	0.98	0.05	50,50,50,50	0
58	MG	1A	3908	1/1	0.98	0.04	24,24,24,24	0
58	MG	1A	3844	1/1	0.98	0.18	38,38,38,38	0
58	MG	1A	3071	1/1	0.98	0.08	21,21,21,21	0
58	MG	2F	305	1/1	0.98	0.08	46,46,46,46	0
58	MG	2A	3500	1/1	0.98	0.11	59,59,59,59	0
58	MG	2A	3618	1/1	0.98	0.14	39,39,39,39	0
58	MG	2A	3739	1/1	0.98	0.05	42,42,42,42	0
58	MG	1F	303	1/1	0.98	0.21	28,28,28,28	0
58	MG	2O	202	1/1	0.98	0.04	58,58,58,58	0
58	MG	1A	3080	1/1	0.98	0.11	31,31,31,31	0
58	MG	1F	305	1/1	0.98	0.10	41,41,41,41	0
58	MG	2A	3504	1/1	0.98	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3205	1/1	0.98	0.16	23,23,23,23	0
58	MG	1a	1650	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3619	1/1	0.98	0.05	32,32,32,32	0
58	MG	2A	3626	1/1	0.98	0.14	46,46,46,46	0
58	MG	1A	3354	1/1	0.98	0.04	40,40,40,40	0
58	MG	1A	3065	1/1	0.98	0.10	34,34,34,34	0
58	MG	1A	3179	1/1	0.98	0.04	30,30,30,30	0
58	MG	1A	3789	1/1	0.98	0.05	45,45,45,45	0
58	MG	1a	1746	1/1	0.98	0.06	53,53,53,53	0
58	MG	2A	3401	1/1	0.98	0.27	40,40,40,40	0
58	MG	2x	103	1/1	0.98	0.13	53,53,53,53	0
58	MG	1A	3414	1/1	0.98	0.12	28,28,28,28	0
58	MG	2A	3755	1/1	0.98	0.11	42,42,42,42	0
58	MG	1A	3992	1/1	0.98	0.05	13,13,13,13	0
58	MG	1A	3257	1/1	0.98	0.06	33,33,33,33	0
58	MG	1A	3921	1/1	0.98	0.03	22,22,22,22	0
58	MG	2A	3102	1/1	0.98	0.05	38,38,38,38	0
61	ZN	1Y	203	1/1	0.98	0.04	61,61,61,61	0
58	MG	1A	3726	1/1	0.98	0.07	36,36,36,36	0
58	MG	1A	3239	1/1	0.98	0.07	23,23,23,23	0
58	MG	1A	3512	1/1	0.98	0.06	33,33,33,33	0
61	ZN	26	501	1/1	0.98	0.07	66,66,66,66	0
58	MG	1A	3925	1/1	0.98	0.07	53,53,53,53	0
58	MG	1A	3029	1/1	0.98	0.07	26,26,26,26	0
62	SF4	1d	302	8/8	0.98	0.05	58,60,65,70	0
58	MG	1A	3448	1/1	0.98	0.21	53,53,53,53	0
58	MG	1a	1699	1/1	0.99	0.05	46,46,46,46	0
58	MG	1A	3287	1/1	0.99	0.07	35,35,35,35	0
58	MG	1A	3183	1/1	0.99	0.12	33,33,33,33	0
58	MG	1A	3737	1/1	0.99	0.07	32,32,32,32	0
58	MG	1A	3123	1/1	0.99	0.15	28,28,28,28	0
58	MG	2A	3772	1/1	0.99	0.06	32,32,32,32	0
58	MG	2A	3531	1/1	0.99	0.11	30,30,30,30	0
58	MG	1A	3739	1/1	0.99	0.04	37,37,37,37	0
58	MG	2A	3533	1/1	0.99	0.16	36,36,36,36	0
58	MG	1A	3119	1/1	0.99	0.15	19,19,19,19	0
58	MG	1A	3670	1/1	0.99	0.06	18,18,18,18	0
58	MG	1A	3692	1/1	0.99	0.04	25,25,25,25	0
58	MG	2A	3779	1/1	0.99	0.06	25,25,25,25	0
58	MG	1T	201	1/1	0.99	0.05	30,30,30,30	0
58	MG	2A	3538	1/1	0.99	0.08	30,30,30,30	0
58	MG	1F	307	1/1	0.99	0.04	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3983	1/1	0.99	0.05	24,24,24,24	0
58	MG	2A	3379	1/1	0.99	0.06	30,30,30,30	0
58	MG	1A	3583	1/1	0.99	0.07	30,30,30,30	0
58	MG	1A	3774	1/1	0.99	0.03	33,33,33,33	0
58	MG	1A	3672	1/1	0.99	0.03	26,26,26,26	0
58	MG	1A	3719	1/1	0.99	0.04	17,17,17,17	0
58	MG	1A	3101	1/1	0.99	0.03	33,33,33,33	0
58	MG	1I	202	1/1	0.99	0.06	39,39,39,39	0
58	MG	1A	3951	1/1	0.99	0.10	16,16,16,16	0
58	MG	13	101	1/1	0.99	0.05	32,32,32,32	0
58	MG	1A	3126	1/1	0.99	0.03	25,25,25,25	0
58	MG	2A	3494	1/1	0.99	0.07	29,29,29,29	0
58	MG	1A	3779	1/1	0.99	0.04	42,42,42,42	0
58	MG	1A	3814	1/1	0.99	0.06	30,30,30,30	0
58	MG	1A	3601	1/1	0.99	0.10	33,33,33,33	0
58	MG	15	101	1/1	0.99	0.08	35,35,35,35	0
58	MG	2A	3499	1/1	0.99	0.07	42,42,42,42	0
58	MG	1A	3363	1/1	0.99	0.04	36,36,36,36	0
58	MG	2A	3737	1/1	0.99	0.04	43,43,43,43	0
58	MG	1A	3920	1/1	0.99	0.04	22,22,22,22	0
58	MG	1A	4036	1/1	0.99	0.05	34,34,34,34	0
58	MG	1A	3620	1/1	0.99	0.07	24,24,24,24	0
58	MG	1A	3074	1/1	0.99	0.02	11,11,11,11	0
58	MG	1A	3146	1/1	0.99	0.04	19,19,19,19	0
58	MG	1A	4040	1/1	0.99	0.04	25,25,25,25	0
58	MG	2A	3682	1/1	0.99	0.05	33,33,33,33	0
58	MG	1a	1780	1/1	0.99	0.04	41,41,41,41	0
58	MG	1A	3092	1/1	0.99	0.05	34,34,34,34	0
58	MG	1A	3606	1/1	0.99	0.07	25,25,25,25	0
58	MG	1A	3296	1/1	0.99	0.09	23,23,23,23	0
58	MG	1A	3445	1/1	0.99	0.04	29,29,29,29	0
58	MG	1A	3663	1/1	0.99	0.04	19,19,19,19	0
58	MG	1W	206	1/1	0.99	0.06	17,17,17,17	0
58	MG	2A	3690	1/1	0.99	0.06	41,41,41,41	0
58	MG	1A	3791	1/1	0.99	0.07	19,19,19,19	0
58	MG	2A	3572	1/1	0.99	0.07	35,35,35,35	0
58	MG	1A	4047	1/1	0.99	0.05	20,20,20,20	0
58	MG	1A	3759	1/1	0.99	0.03	38,38,38,38	0
58	MG	1A	3793	1/1	0.99	0.04	19,19,19,19	0
58	MG	1A	3520	1/1	0.99	0.14	37,37,37,37	0
58	MG	2X	102	1/1	0.99	0.04	63,63,63,63	0
58	MG	1A	3761	1/1	0.99	0.07	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	ZN	19	102	1/1	0.99	0.05	43,43,43,43	0
61	ZN	1n	103	1/1	0.99	0.03	56,56,56,56	0
58	MG	1A	3494	1/1	0.99	0.11	30,30,30,30	0
58	MG	1A	4053	1/1	0.99	0.03	27,27,27,27	0
61	ZN	25	104	1/1	0.99	0.04	70,70,70,70	0
58	MG	1A	3763	1/1	0.99	0.04	58,58,58,58	0
58	MG	1A	4012	1/1	0.99	0.03	16,16,16,16	0
58	MG	2A	3640	1/1	0.99	0.05	59,59,59,59	0
58	MG	1A	3900	1/1	0.99	0.03	24,24,24,24	0
58	MG	1A	3709	1/1	0.99	0.07	22,22,22,22	0
58	MG	1A	3993	1/1	1.00	0.03	27,27,27,27	0
58	MG	1A	3748	1/1	1.00	0.09	34,34,34,34	0
58	MG	1A	3718	1/1	1.00	0.01	20,20,20,20	0
58	MG	1A	3782	1/1	1.00	0.06	15,15,15,15	0
61	ZN	15	109	1/1	1.00	0.01	42,42,42,42	0
61	ZN	16	103	1/1	1.00	0.04	38,38,38,38	0
58	MG	2A	3675	1/1	1.00	0.06	19,19,19,19	0
58	MG	1a	1734	1/1	1.00	0.09	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.