



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2025 – 07:16 PM EDT

PDB ID : 9O3J / pdb_00009o3j
Title : Crystal structure of the wild-type drug-free *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Lys-tRNA^{Lys}, P-site fM RC-peptidyl-tRNA^{Met}, and deacylated E-site tRNA^{Lys} at 2.60Å 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 : 2.60 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

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

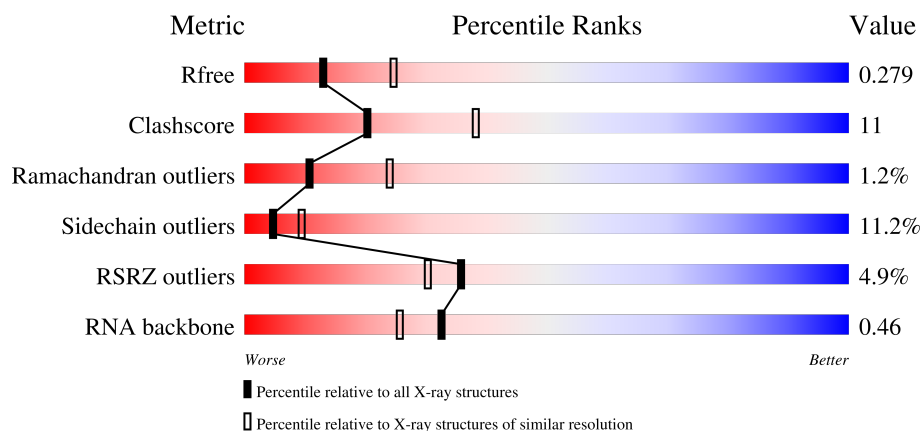
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)
RNA backbone	3690	1025 (2.88-2.32)

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>3%</div> <div>59%</div> <div>31%</div> <div>8%</div> <div>.</div> </div>
1	2A	2915	<div> <div>3%</div> <div>52%</div> <div>37%</div> <div>8%</div> <div>.</div> </div>
2	1B	121	<div> <div>%</div> <div>59%</div> <div>37%</div> <div>.</div> <div>.</div> </div>












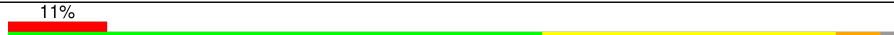

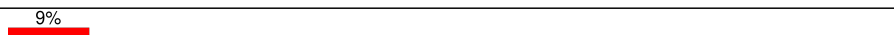
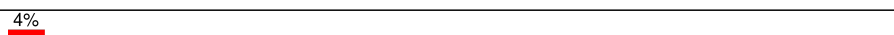
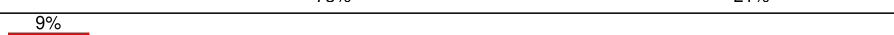

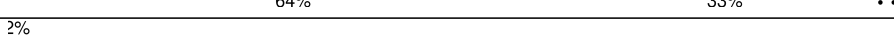







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Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141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



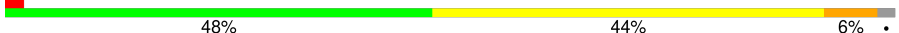








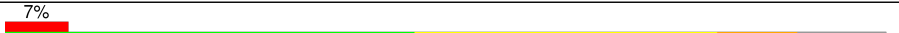













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Mol	Chain	Length	Quality of chain
15	1T	146	% 
15	2T	146	% 
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	5% 
18	1W	113	
18	2W	113	2% 
19	1X	96	% 
19	2X	96	% 
20	1Y	110	
20	2Y	110	11% 
21	1Z	206	7% 
21	2Z	206	9% 
22	10	85	4% 
22	20	85	9% 
23	11	98	% 
23	21	98	2% 
24	12	72	% 
24	22	72	
25	13	60	
25	23	60	
26	14	71	10% 
26	24	71	10% 
27	15	60	2% 

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Mol	Chain	Length	Quality of chain
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	
39	2h	138	

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Mol	Chain	Length	Quality of chain
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	
52	1u	27	

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Mol	Chain	Length	Quality of chain
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	1U	208	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 299808 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	1096	Total	Mg	0	0
			1096	1096		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	37	Total 37	Mg 37	0	0
58	1D	13	Total 13	Mg 13	0	0
58	1E	16	Total 16	Mg 16	0	0
58	1F	13	Total 13	Mg 13	0	0
58	1G	5	Total 5	Mg 5	0	0
58	1H	1	Total 1	Mg 1	0	0
58	1I	1	Total 1	Mg 1	0	0
58	1N	5	Total 5	Mg 5	0	0
58	1O	4	Total 4	Mg 4	0	0
58	1P	6	Total 6	Mg 6	0	0
58	1Q	7	Total 7	Mg 7	0	0
58	1R	4	Total 4	Mg 4	0	0
58	1S	3	Total 3	Mg 3	0	0
58	1T	2	Total 2	Mg 2	0	0
58	1U	9	Total 9	Mg 9	0	0
58	1V	9	Total 9	Mg 9	0	0
58	1W	7	Total 7	Mg 7	0	0
58	1X	5	Total 5	Mg 5	0	0
58	1Y	3	Total 3	Mg 3	0	0
58	1Z	2	Total 2	Mg 2	0	0
58	10	9	Total 9	Mg 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	11	5	Total 5	Mg 5	0	0
58	12	2	Total 2	Mg 2	0	0
58	13	5	Total 5	Mg 5	0	0
58	14	1	Total 1	Mg 1	0	0
58	15	6	Total 6	Mg 6	0	0
58	16	2	Total 2	Mg 2	0	0
58	17	6	Total 6	Mg 6	0	0
58	18	9	Total 9	Mg 9	0	0
58	1a	210	Total 210	Mg 210	0	0
58	1b	1	Total 1	Mg 1	0	0
58	1d	1	Total 1	Mg 1	0	0
58	1e	2	Total 2	Mg 2	0	0
58	1f	1	Total 1	Mg 1	0	0
58	1k	1	Total 1	Mg 1	0	0
58	1l	2	Total 2	Mg 2	0	0
58	1m	1	Total 1	Mg 1	0	0
58	1n	2	Total 2	Mg 2	0	0
58	1p	1	Total 1	Mg 1	0	0
58	1t	1	Total 1	Mg 1	0	0
58	1v	1	Total 1	Mg 1	0	0
58	1w	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1x	11	Total 11	Mg 11	0	0
58	2A	863	Total 863	Mg 863	0	0
58	2B	20	Total 20	Mg 20	0	0
58	2D	7	Total 7	Mg 7	0	0
58	2E	7	Total 7	Mg 7	0	0
58	2F	7	Total 7	Mg 7	0	0
58	2G	1	Total 1	Mg 1	0	0
58	2O	2	Total 2	Mg 2	0	0
58	2P	3	Total 3	Mg 3	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	2	Total 2	Mg 2	0	0
58	2V	2	Total 2	Mg 2	0	0
58	2W	2	Total 2	Mg 2	0	0
58	2X	1	Total 1	Mg 1	0	0
58	2Y	1	Total 1	Mg 1	0	0
58	2Z	1	Total 1	Mg 1	0	0
58	20	4	Total 4	Mg 4	0	0
58	23	4	Total 4	Mg 4	0	0
58	25	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	27	3	Total 3	Mg 3	0	0
58	28	1	Total 1	Mg 1	0	0
58	2a	230	Total 230	Mg 230	0	0
58	2d	2	Total 2	Mg 2	0	0
58	2e	1	Total 1	Mg 1	0	0
58	2f	2	Total 2	Mg 2	0	0
58	2g	1	Total 1	Mg 1	0	0
58	2i	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	2n	1	Total 1	Mg 1	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	4	Total 4	Mg 4	0	0
58	2w	1	Total 1	Mg 1	0	0
58	2x	6	Total 6	Mg 6	0	0
58	2y	1	Total 1	Mg 1	0	0

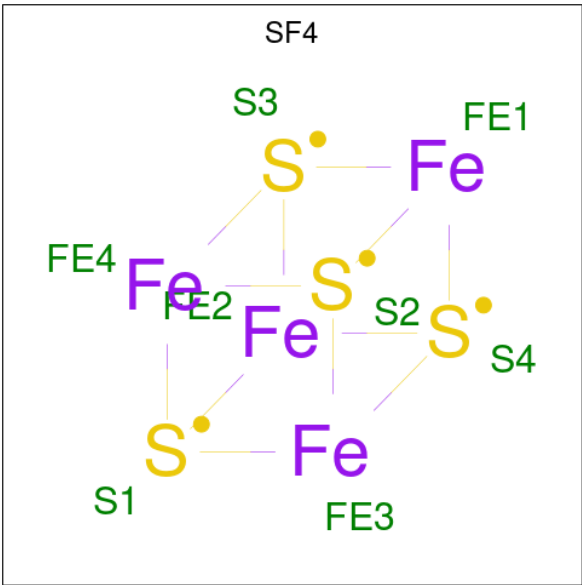
- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	1d	1	Total	Fe	S	0	0
			8	4	4		
61	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1886	Total	O	0	0
			1886	1886		
62	1B	61	Total	O	0	0
			61	61		
62	1D	28	Total	O	0	0
			28	28		
62	1E	29	Total	O	0	0
			29	29		
62	1F	15	Total	O	0	0
			15	15		
62	1G	3	Total	O	0	0
			3	3		
62	1H	2	Total	O	0	0
			2	2		
62	1I	1	Total	O	0	0
			1	1		
62	1N	4	Total	O	0	0
			4	4		
62	1O	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1P	23	Total 23	O 23	0	0
62	1Q	8	Total 8	O 8	0	0
62	1R	16	Total 16	O 16	0	0
62	1S	5	Total 5	O 5	0	0
62	1T	8	Total 8	O 8	0	0
62	1U	10	Total 10	O 10	0	0
62	1V	11	Total 11	O 11	0	0
62	1W	6	Total 6	O 6	0	0
62	1X	7	Total 7	O 7	0	0
62	1Y	1	Total 1	O 1	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	10	Total 10	O 10	0	0
62	11	12	Total 12	O 12	0	0
62	12	3	Total 3	O 3	0	0
62	13	4	Total 4	O 4	0	0
62	14	1	Total 1	O 1	0	0
62	15	7	Total 7	O 7	0	0
62	16	2	Total 2	O 2	0	0
62	17	11	Total 11	O 11	0	0
62	18	11	Total 11	O 11	0	0
62	1a	308	Total 308	O 308	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1b	1	Total 1	O 1	0	0
62	1e	1	Total 1	O 1	0	0
62	1f	1	Total 1	O 1	0	0
62	1i	1	Total 1	O 1	0	0
62	1l	7	Total 7	O 7	0	0
62	1m	2	Total 2	O 2	0	0
62	1o	1	Total 1	O 1	0	0
62	1q	2	Total 2	O 2	0	0
62	1u	1	Total 1	O 1	0	0
62	1v	5	Total 5	O 5	0	0
62	1w	8	Total 8	O 8	0	0
62	1x	6	Total 6	O 6	0	0
62	1z	1	Total 1	O 1	0	0
62	1y	1	Total 1	O 1	0	0
62	2A	1000	Total 1000	O 1000	0	0
62	2B	22	Total 22	O 22	0	0
62	2D	24	Total 24	O 24	0	0
62	2E	9	Total 9	O 9	0	0
62	2F	15	Total 15	O 15	0	0
62	2N	1	Total 1	O 1	0	0
62	2O	2	Total 2	O 2	0	0

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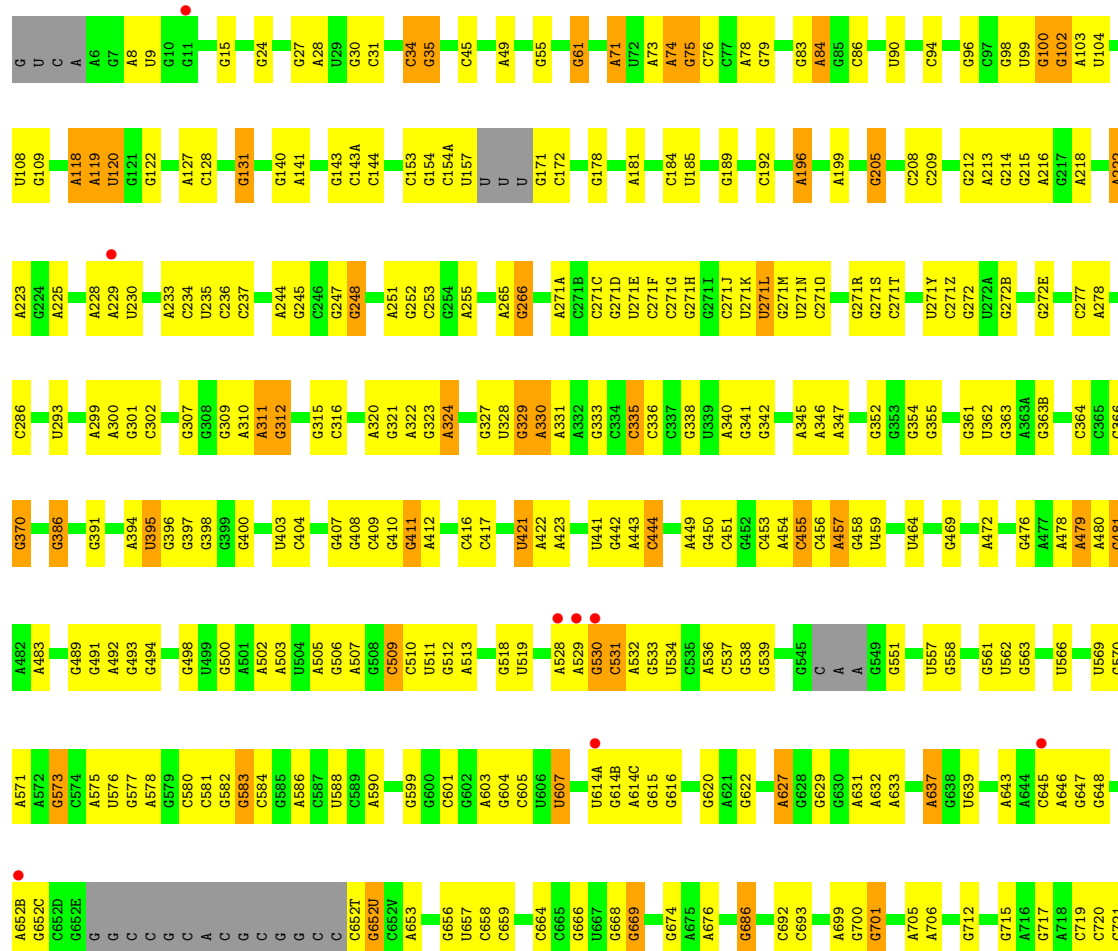
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62	2P	11	Total 11	O 11	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	3	Total 3	O 3	0	0
62	2T	5	Total 5	O 5	0	0
62	2U	3	Total 3	O 3	0	0
62	2W	3	Total 3	O 3	0	0
62	2X	4	Total 4	O 4	0	0
62	2Y	1	Total 1	O 1	0	0
62	2Z	1	Total 1	O 1	0	0
62	20	5	Total 5	O 5	0	0
62	21	13	Total 13	O 13	0	0
62	25	2	Total 2	O 2	0	0
62	27	1	Total 1	O 1	0	0
62	28	3	Total 3	O 3	0	0
62	29	1	Total 1	O 1	0	0
62	2a	198	Total 198	O 198	0	0
62	2d	1	Total 1	O 1	0	0
62	2e	1	Total 1	O 1	0	0
62	2j	1	Total 1	O 1	0	0
62	2l	4	Total 4	O 4	0	0
62	2p	2	Total 2	O 2	0	0

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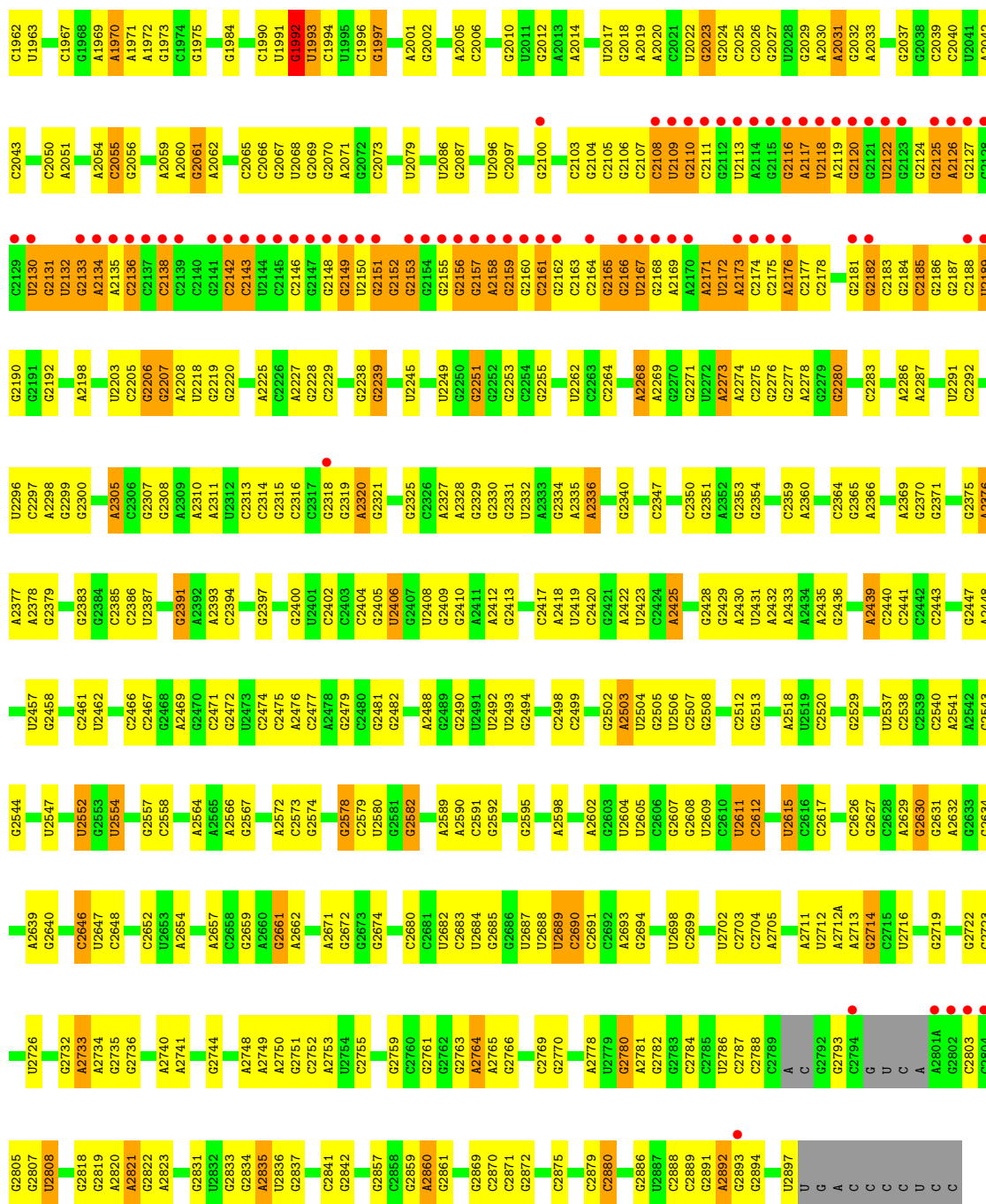
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2r	1	Total	O	0	0
			1	1		
62	2t	1	Total	O	0	0
			1	1		
62	2v	2	Total	O	0	0
			2	2		
62	2w	3	Total	O	0	0
			3	3		
62	2x	5	Total	O	0	0
			5	5		





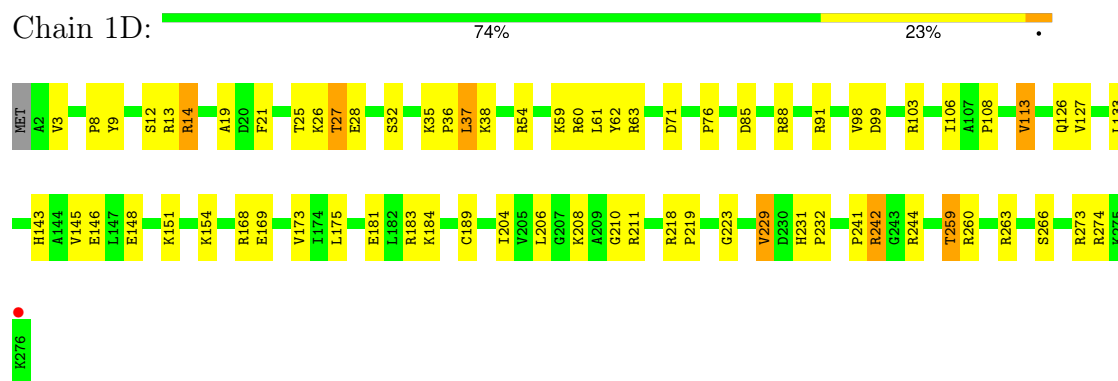
A1876	G1756	C1532	C1450A	A1379	G1183	C	G1042	C888	G808	A722
A1877	U1757	G1533	C1451	G1380	G1183	A	G	C889	G809	G723
G1878	G1758	U	A1452	U1263	G1186	C	G	A890	U811	U724
A1759	A1759	A	G1640	A1384	G1187	U	A	G892	C812	U725
			G1641	G1385	U1188	G	A	A890	G893	G726
			G1642	G1266	U1188	G	A	A891	G894	A727
C1882	A1762	G1536	A1459	U1267	G1191	U	A	C882	A819	G728
G1883	G1763	G1537	C1463	U1268	G1191	C	C	A883	A820	G729
A1884	G1764	G1538	C1464	G1388	G1191	G	A	C887	C731	
A1885	G1647	G1539	C1464	G1389	G1191	A	A	A896		
	G1648	U1540			G1195	A	G	C898	A824	
A1889	G1651	A1544	C1467	U1394	G1195	A	G	A899	A825	
A1890	A1652	A1545	C1468	A1395	C1196	C	C	A900	U826	U740
	G1653	A1546	A1469	U1396	U1113	C	C	A901	U827	G741
C1884	A1654	C1547	A1470	A1274	U1198	A	A	C991	U827	
C1895	A1655	C1548	G1400	A1275	U1199	G	G	C992	U828	G742
			G1401	A1276	C1200	G	A	C993		
			A1471	G1277	C1201	G	A	C994	G831	G743
A1784	A1472	G1473	A1472	G1277	C1201	G	A	C995	G744	
A1785	G1473		C1403	A1278	G1117	G	A	U907	A745	
A1786	C1404	A1557	C1404	A1287	G1202	G	G	A996	C995	
	U1659	A1558	U1405	U1288	A1204	U	U	C997	U839	A746
		G1559	U1406	G1296	U1205	C	C	C998	U747	U747
	G1662	G1560	C1407	G1296	G1206	A	A	A910	G748	
G1790	G1667	A1566	C1408	G1296	A1210	G	G	A911		
A1791	C1670	A1567	C1409	G1296	U1211	C	C	C912	A752	
G1792	G1674	G1568	G1410	A1300	G1218	G	G	U913	C753	
U1911		A1569	C1411	A1301	G1219	C	C	C914	A849	
A1912	U1680	A1570	A1412	A1302	A1220	U	U	C915	U851	G760
A1913	U1680	A1571	G1413	G1303	C1221	A	A	C916	G852	A761
C1914					C1221A	G	G	C917	G853	
U1915					G1222	C	C	C918	G854	A764
A1916					G1223	A	A	C919	G855	
U1917					U1420	G	G	C920	G856	G771
A1918					C1224	C	C	C921	G857	G772
A1919					A1421	G	G	C922	U858	U773
C1920					A1422	C	C	C923	G859	A774
					G1225	A	A	C924	U860	G775
					A1226	C	C	C925	A861	G776
C1924					G1229	A	A	C926	G862	
U1925					G1230	U	U	C927	A863	U779
A1926					G1231	C	C	C928	G864	G780
A1927					G1231	C	C	C929	G865	A781
A1928					G1231	C	C	C930	G866	A782
G1929					G1231	C	C	C931	G867	A783
G1930					G1231	C	C	C932	U868	A784
U1931					G1231	C	C	C933	G869	G785
					G1231	C	C	C934	A870	
A1936					G1231	C	C	C935	U871	A788
A1937					G1231	C	C	C936	A872	A789
A1938					G1231	C	C	C937	G873	C790
U1939					G1231	C	C	C938	G874	C791
					G1231	C	C	C939	U877	G792
					G1231	C	C	C940	A793	
C1942					G1231	C	C	C941		
					G1231	C	C	C942		
U1946					G1231	C	C	C943		
C1947					G1231	C	C	C944		
U1951					G1231	C	C	C945		
A1952					G1231	C	C	C946		
A1953					G1231	C	C	C947		
U1955					G1231	C	C	C948		
					G1231	C	C	C949		
G1959					G1231	C	C	C950		
					G1231	C	C	C951		
					G1231	C	C	C952		
					G1231	C	C	C953		
					G1231	C	C	C954		
					G1231	C	C	C955		
					G1231	C	C	C956		
					G1231	C	C	C957		
					G1231	C	C	C958		
					G1231	C	C	C959		
					G1231	C	C	C960		
					G1231	C	C	C961		
					G1231	C	C	C962		
					G1231	C	C	C963		
					G1231	C	C	C964		
					G1231	C	C	C965		
					G1231	C	C	C966		
					G1231	C	C	C967		
					G1231	C	C	C968		
					G1231	C	C	C969		
					G1231	C	C	C970		
					G1231	C	C	C971		
					G1231	C	C	C972		
					G1231	C	C	C973		
					G1231	C	C	C974		
					G1231	C	C	C975		
					G1231	C	C	C976		
					G1231	C	C	C977		
					G1231	C	C	C978		
					G1231	C	C	C979		
					G1231	C	C	C980		
					G1231	C	C	C981		
					G1231	C	C	C982		
					G1231	C	C	C983		
					G1231	C	C	C984		
					G1231	C	C	C985		
					G1231	C	C	C986		
					G1231	C	C	C987		
					G1231	C	C	C988		
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					G1231	C	C	C1001		
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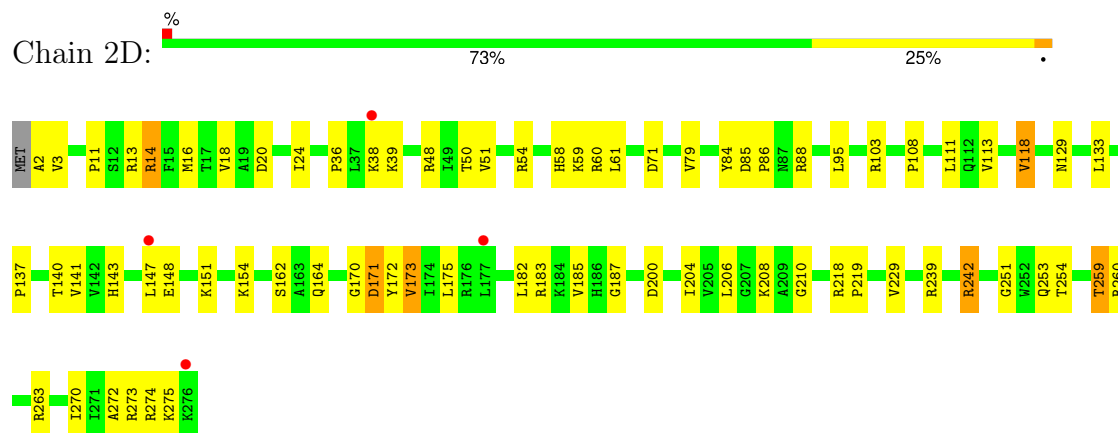
- Molecule 2: 5S Ribosomal RNA



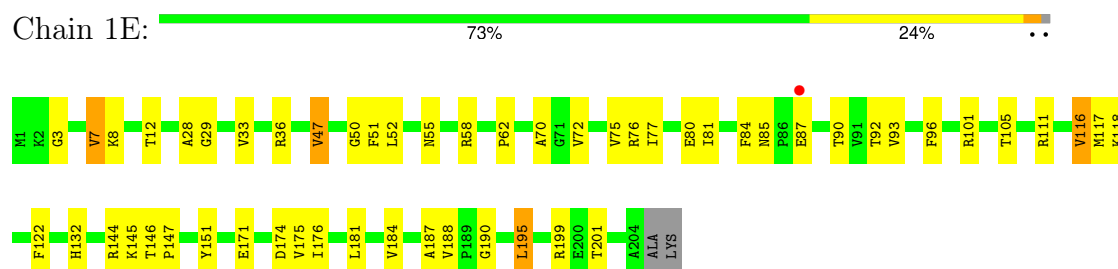
- Molecule 3: 50S ribosomal protein L2



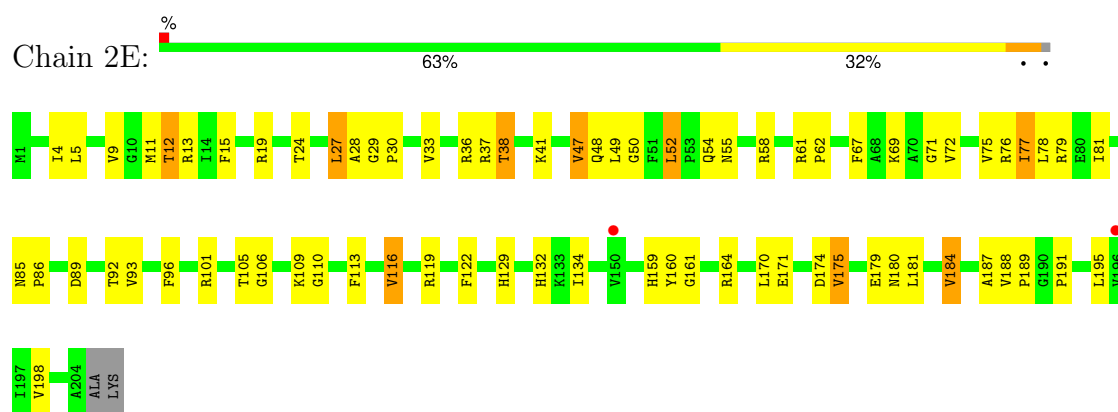
- Molecule 3: 50S ribosomal protein L2



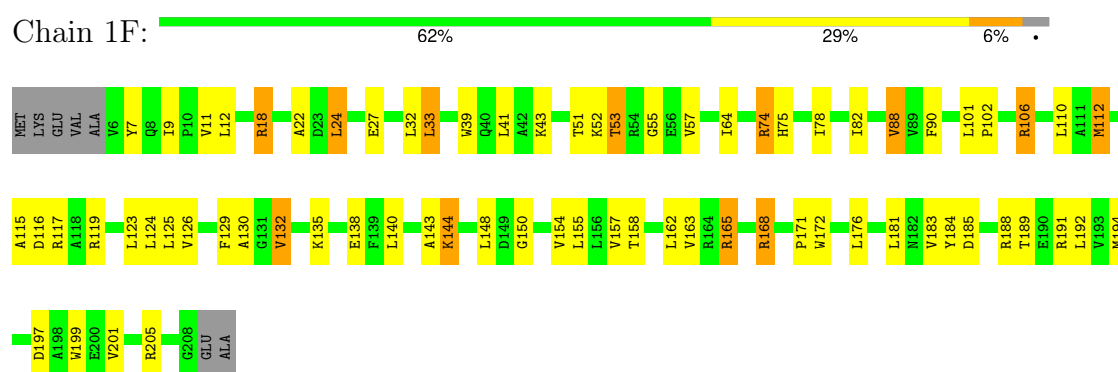
- Molecule 4: 50S ribosomal protein L3



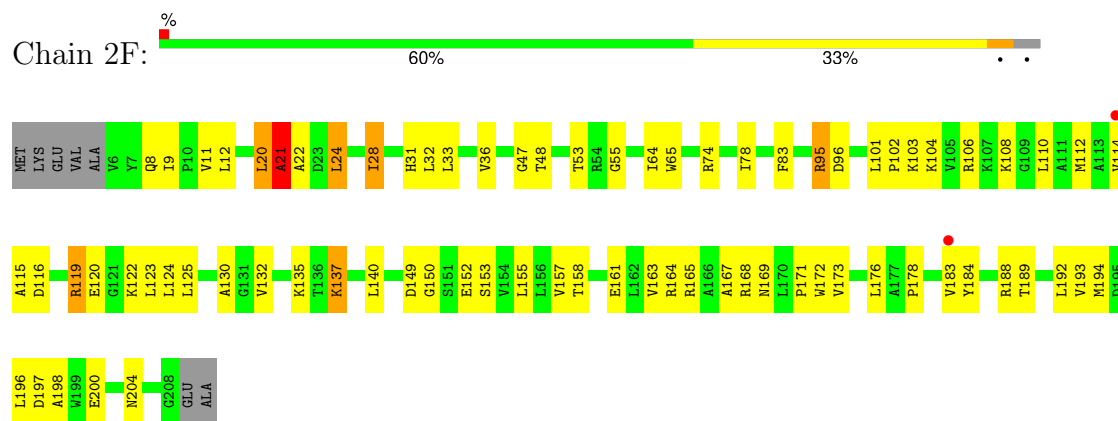
- Molecule 4: 50S ribosomal protein L3



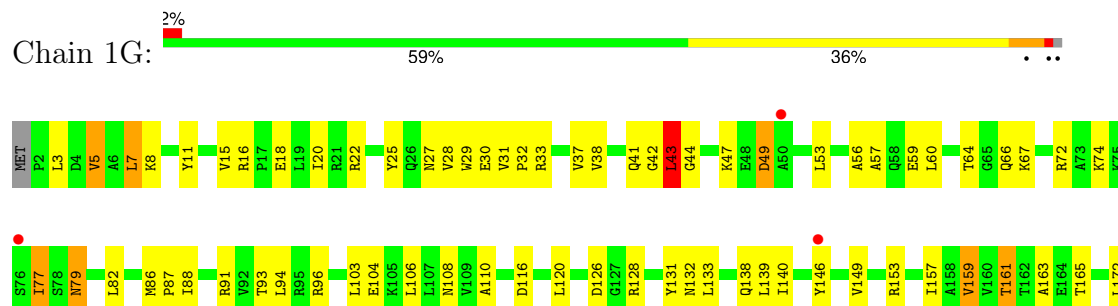
• Molecule 5: 50S ribosomal protein L4

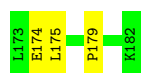


• Molecule 5: 50S ribosomal protein L4

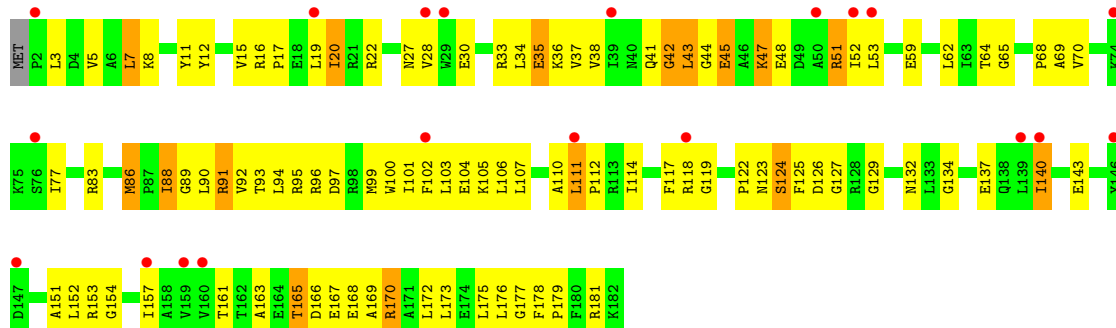
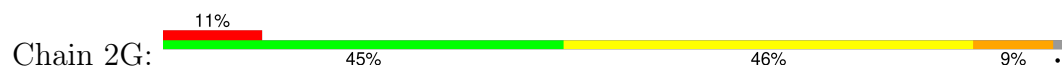


• Molecule 6: 50S ribosomal protein L5

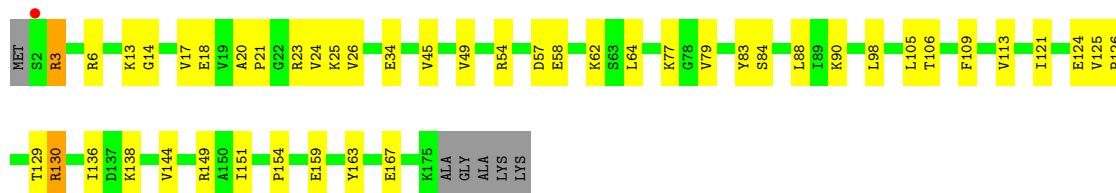




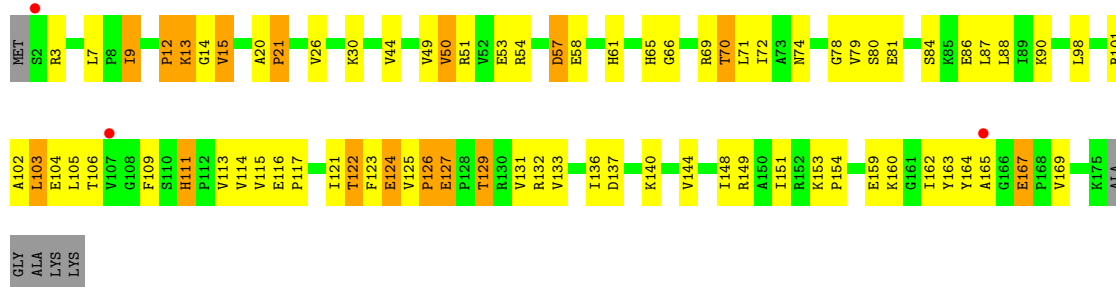
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

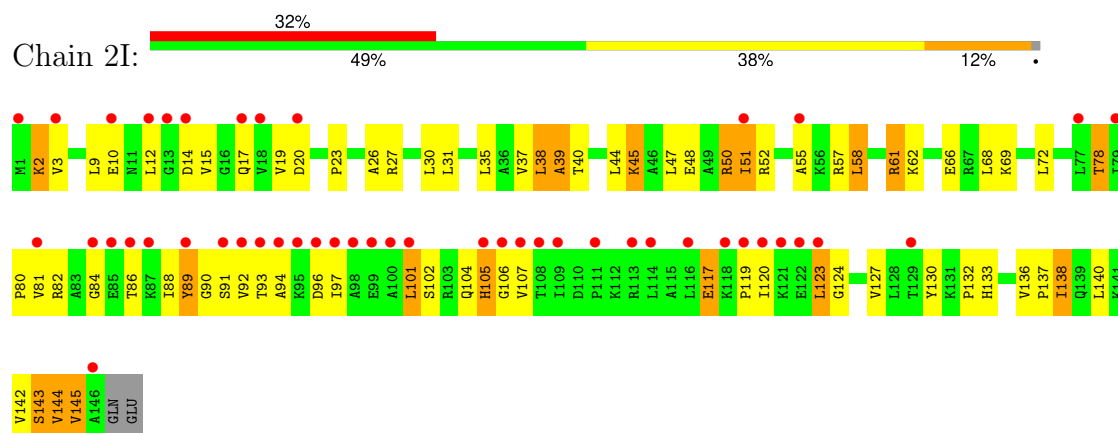


• Molecule 8: 50S ribosomal protein L9

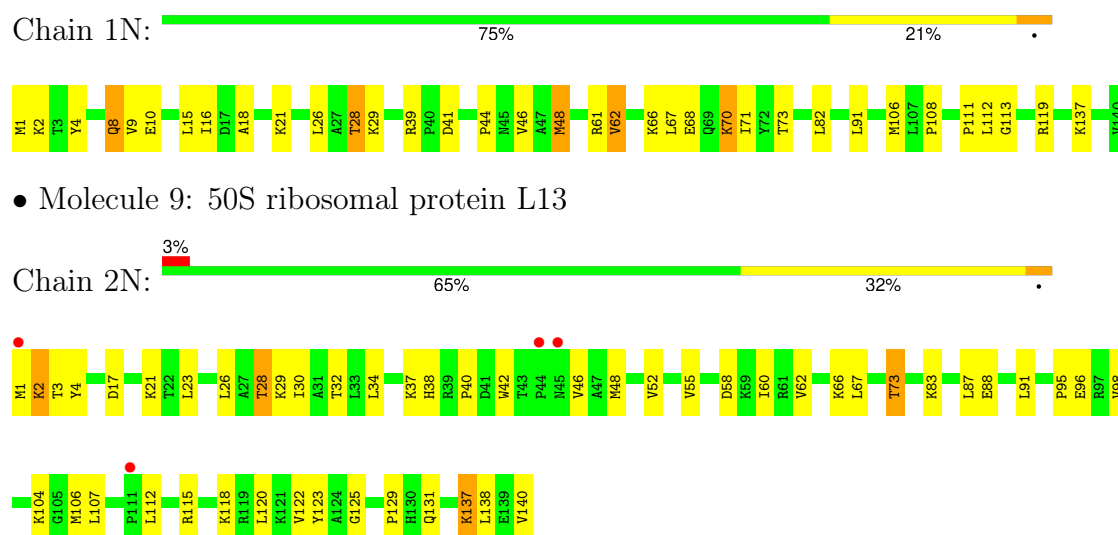




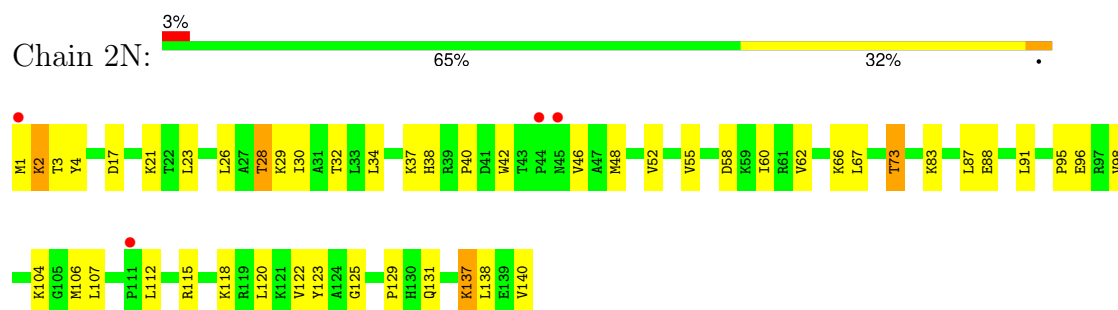
• Molecule 8: 50S ribosomal protein L9



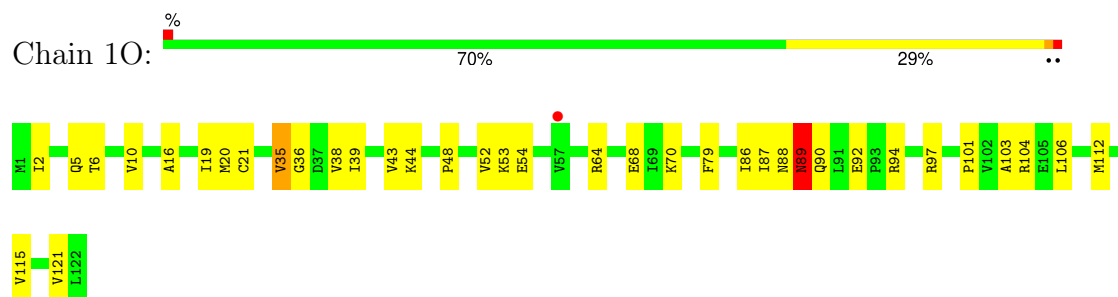
• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13

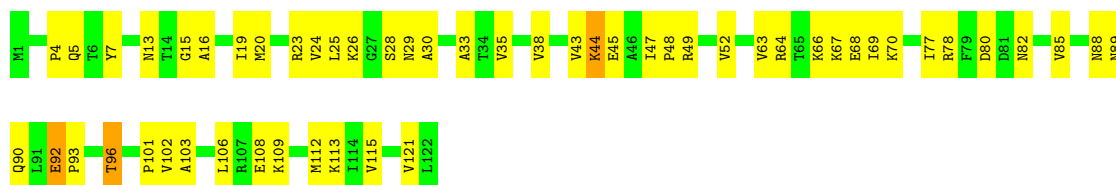


• Molecule 10: 50S ribosomal protein L14



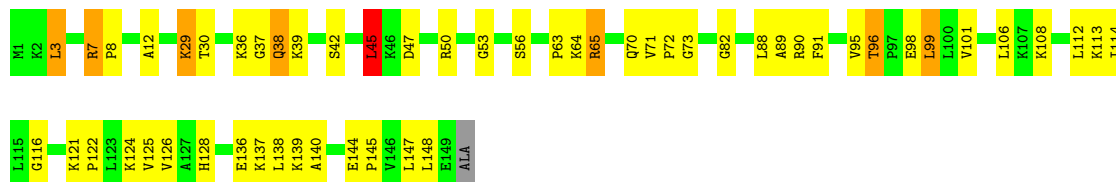
• Molecule 10: 50S ribosomal protein L14





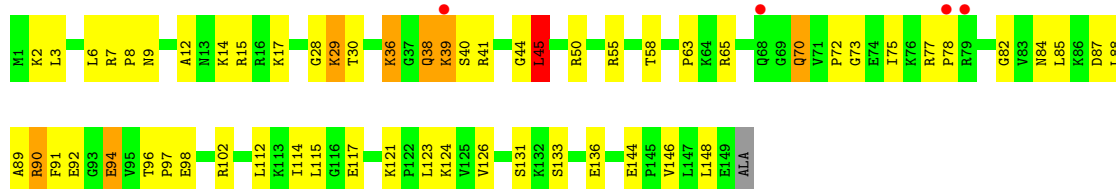
• Molecule 11: 50S ribosomal protein L15

Chain 1P: 63% 31% 5% ..



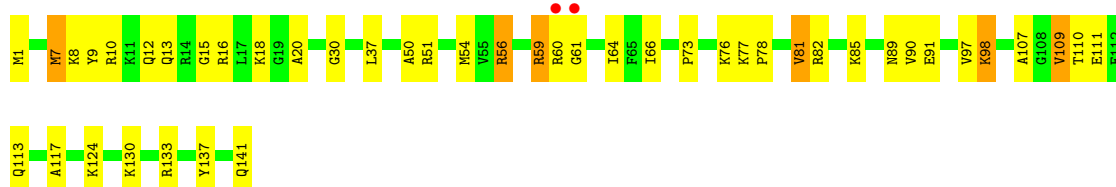
• Molecule 11: 50S ribosomal protein L15

Chain 2P: 3% 60% 34% 5% ..



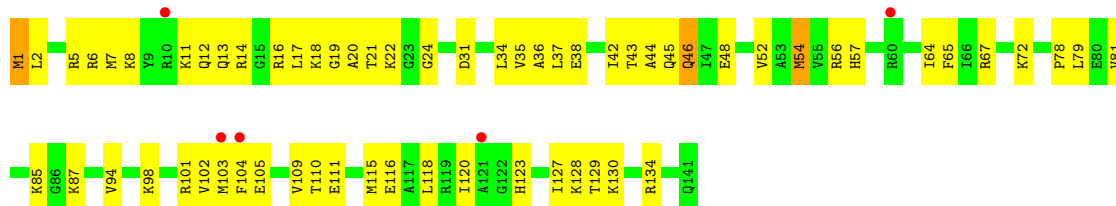
• Molecule 12: 50S ribosomal protein L16

Chain 1Q: 68% 28% .




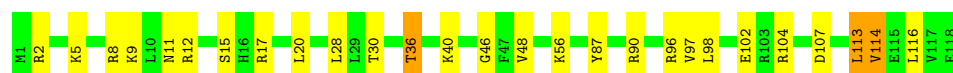
• Molecule 12: 50S ribosomal protein L16

Chain 2Q: 4% 55% 43% .



• Molecule 13: 50S ribosomal protein L17

Chain 1R:  77% 20% .



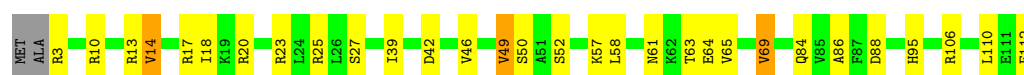
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  2% 74% 25% .



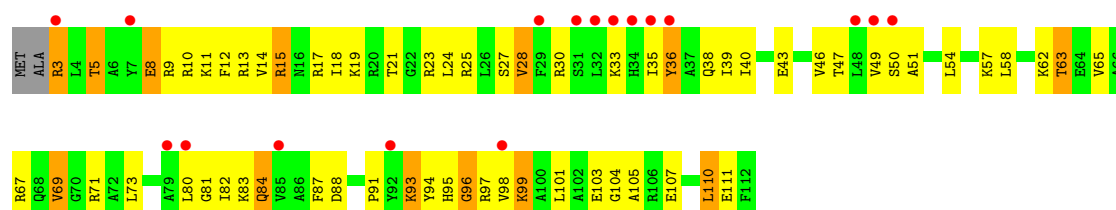
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  71% 24% . .



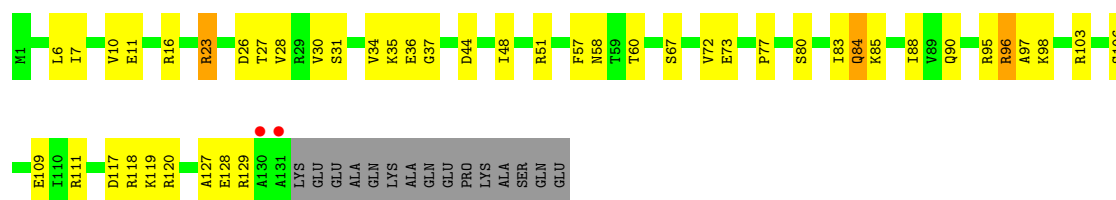
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  15% 41% 46% 12% .



- Molecule 15: 50S ribosomal protein L19

Chain 1T:  58% 29% 10% .



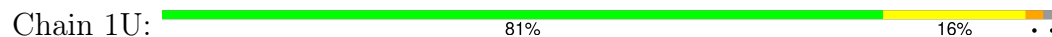
- Molecule 15: 50S ribosomal protein L19

Chain 2T:  55% 34% 10% .





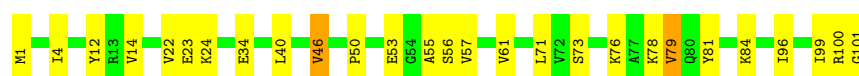
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



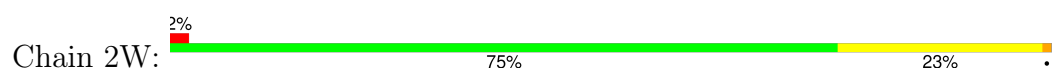
- Molecule 17: 50S ribosomal protein L21



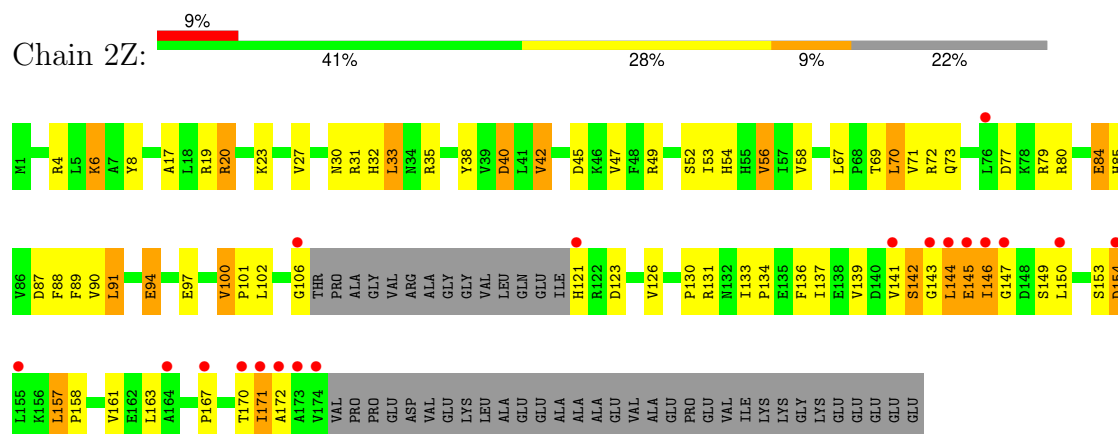
- Molecule 18: 50S ribosomal protein L22



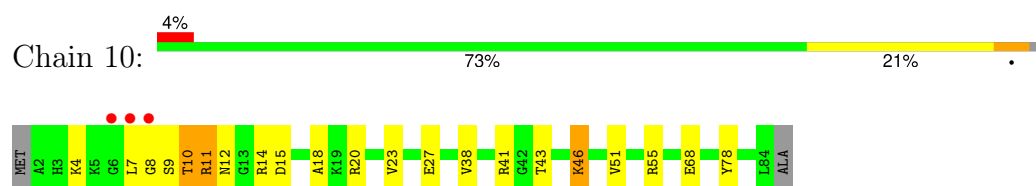
- Molecule 18: 50S ribosomal protein L22



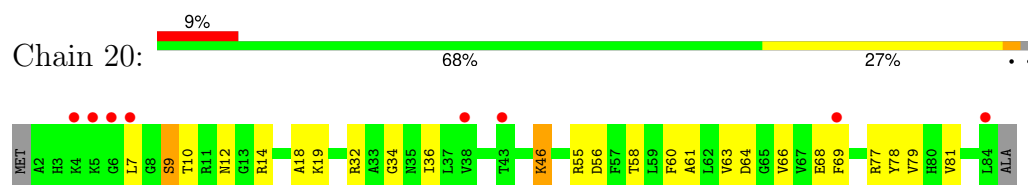
- Molecule 21: 50S ribosomal protein L25



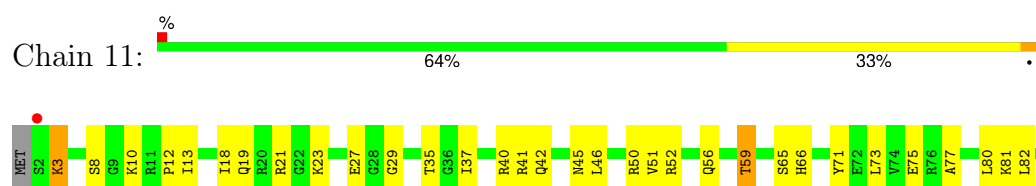
- Molecule 22: 50S ribosomal protein L27



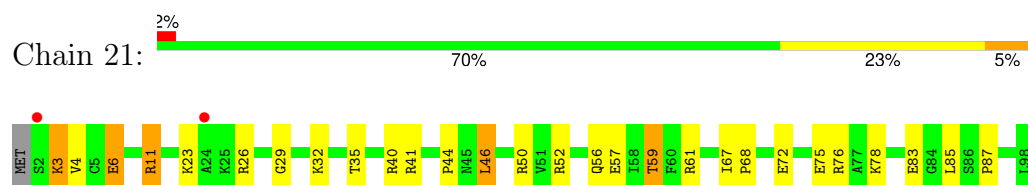
- Molecule 22: 50S ribosomal protein L27



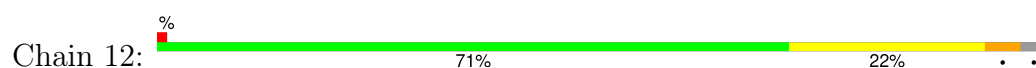
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

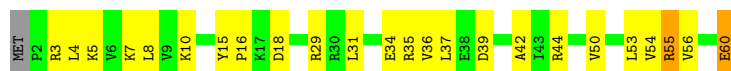




- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



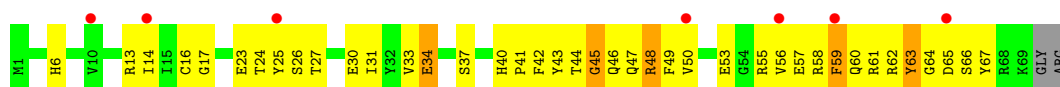
- Molecule 25: 50S ribosomal protein L30



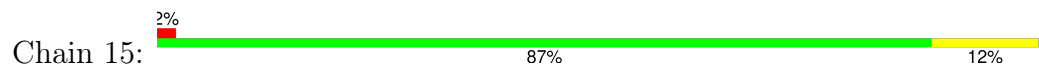
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



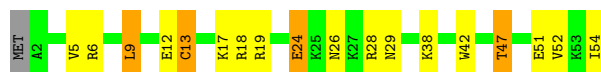
- Molecule 27: 50S ribosomal protein L32





- Molecule 28: 50S ribosomal protein L33

Chain 16: 65% 26% 7% .



- Molecule 28: 50S ribosomal protein L33

Chain 26: 2% 48% 44% 6% .



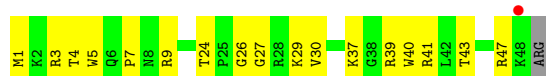
- Molecule 29: 50S ribosomal protein L34

Chain 17: 78% 18% . .



- Molecule 29: 50S ribosomal protein L34

Chain 27: 2% 63% 35% .



- Molecule 30: 50S ribosomal protein L35

Chain 18: 66% 31% . .



- Molecule 30: 50S ribosomal protein L35

Chain 28: 2% 65% 34% .

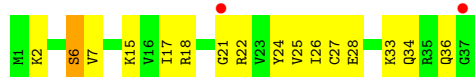


- Molecule 31: 50S ribosomal protein L36

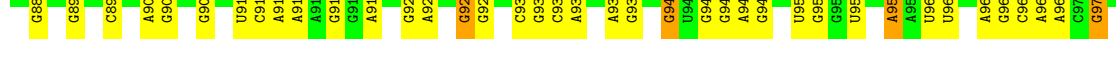
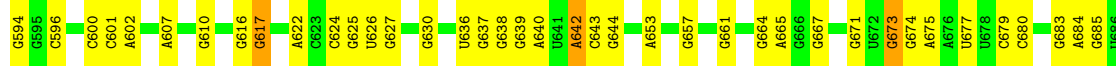
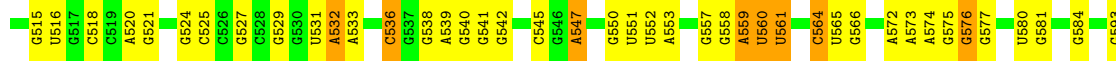
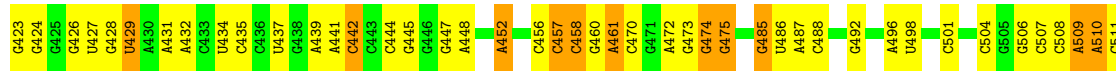
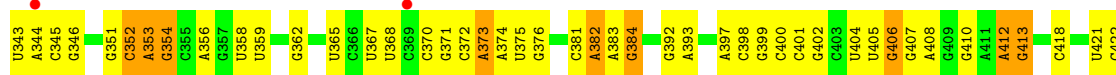
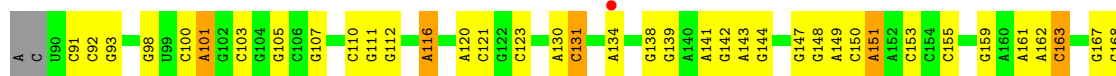
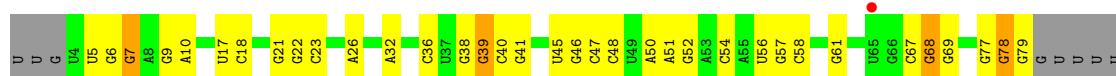
Chain 19: 92% 8%

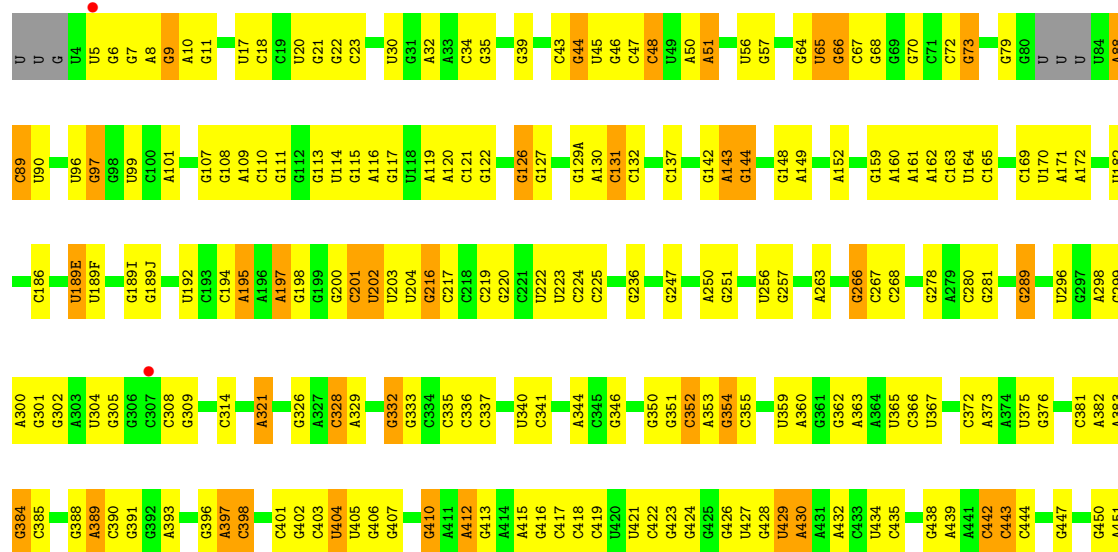


- Molecule 31: 50S ribosomal protein L36



- Molecule 32: 16S Ribosomal RNA

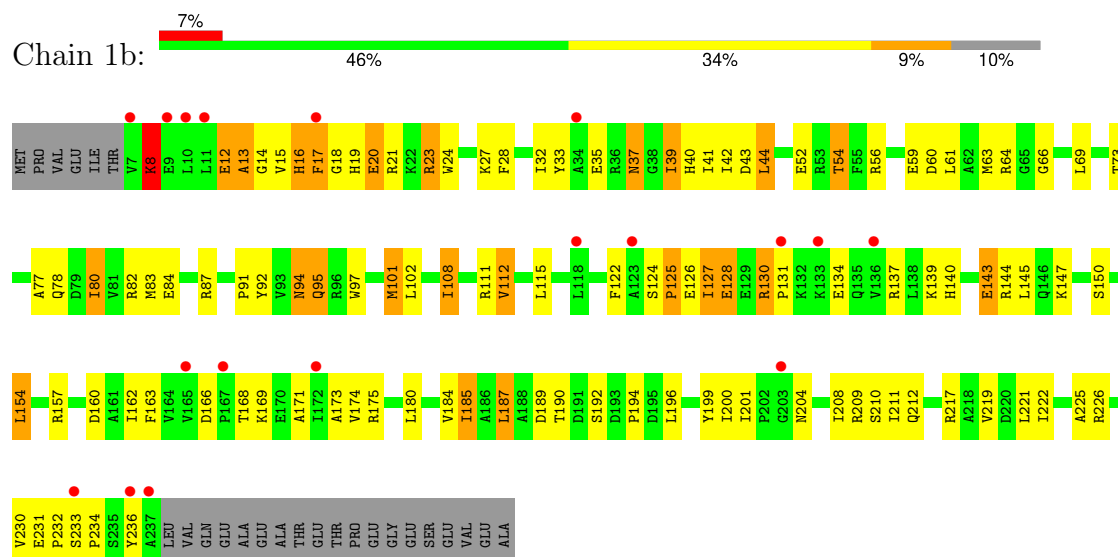




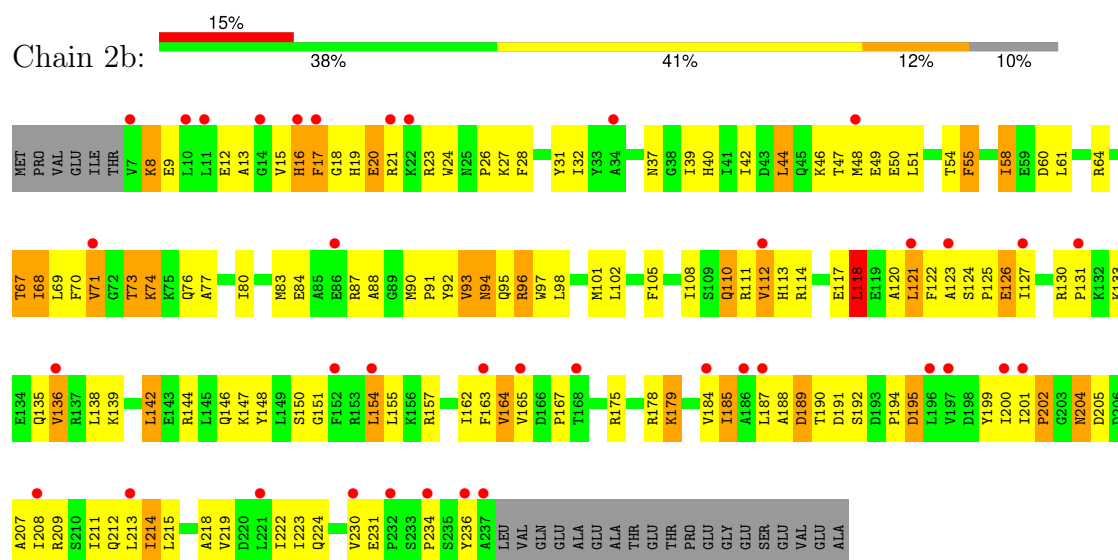
WORLDWIDE
PDB
PROTEIN DATA BANK



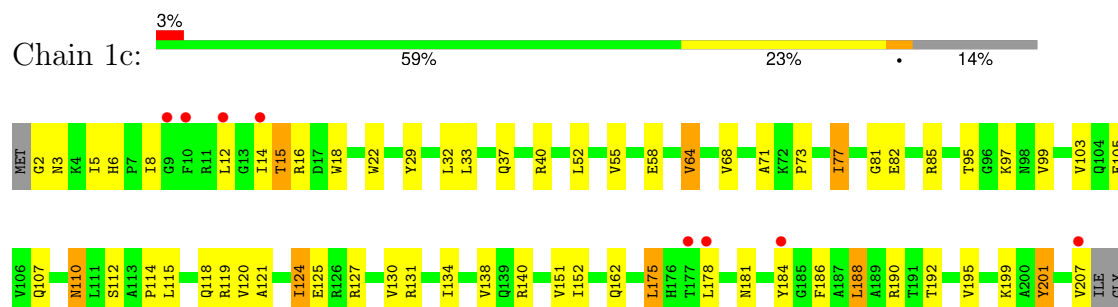
• Molecule 33: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S2

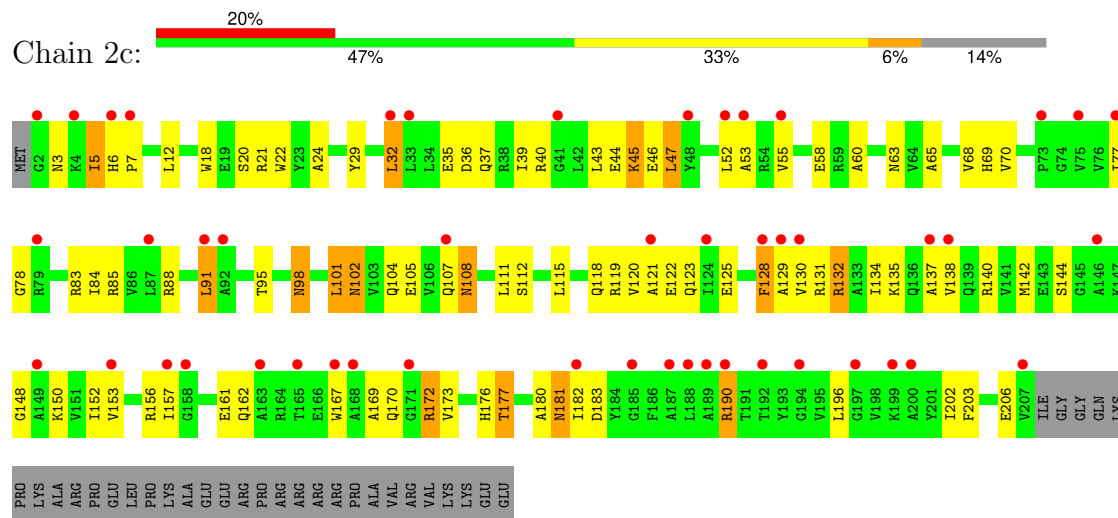


• Molecule 34: 30S ribosomal protein S3

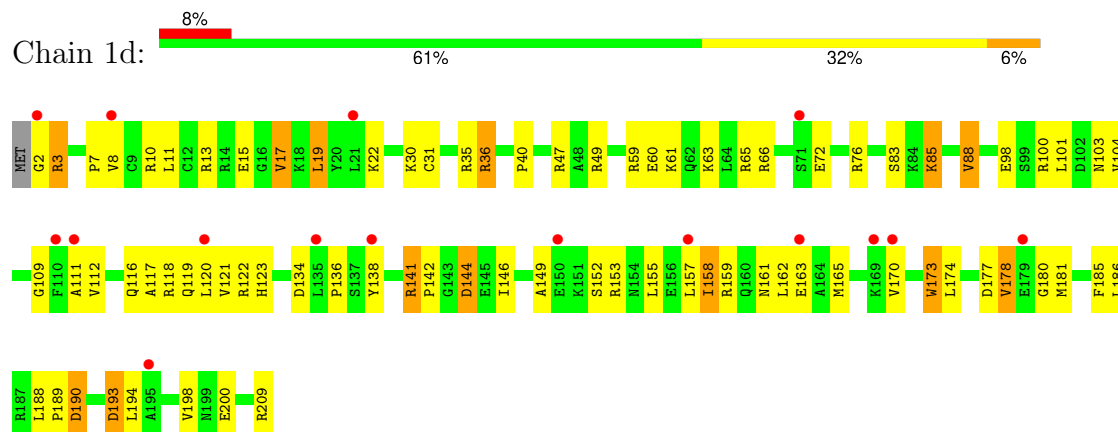


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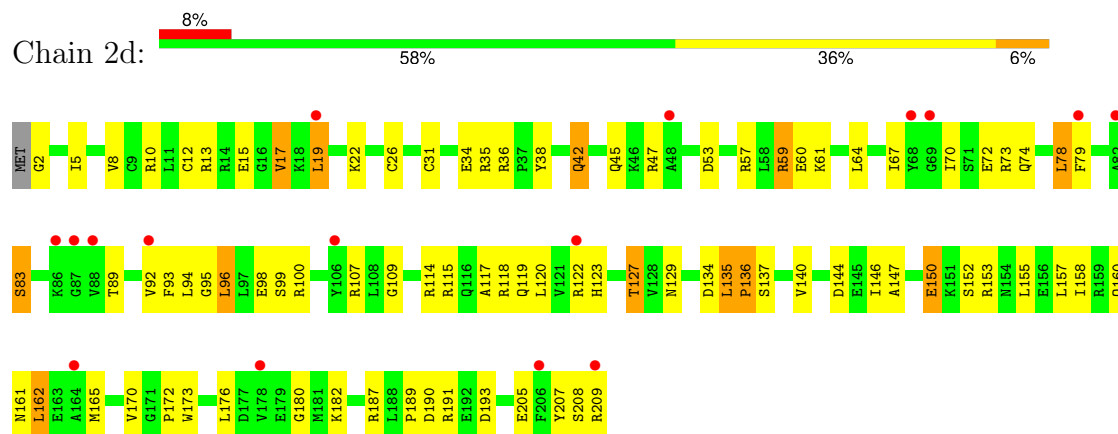
• Molecule 34: 30S ribosomal protein S3



• Molecule 35: 30S ribosomal protein S4

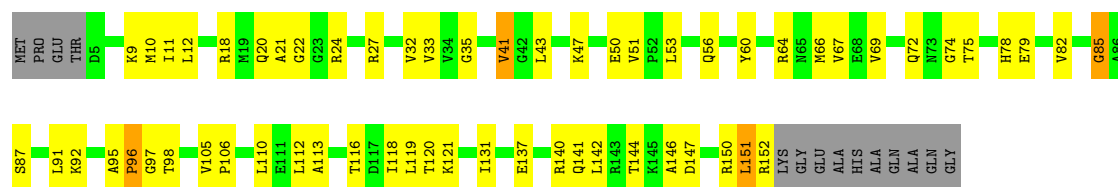


• Molecule 35: 30S ribosomal protein S4



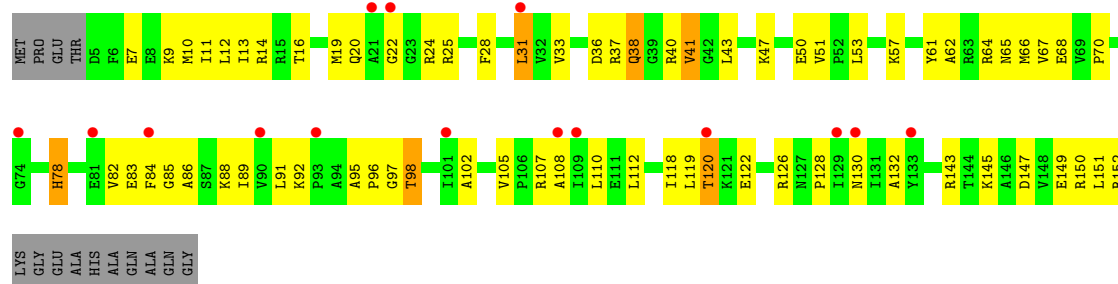
• Molecule 36: 30S ribosomal protein S5

Chain 1e: 



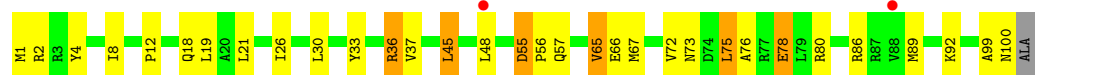
• Molecule 36: 30S ribosomal protein S5

Chain 2e: 



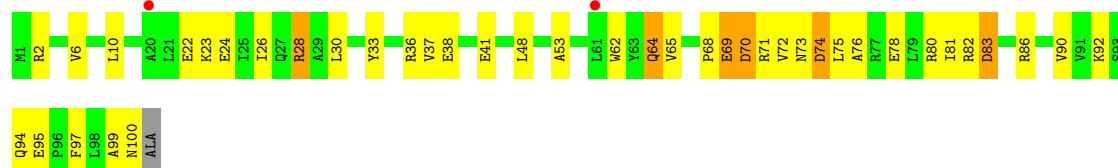
• Molecule 37: 30S ribosomal protein S6

Chain 1f: 



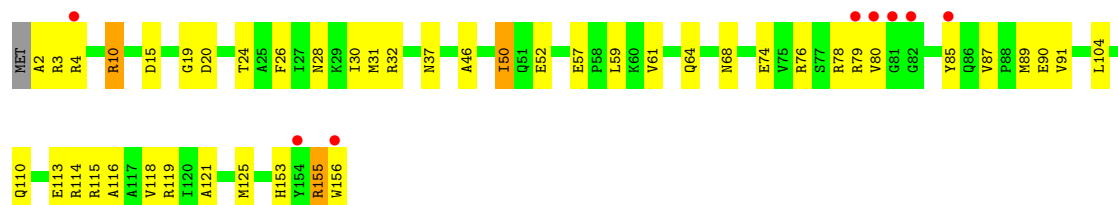
• Molecule 37: 30S ribosomal protein S6

Chain 2f: 

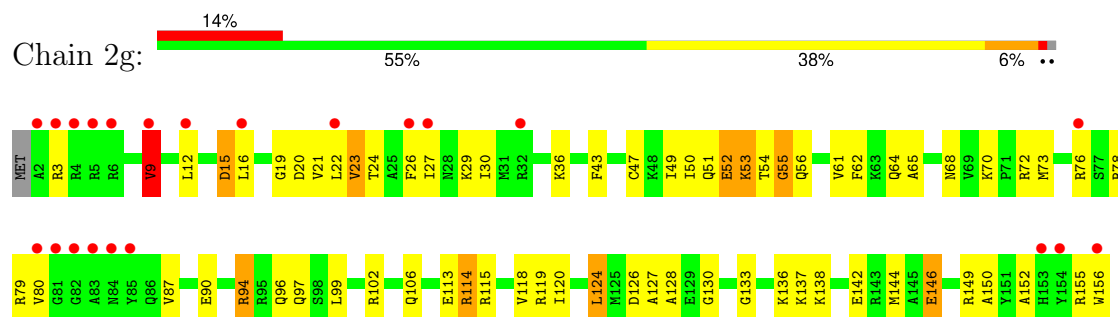


• Molecule 38: 30S ribosomal protein S7

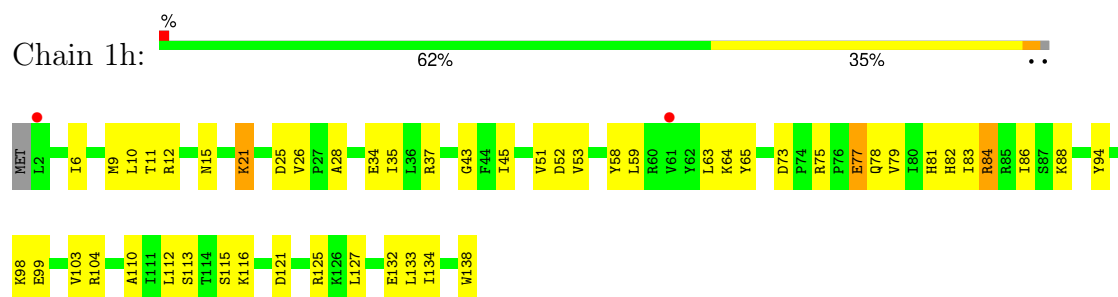
Chain 1g: 



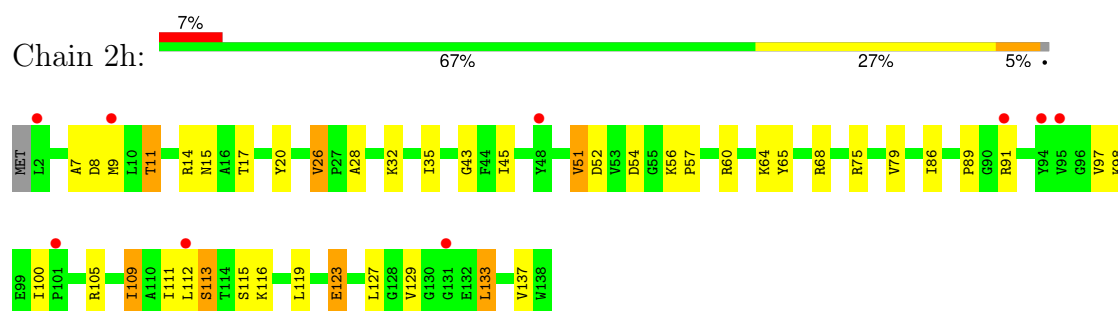
- Molecule 38: 30S ribosomal protein S7



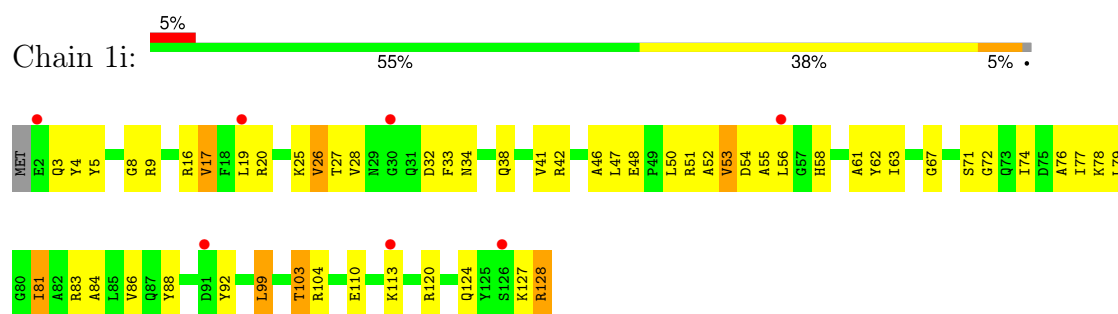
- Molecule 39: 30S ribosomal protein S8



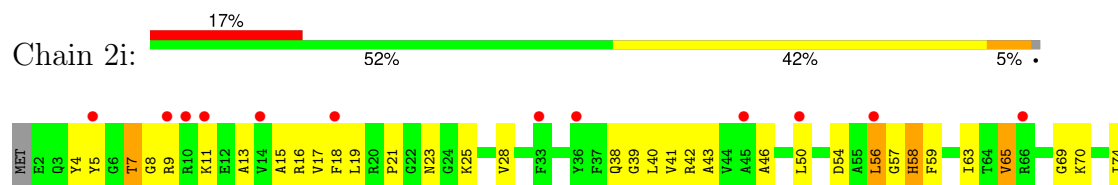
- Molecule 39: 30S ribosomal protein S8

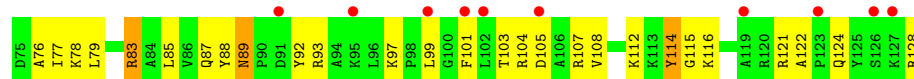


- Molecule 40: 30S ribosomal protein S9

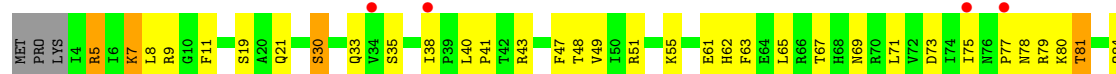


- Molecule 40: 30S ribosomal protein S9

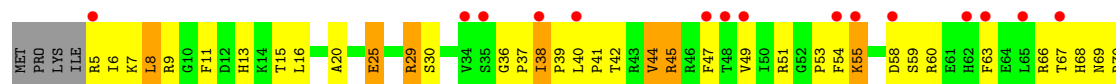




- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S11

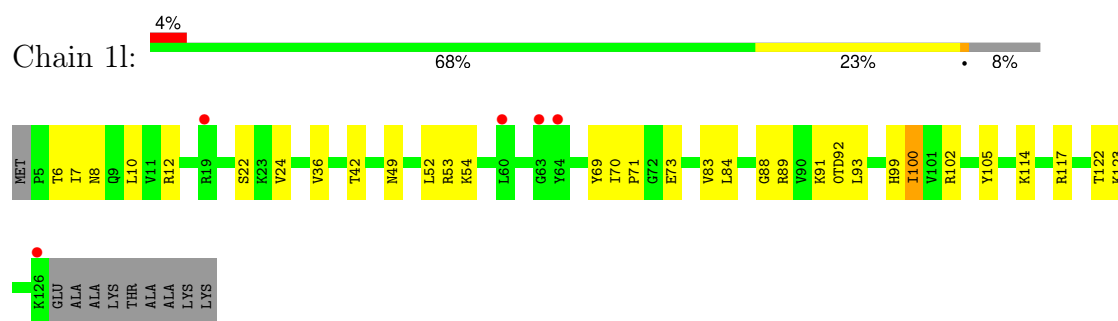


- Molecule 42: 30S ribosomal protein S11

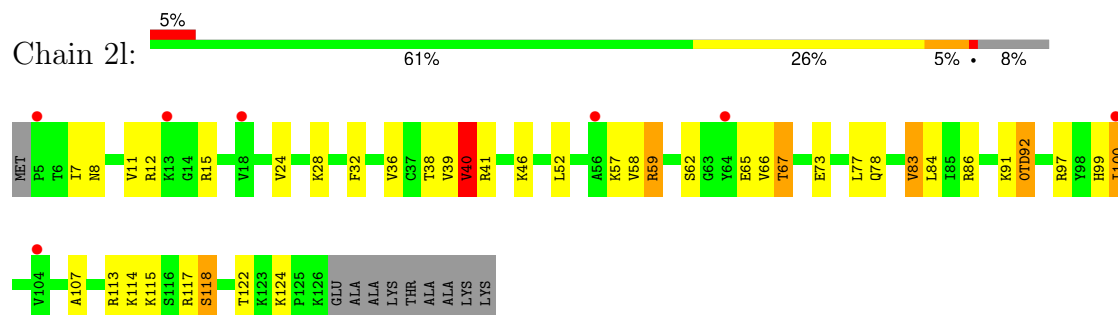


- Molecule 43: 30S ribosomal protein S12

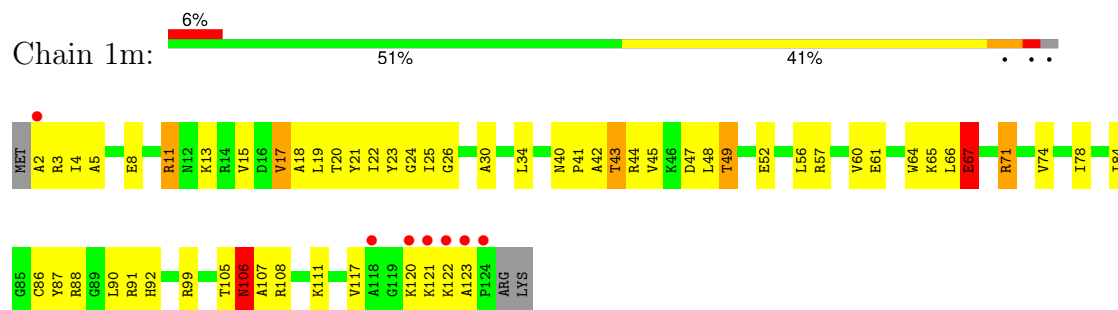




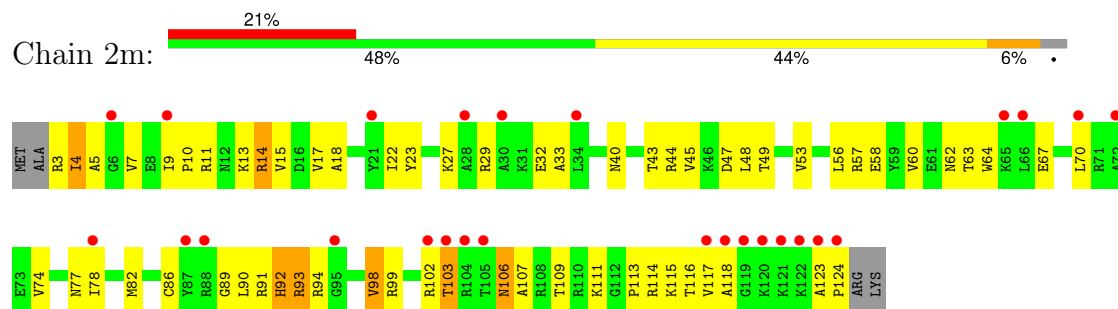
- Molecule 43: 30S ribosomal protein S12



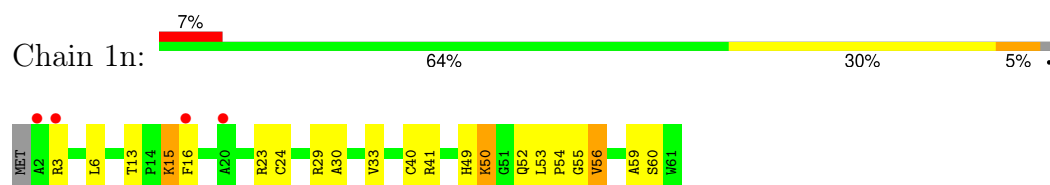
- Molecule 44: 30S ribosomal protein S13



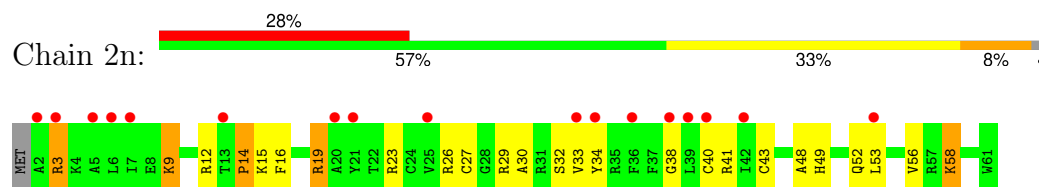
- Molecule 44: 30S ribosomal protein S13



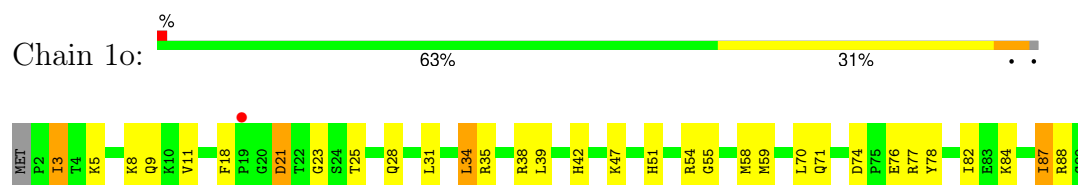
- Molecule 45: 30S ribosomal protein S14 type Z



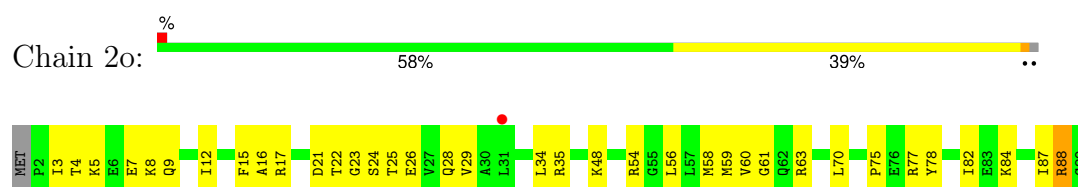
- Molecule 45: 30S ribosomal protein S14 type Z



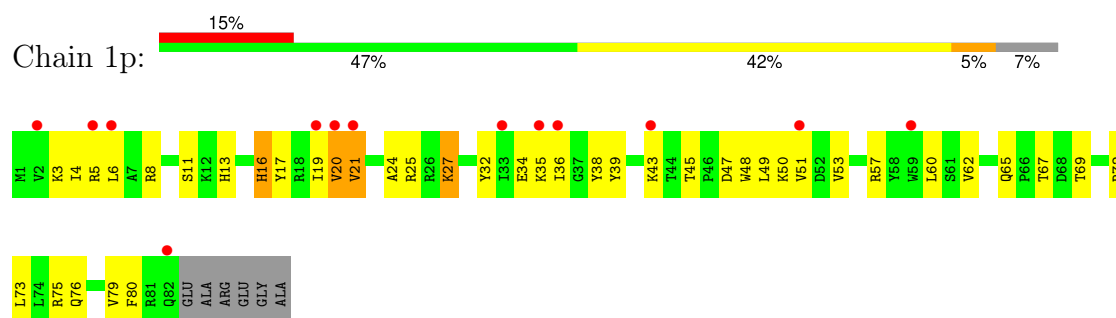
- Molecule 46: 30S ribosomal protein S15



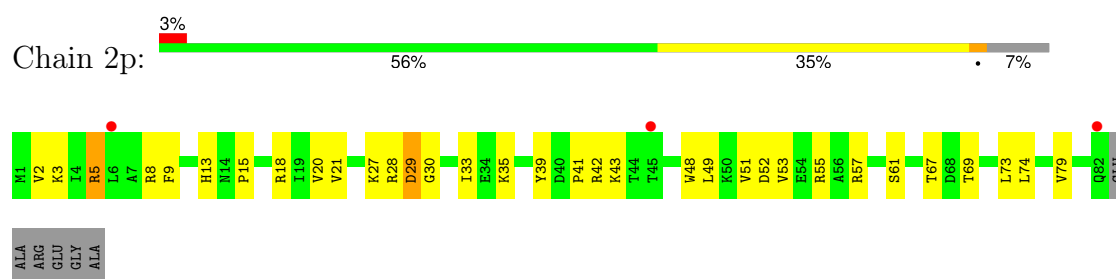
- Molecule 46: 30S ribosomal protein S15



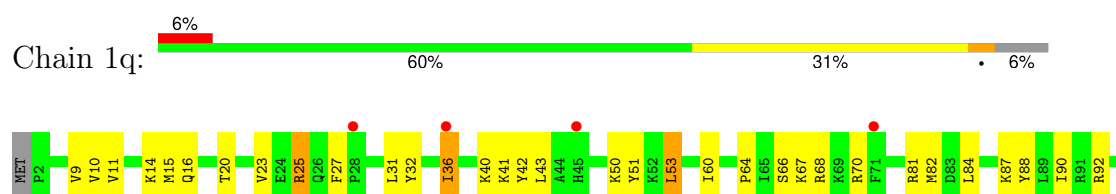
- Molecule 47: 30S ribosomal protein S16

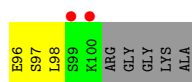


- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17





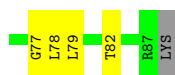
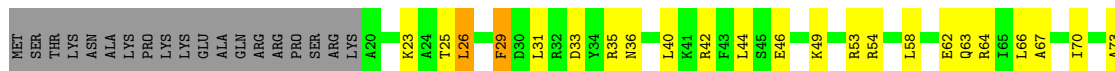
• Molecule 48: 30S ribosomal protein S17



• Molecule 49: 30S ribosomal protein S18



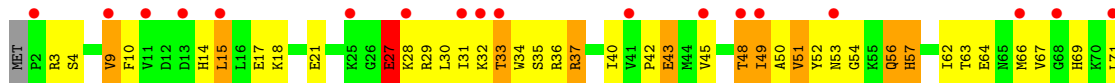
• Molecule 49: 30S ribosomal protein S18

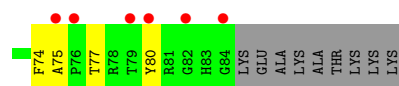


• Molecule 50: 30S ribosomal protein S19



• Molecule 50: 30S ribosomal protein S19

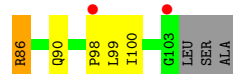
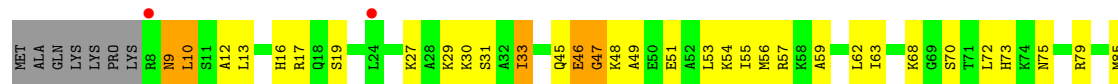




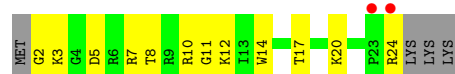
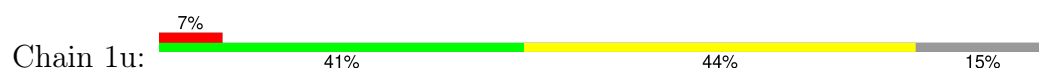
- Molecule 51: 30S ribosomal protein S20



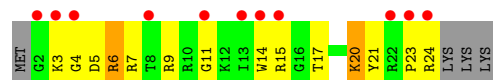
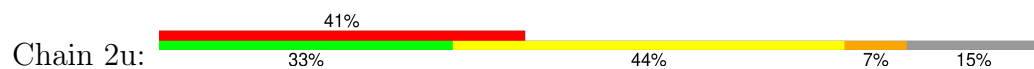
- Molecule 51: 30S ribosomal protein S20



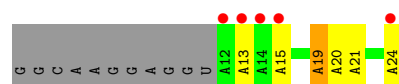
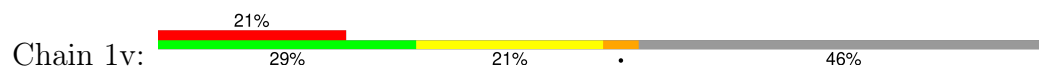
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx

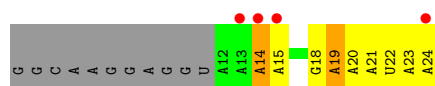


- Molecule 53: MET-LYS-mRNA

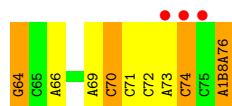


- Molecule 53: MET-LYS-mRNA

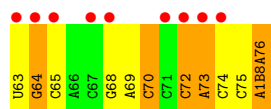
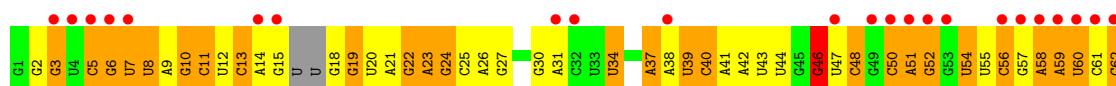
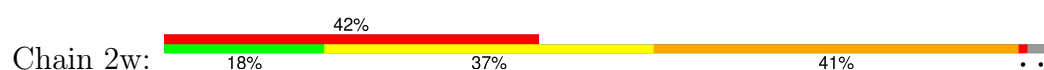




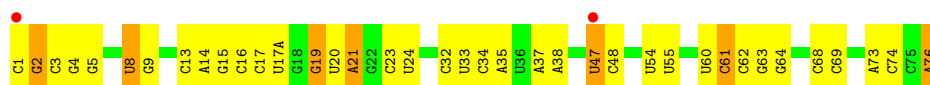
● Molecule 54: A-site Aminoacyl-tRNA Lys-tRNA_{Lys}



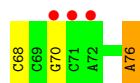
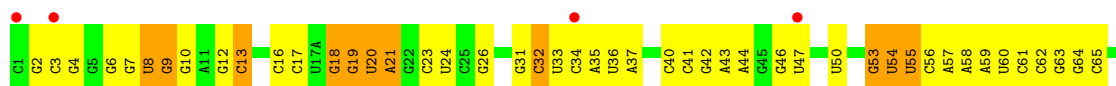
● Molecule 54: A-site Aminoacyl-tRNA Lys-tRNA_{Lys}



● Molecule 55: P-site Peptidyl-tRNA fMRC-tRNA_{Cys} RNA-part

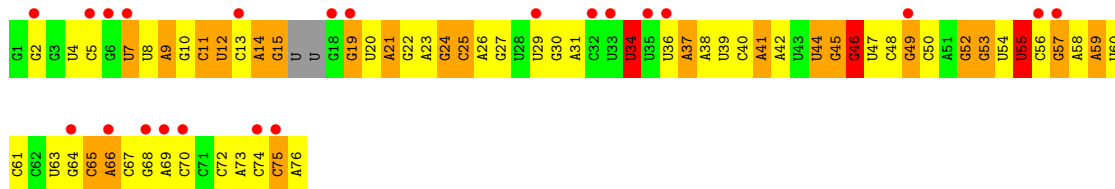


● Molecule 55: P-site Peptidyl-tRNA fMRC-tRNA_{Cys} RNA-part



● Molecule 56: P-site Peptidyl-tRNA fMRC-tRNA_{Cys} Peptide-part





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.56Å 449.05Å 616.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.94 – 2.60 123.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (123.94-2.60) 99.9 (123.94-2.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.229 , 0.278 0.232 , 0.279	Depositor DCC
R_{free} test set	87814 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	299808	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: OMC, 2MG, U8U, OMG, UR3, 2MA, M2G, K, 5MU, 4OC, 0TD, A1B8A, 8AN, SF4, 5MC, ZN, OMU, MA6, 4SU, FME, MG, T6A, PSU, G7M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.29	1/69011 (0.0%)	0.47	1/107720 (0.0%)
1	2A	0.22	1/67295 (0.0%)	0.41	1/105042 (0.0%)
2	1B	0.24	0/2882	0.42	0/4494
2	2B	0.19	0/2879	0.37	0/4487
3	1D	0.29	0/2186	0.51	0/2944
3	2D	0.23	0/2186	0.47	0/2944
4	1E	0.26	0/1592	0.54	0/2149
4	2E	0.21	0/1592	0.45	0/2149
5	1F	0.25	0/1619	0.48	0/2193
5	2F	0.22	0/1615	0.47	3/2188 (0.1%)
6	1G	0.22	0/1448	0.47	1/1957 (0.1%)
6	2G	0.23	0/1453	0.50	1/1963 (0.1%)
7	1H	0.23	0/1356	0.43	0/1834
7	2H	0.19	0/1356	0.40	0/1834
8	1I	0.18	0/1112	0.42	0/1514
8	2I	0.22	0/1079	0.48	0/1475
9	1N	0.25	0/1144	0.49	0/1543
9	2N	0.20	0/1144	0.40	0/1543
10	1O	0.28	0/943	0.49	0/1269
10	2O	0.22	0/943	0.50	0/1269
11	1P	0.26	0/1152	0.50	0/1533
11	2P	0.21	0/1152	0.48	0/1533
12	1Q	0.28	0/1143	0.49	0/1527
12	2Q	0.22	0/1143	0.47	0/1527
13	1R	0.27	0/982	0.50	0/1312
13	2R	0.22	0/982	0.46	0/1312
14	1S	0.21	0/883	0.48	0/1176
14	2S	0.21	0/880	0.46	0/1172
15	1T	0.25	0/1105	0.48	0/1477
15	2T	0.22	0/1097	0.48	0/1468
16	1U	0.28	0/977	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.41	0/1301
17	1V	0.26	0/782	0.47	0/1049
17	2V	0.18	0/782	0.39	0/1049
18	1W	0.27	0/897	0.45	0/1205
18	2W	0.21	0/897	0.44	0/1205
19	1X	0.26	0/764	0.55	2/1025 (0.2%)
19	2X	0.23	0/764	0.61	2/1025 (0.2%)
20	1Y	0.23	0/819	0.44	0/1095
20	2Y	0.20	0/819	0.47	1/1095 (0.1%)
21	1Z	0.23	0/1267	0.48	0/1717
21	2Z	0.22	0/1299	0.42	0/1763
22	10	0.27	0/662	0.52	0/881
22	20	0.23	0/662	0.53	0/881
23	11	0.27	0/762	0.46	0/1014
23	21	0.21	0/762	0.41	0/1014
24	12	0.23	0/590	0.43	0/781
24	22	0.22	0/590	0.42	0/781
25	13	0.26	0/474	0.45	0/635
25	23	0.18	0/469	0.39	0/630
26	14	0.25	0/565	0.58	1/761 (0.1%)
26	24	0.28	0/545	0.56	0/737
27	15	0.27	0/469	0.47	0/635
27	25	0.23	0/469	0.48	0/635
28	16	0.29	0/460	0.50	0/613
28	26	0.21	0/456	0.45	0/608
29	17	0.33	0/426	0.56	0/561
29	27	0.25	0/426	0.51	0/561
30	18	0.28	0/525	0.52	0/691
30	28	0.21	0/525	0.42	0/691
31	19	0.27	0/310	0.56	0/407
31	29	0.20	0/310	0.42	0/407
32	1a	0.20	0/35795	0.39	0/55864
32	2a	0.19	0/35886	0.38	1/56005 (0.0%)
33	1b	0.21	0/1881	0.47	0/2542
33	2b	0.26	0/1860	0.52	0/2518
34	1c	0.18	0/1572	0.39	0/2126
34	2c	0.23	0/1566	0.51	1/2119 (0.0%)
35	1d	0.20	0/1685	0.45	0/2262
35	2d	0.21	0/1704	0.46	0/2284
36	1e	0.22	0/1145	0.47	0/1543
36	2e	0.21	0/1149	0.48	0/1548
37	1f	0.18	0/823	0.39	0/1115
37	2f	0.20	0/829	0.43	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.20	0/1250	0.42	0/1679
38	2g	0.20	0/1254	0.41	0/1683
39	1h	0.19	0/1108	0.41	0/1494
39	2h	0.19	0/1108	0.43	0/1494
40	1i	0.21	0/1002	0.49	0/1346
40	2i	0.23	0/997	0.55	0/1343
41	1j	0.22	0/722	0.47	0/982
41	2j	0.21	0/727	0.46	0/988
42	1k	0.23	0/844	0.43	0/1145
42	2k	0.20	0/848	0.41	0/1149
43	1l	0.20	0/937	0.42	0/1260
43	2l	0.20	0/937	0.45	0/1260
44	1m	0.21	0/969	0.51	0/1302
44	2m	0.21	0/961	0.45	0/1291
45	1n	0.19	0/501	0.41	0/664
45	2n	0.20	0/501	0.45	0/664
46	1o	0.19	0/739	0.43	0/985
46	2o	0.18	0/739	0.40	0/985
47	1p	0.20	0/697	0.45	0/939
47	2p	0.19	0/693	0.49	0/935
48	1q	0.20	0/836	0.42	0/1117
48	2q	0.21	0/836	0.46	0/1117
49	1r	0.20	0/560	0.45	0/746
49	2r	0.19	0/560	0.47	0/746
50	1s	0.19	0/667	0.50	0/900
50	2s	0.24	0/661	0.58	2/893 (0.2%)
51	1t	0.21	0/730	0.48	0/965
51	2t	0.21	0/729	0.48	0/965
52	1u	0.19	0/203	0.43	0/266
52	2u	0.36	0/203	0.58	0/266
53	1v	0.23	0/319	0.40	0/495
53	2v	0.21	0/319	0.44	0/495
54	1w	0.32	2/1593 (0.1%)	0.39	0/2474
54	2w	0.36	2/1593 (0.1%)	0.52	0/2474
55	1x	0.27	0/1723	0.41	0/2684
55	2x	0.25	0/1723	0.40	0/2684
56	1z	0.54	0/16	0.89	0/19
56	2z	0.57	0/16	0.63	0/19
57	1y	0.31	1/1618 (0.1%)	0.45	0/2513
57	2y	0.35	2/1618 (0.1%)	0.53	0/2513
All	All	0.24	9/316807 (0.0%)	0.44	17/474290 (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
12	1Q	0	1
26	24	0	1
33	1b	0	1
33	2b	0	1
51	1t	0	1
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	46	G7M	O3'-P	6.04	1.62	1.56
54	2w	46	G7M	O3'-P	5.90	1.62	1.56
57	2y	46	G7M	O3'-P	5.57	1.61	1.56
1	1A	2552	OMU	O3'-P	5.55	1.61	1.56
54	2w	37	T6A	O3'-P	5.41	1.61	1.56

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2X	94	GLY	CA-C-N	8.05	136.18	121.70
19	2X	94	GLY	C-N-CA	8.05	136.18	121.70
34	2c	84	ILE	N-CA-C	-6.13	105.04	113.00
6	1G	96	ARG	CB-CA-C	-5.96	109.69	116.54
1	1A	1992	G	C2'-C3'-O3'	5.83	118.25	109.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	1Q	15	GLY	Peptide
33	1b	130	ARG	Peptide
51	1t	99	LEU	Peptide
26	24	59	PHE	Peptide
33	2b	118	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	31192	762	0
1	2A	60322	0	30422	849	0
2	1B	2577	0	1304	30	0
2	2B	2575	0	1303	61	0
3	1D	2136	0	2218	54	0
3	2D	2136	0	2218	55	0
4	1E	1559	0	1618	32	0
4	2E	1559	0	1618	49	0
5	1F	1584	0	1625	50	0
5	2F	1580	0	1619	55	0
6	1G	1423	0	1436	47	0
6	2G	1428	0	1438	73	0
7	1H	1330	0	1407	20	0
7	2H	1330	0	1407	48	0
8	1I	1097	0	1140	38	0
8	2I	1064	0	1082	55	0
9	1N	1117	0	1184	23	0
9	2N	1117	0	1184	33	0
10	1O	933	0	996	25	0
10	2O	933	0	996	33	0
11	1P	1135	0	1212	40	0
11	2P	1135	0	1212	44	0
12	1Q	1122	0	1179	30	0
12	2Q	1122	0	1179	47	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	20	0
14	1S	873	0	927	19	0
14	2S	870	0	923	54	0
15	1T	1091	0	1151	30	0
15	2T	1083	0	1136	38	0
16	1U	959	0	1019	20	0
16	2U	959	0	1019	30	0
17	1V	771	0	830	16	0
17	2V	771	0	830	29	0
18	1W	886	0	940	18	0
18	2W	886	0	940	15	0
19	1X	750	0	814	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	813	23	0
20	1Y	806	0	881	22	0
20	2Y	806	0	881	23	0
21	1Z	1240	0	1240	38	0
21	2Z	1271	0	1273	56	0
22	10	653	0	674	21	0
22	20	653	0	674	18	0
23	11	755	0	826	24	0
23	21	755	0	825	20	0
24	12	588	0	643	9	0
24	22	588	0	643	22	0
25	13	469	0	518	18	0
25	23	464	0	514	13	0
26	14	552	0	533	21	0
26	24	532	0	503	32	0
27	15	455	0	465	4	0
27	25	455	0	465	11	0
28	16	453	0	473	10	0
28	26	449	0	469	16	0
29	17	418	0	467	6	0
29	27	418	0	467	11	0
30	18	517	0	582	14	0
30	28	517	0	582	14	0
31	19	307	0	335	2	0
31	29	307	0	335	13	0
32	1a	32246	0	16293	497	0
32	2a	32327	0	16338	653	0
33	1b	1846	0	1867	68	0
33	2b	1825	0	1828	93	0
34	1c	1548	0	1535	43	0
34	2c	1542	0	1517	69	0
35	1d	1655	0	1672	56	0
35	2d	1674	0	1714	63	0
36	1e	1129	0	1185	43	0
36	2e	1133	0	1191	48	0
37	1f	810	0	804	22	0
37	2f	816	0	808	27	0
38	1g	1231	0	1238	31	0
38	2g	1235	0	1249	47	0
39	1h	1088	0	1126	31	0
39	2h	1088	0	1126	28	0
40	1i	983	0	986	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	978	0	966	53	0
41	1j	709	0	650	31	0
41	2j	714	0	672	39	0
42	1k	829	0	825	23	0
42	2k	833	0	834	26	0
43	1l	932	0	981	21	0
43	2l	932	0	981	32	0
44	1m	958	0	1002	40	0
44	2m	950	0	988	46	0
45	1n	492	0	529	21	0
45	2n	492	0	529	25	0
46	1o	728	0	760	21	0
46	2o	728	0	760	22	0
47	1p	681	0	697	33	0
47	2p	677	0	686	22	0
48	1q	823	0	891	24	0
48	2q	823	0	891	26	0
49	1r	555	0	618	20	0
49	2r	555	0	618	19	0
50	1s	652	0	662	21	0
50	2s	646	0	644	38	0
51	1t	728	0	798	29	0
51	2t	727	0	796	26	0
52	1u	199	0	208	9	0
52	2u	199	0	208	11	0
53	1v	283	0	142	8	0
53	2v	283	0	141	7	0
54	1w	1599	0	801	35	0
54	2w	1599	0	801	65	0
55	1x	1646	0	839	22	0
55	2x	1646	0	839	33	0
56	1z	27	0	28	1	0
56	2z	27	0	28	1	0
57	1y	1577	0	799	42	0
57	2y	1577	0	798	47	0
58	10	9	0	0	0	0
58	11	5	0	0	0	0
58	12	2	0	0	0	0
58	13	5	0	0	0	0
58	14	1	0	0	0	0
58	15	6	0	0	0	0
58	16	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	17	6	0	0	0	0
58	18	9	0	0	0	0
58	1A	1096	0	0	0	0
58	1B	37	0	0	0	0
58	1D	13	0	0	0	0
58	1E	16	0	0	0	0
58	1F	13	0	0	0	0
58	1G	5	0	0	0	0
58	1H	1	0	0	0	0
58	1I	1	0	0	0	0
58	1N	5	0	0	0	0
58	1O	4	0	0	0	0
58	1P	6	0	0	0	0
58	1Q	7	0	0	0	0
58	1R	4	0	0	0	0
58	1S	3	0	0	0	0
58	1T	2	0	0	0	0
58	1U	9	0	0	0	0
58	1V	9	0	0	0	0
58	1W	7	0	0	0	0
58	1X	5	0	0	0	0
58	1Y	3	0	0	0	0
58	1Z	2	0	0	0	0
58	1a	210	0	0	0	0
58	1b	1	0	0	0	0
58	1d	1	0	0	0	0
58	1e	2	0	0	0	0
58	1f	1	0	0	0	0
58	1k	1	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	1	0	0	0	0
58	1t	1	0	0	0	0
58	1v	1	0	0	0	0
58	1w	3	0	0	0	0
58	1x	11	0	0	0	0
58	20	4	0	0	0	0
58	23	4	0	0	0	0
58	25	5	0	0	0	0
58	27	3	0	0	0	0
58	28	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2A	863	0	0	0	0
58	2B	20	0	0	0	0
58	2D	7	0	0	0	0
58	2E	7	0	0	0	0
58	2F	7	0	0	0	0
58	2G	1	0	0	0	0
58	2O	2	0	0	0	0
58	2P	3	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	2	0	0	0	0
58	2V	2	0	0	0	0
58	2W	2	0	0	0	0
58	2X	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	230	0	0	0	0
58	2d	2	0	0	0	0
58	2e	1	0	0	0	0
58	2f	2	0	0	0	0
58	2g	1	0	0	0	0
58	2i	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	2n	1	0	0	0	0
58	2q	2	0	0	0	0
58	2r	1	0	0	0	0
58	2t	1	0	0	0	0
58	2v	4	0	0	0	0
58	2w	1	0	0	0	0
58	2x	6	0	0	0	0
58	2y	1	0	0	0	0
59	1A	1	0	0	0	0
59	2A	1	0	0	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	10	10	0	0	1	0
62	11	12	0	0	0	0
62	12	3	0	0	0	0
62	13	4	0	0	0	0
62	14	1	0	0	0	0
62	15	7	0	0	0	0
62	16	2	0	0	0	0
62	17	11	0	0	1	0
62	18	11	0	0	1	0
62	1A	1886	0	0	92	0
62	1B	61	0	0	1	0
62	1D	28	0	0	2	0
62	1E	29	0	0	2	0
62	1F	15	0	0	1	0
62	1G	3	0	0	0	0
62	1H	2	0	0	0	0
62	1I	1	0	0	0	0
62	1N	4	0	0	0	0
62	1O	4	0	0	0	0
62	1P	23	0	0	1	0
62	1Q	8	0	0	0	0
62	1R	16	0	0	2	0
62	1S	5	0	0	0	0
62	1T	8	0	0	0	0
62	1U	10	0	0	0	0
62	1V	11	0	0	1	0
62	1W	6	0	0	1	0
62	1X	7	0	0	0	0
62	1Y	1	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	308	0	0	25	0
62	1b	1	0	0	0	0
62	1e	1	0	0	0	0
62	1f	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1i	1	0	0	0	0
62	1l	7	0	0	0	0
62	1m	2	0	0	0	0
62	1o	1	0	0	0	0
62	1q	2	0	0	0	0
62	1u	1	0	0	0	0
62	1v	5	0	0	0	0
62	1w	8	0	0	1	0
62	1x	6	0	0	0	0
62	1y	1	0	0	0	0
62	1z	1	0	0	1	0
62	20	5	0	0	0	0
62	21	13	0	0	1	0
62	25	2	0	0	1	0
62	27	1	0	0	0	0
62	28	3	0	0	0	0
62	29	1	0	0	0	0
62	2A	1000	0	0	92	0
62	2B	22	0	0	3	0
62	2D	24	0	0	1	0
62	2E	9	0	0	1	0
62	2F	15	0	0	0	0
62	2N	1	0	0	0	0
62	2O	2	0	0	0	0
62	2P	11	0	0	1	0
62	2Q	1	0	0	0	0
62	2R	3	0	0	0	0
62	2T	5	0	0	0	0
62	2U	3	0	0	2	0
62	2W	3	0	0	0	0
62	2X	4	0	0	0	0
62	2Y	1	0	0	0	0
62	2Z	1	0	0	0	0
62	2a	198	0	0	20	0
62	2d	1	0	0	0	0
62	2e	1	0	0	0	0
62	2j	1	0	0	0	0
62	2l	4	0	0	1	0
62	2p	2	0	0	0	0
62	2r	1	0	0	0	0
62	2t	1	0	0	0	0
62	2v	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2w	3	0	0	0	0
62	2x	5	0	0	0	0
All	All	299808	0	196752	5317	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 11.

The worst 5 of 5317 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	1.22	1.38
54:2w:51:A:N6	54:2w:63:U:H3	1.37	1.22
54:2w:51:A:N6	54:2w:63:U:N3	1.94	1.14
1:1A:1082:U:O4	1:1A:1086:A:N1	1.87	1.06
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.44	0.99

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%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	246 (90%)	26 (10%)	1 (0%)	30	52
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	25	47
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	25	47
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	25	47
5	2F	201/210 (96%)	187 (93%)	12 (6%)	2 (1%)	13	29
6	1G	179/182 (98%)	165 (92%)	11 (6%)	3 (2%)	7	16
6	2G	179/182 (98%)	146 (82%)	29 (16%)	4 (2%)	5	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	1H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	22	43
7	2H	172/180 (96%)	153 (89%)	16 (9%)	3 (2%)	7	16
8	1I	144/148 (97%)	125 (87%)	19 (13%)	0	100	100
8	2I	144/148 (97%)	119 (83%)	20 (14%)	5 (4%)	3	4
9	1N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	19	38
9	2N	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	19	38
10	1O	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	7	16
10	2O	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
11	1P	147/150 (98%)	131 (89%)	10 (7%)	6 (4%)	2	3
11	2P	147/150 (98%)	126 (86%)	17 (12%)	4 (3%)	4	7
12	1Q	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	19	38
12	2Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	3 (3%)	1 (1%)	14	31
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	96 (89%)	9 (8%)	3 (3%)	4	7
15	1T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	16	34
15	2T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	2 (2%)	2 (2%)	6	12
17	2V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6	12
18	1W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	12	26
19	2X	93/96 (97%)	83 (89%)	9 (10%)	1 (1%)	12	26
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	148/206 (72%)	126 (85%)	21 (14%)	1 (1%)	19	38
21	2Z	156/206 (76%)	125 (80%)	27 (17%)	4 (3%)	4	7
22	10	81/85 (95%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	20	81/85 (95%)	73 (90%)	8 (10%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12	26
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12	26
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1
26	24	67/71 (94%)	47 (70%)	17 (25%)	3 (4%)	2	2
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	43 (84%)	8 (16%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	195 (85%)	23 (10%)	11 (5%)	2	2
33	2b	229/256 (90%)	182 (80%)	37 (16%)	10 (4%)	2	2
34	1c	204/239 (85%)	180 (88%)	21 (10%)	3 (2%)	8	18
34	2c	204/239 (85%)	160 (78%)	37 (18%)	7 (3%)	3	5
35	1d	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	25	47
35	2d	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	25	47
36	1e	146/162 (90%)	128 (88%)	16 (11%)	2 (1%)	9	19
36	2e	146/162 (90%)	124 (85%)	19 (13%)	3 (2%)	5	11
37	1f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	13	29
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	136 (89%)	16 (10%)	1 (1%)	19	38
38	2g	153/156 (98%)	135 (88%)	14 (9%)	4 (3%)	4	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
39	2h	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
40	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16	34
40	2i	125/128 (98%)	107 (86%)	16 (13%)	2 (2%)	8	17
41	1j	95/105 (90%)	77 (81%)	13 (14%)	5 (5%)	1	1
41	2j	94/105 (90%)	76 (81%)	15 (16%)	3 (3%)	3	5
42	1k	112/129 (87%)	98 (88%)	12 (11%)	2 (2%)	7	14
42	2k	112/129 (87%)	96 (86%)	12 (11%)	4 (4%)	3	4
43	1l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
43	2l	119/132 (90%)	101 (85%)	16 (13%)	2 (2%)	7	16
44	1m	121/126 (96%)	106 (88%)	13 (11%)	2 (2%)	7	16
44	2m	120/126 (95%)	101 (84%)	18 (15%)	1 (1%)	16	34
45	1n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
45	2n	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	16
46	1o	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	11	24
47	1p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
47	2p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	10	21
48	1q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
48	2q	97/105 (92%)	84 (87%)	12 (12%)	1 (1%)	13	29
49	1r	66/88 (75%)	58 (88%)	7 (11%)	1 (2%)	8	18
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
50	2s	81/93 (87%)	67 (83%)	13 (16%)	1 (1%)	11	24
51	1t	94/106 (89%)	82 (87%)	9 (10%)	3 (3%)	3	5
51	2t	94/106 (89%)	84 (89%)	8 (8%)	2 (2%)	5	11
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	1 (5%)	2 (10%)	0	0
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%)	10242 (90%)	989 (9%)	141 (1%)	11	24

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	38	GLN
23	11	3	LYS
26	14	49	PHE
36	1e	96	PRO

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%)	202 (94%)	13 (6%)	16	35
3	2D	215/218 (99%)	200 (93%)	15 (7%)	12	27
4	1E	164/166 (99%)	152 (93%)	12 (7%)	11	25
4	2E	164/166 (99%)	151 (92%)	13 (8%)	10	21
5	1F	160/166 (96%)	142 (89%)	18 (11%)	4	9
5	2F	159/166 (96%)	145 (91%)	14 (9%)	8	17
6	1G	143/156 (92%)	123 (86%)	20 (14%)	3	5
6	2G	143/156 (92%)	121 (85%)	22 (15%)	2	4
7	1H	144/148 (97%)	130 (90%)	14 (10%)	6	14
7	2H	144/148 (97%)	123 (85%)	21 (15%)	2	4
8	1I	113/124 (91%)	90 (80%)	23 (20%)	1	1
8	2I	105/124 (85%)	83 (79%)	22 (21%)	1	1
9	1N	118/119 (99%)	106 (90%)	12 (10%)	6	12
9	2N	118/119 (99%)	105 (89%)	13 (11%)	5	10
10	1O	100/100 (100%)	96 (96%)	4 (4%)	27	52
10	2O	100/100 (100%)	91 (91%)	9 (9%)	8	16
11	1P	115/116 (99%)	105 (91%)	10 (9%)	8	17
11	2P	115/116 (99%)	99 (86%)	16 (14%)	3	5
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	8	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	8	16
13	1R	101/101 (100%)	94 (93%)	7 (7%)	13	28
13	2R	101/101 (100%)	95 (94%)	6 (6%)	16	35
14	1S	86/88 (98%)	76 (88%)	10 (12%)	4	9
14	2S	85/88 (97%)	67 (79%)	18 (21%)	1	1
15	1T	115/127 (91%)	104 (90%)	11 (10%)	7	14
15	2T	113/127 (89%)	107 (95%)	6 (5%)	19	40
16	1U	93/94 (99%)	88 (95%)	5 (5%)	18	39
16	2U	93/94 (99%)	81 (87%)	12 (13%)	3	6
17	1V	80/82 (98%)	76 (95%)	4 (5%)	20	43
17	2V	80/82 (98%)	70 (88%)	10 (12%)	3	7
18	1W	90/92 (98%)	86 (96%)	4 (4%)	24	48
18	2W	90/92 (98%)	84 (93%)	6 (7%)	13	29
19	1X	77/78 (99%)	73 (95%)	4 (5%)	19	41
19	2X	77/78 (99%)	72 (94%)	5 (6%)	14	31
20	1Y	85/91 (93%)	72 (85%)	13 (15%)	2	4
20	2Y	85/91 (93%)	68 (80%)	17 (20%)	1	2
21	1Z	135/179 (75%)	110 (82%)	25 (18%)	1	2
21	2Z	137/179 (76%)	112 (82%)	25 (18%)	1	2
22	10	65/67 (97%)	62 (95%)	3 (5%)	23	46
22	20	65/67 (97%)	60 (92%)	5 (8%)	10	22
23	11	80/83 (96%)	75 (94%)	5 (6%)	15	32
23	21	80/83 (96%)	71 (89%)	9 (11%)	4	9
24	12	65/67 (97%)	58 (89%)	7 (11%)	5	10
24	22	65/67 (97%)	58 (89%)	7 (11%)	5	10
25	13	51/52 (98%)	47 (92%)	4 (8%)	10	22
25	23	50/52 (96%)	46 (92%)	4 (8%)	10	21
26	14	59/63 (94%)	49 (83%)	10 (17%)	1	3
26	24	53/63 (84%)	45 (85%)	8 (15%)	2	4
27	15	50/52 (96%)	46 (92%)	4 (8%)	10	21
27	25	50/52 (96%)	46 (92%)	4 (8%)	10	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	16	51/52 (98%)	45 (88%)	6 (12%)	4	8
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	5
29	17	41/42 (98%)	37 (90%)	4 (10%)	6	13
29	27	41/42 (98%)	36 (88%)	5 (12%)	4	8
30	18	54/55 (98%)	51 (94%)	3 (6%)	17	38
30	28	54/55 (98%)	51 (94%)	3 (6%)	17	38
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	64
31	29	34/34 (100%)	31 (91%)	3 (9%)	8	17
33	1b	192/220 (87%)	161 (84%)	31 (16%)	2	3
33	2b	187/220 (85%)	146 (78%)	41 (22%)	1	1
34	1c	142/188 (76%)	124 (87%)	18 (13%)	3	7
34	2c	140/188 (74%)	120 (86%)	20 (14%)	2	5
35	1d	169/181 (93%)	142 (84%)	27 (16%)	2	3
35	2d	173/181 (96%)	150 (87%)	23 (13%)	3	6
36	1e	113/123 (92%)	101 (89%)	12 (11%)	5	11
36	2e	114/123 (93%)	100 (88%)	14 (12%)	4	8
37	1f	84/90 (93%)	75 (89%)	9 (11%)	5	11
37	2f	85/90 (94%)	74 (87%)	11 (13%)	3	6
38	1g	119/127 (94%)	106 (89%)	13 (11%)	5	10
38	2g	120/127 (94%)	104 (87%)	16 (13%)	3	6
39	1h	114/119 (96%)	105 (92%)	9 (8%)	10	21
39	2h	114/119 (96%)	100 (88%)	14 (12%)	4	8
40	1i	90/99 (91%)	78 (87%)	12 (13%)	3	6
40	2i	89/99 (90%)	82 (92%)	7 (8%)	10	21
41	1j	66/92 (72%)	59 (89%)	7 (11%)	5	11
41	2j	69/92 (75%)	55 (80%)	14 (20%)	1	1
42	1k	82/99 (83%)	71 (87%)	11 (13%)	3	6
42	2k	83/99 (84%)	78 (94%)	5 (6%)	16	35
43	1l	96/108 (89%)	92 (96%)	4 (4%)	25	50
43	2l	96/108 (89%)	86 (90%)	10 (10%)	5	11
44	1m	93/101 (92%)	82 (88%)	11 (12%)	4	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	2m	92/101 (91%)	78 (85%)	14 (15%)	2	4
45	1n	49/50 (98%)	45 (92%)	4 (8%)	9	20
45	2n	49/50 (98%)	42 (86%)	7 (14%)	2	5
46	1o	78/80 (98%)	71 (91%)	7 (9%)	8	16
46	2o	78/80 (98%)	73 (94%)	5 (6%)	14	32
47	1p	69/74 (93%)	59 (86%)	10 (14%)	2	4
47	2p	68/74 (92%)	62 (91%)	6 (9%)	8	17
48	1q	94/97 (97%)	84 (89%)	10 (11%)	5	11
48	2q	94/97 (97%)	85 (90%)	9 (10%)	7	14
49	1r	59/77 (77%)	53 (90%)	6 (10%)	6	12
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	5
50	1s	69/80 (86%)	63 (91%)	6 (9%)	8	17
50	2s	67/80 (84%)	53 (79%)	14 (21%)	1	1
51	1t	70/82 (85%)	61 (87%)	9 (13%)	3	6
51	2t	70/82 (85%)	61 (87%)	9 (13%)	3	6
52	1u	18/22 (82%)	16 (89%)	2 (11%)	5	10
52	2u	18/22 (82%)	17 (94%)	1 (6%)	17	38
56	1z	2/2 (100%)	2 (100%)	0	100	100
56	2z	2/2 (100%)	2 (100%)	0	100	100
All	All	9307/10068 (92%)	8260 (89%)	1047 (11%)	5	9

5 of 1047 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	2h	26	VAL
41	2j	58	ASP
39	2h	11	THR
51	2t	45	GLN
40	1i	25	LYS

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	42	GLN

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Mol	Chain	Res	Type
50	2s	83	HIS
35	2d	129	ASN
40	2i	87	GLN
35	1d	161	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	494 (17%)	22 (0%)
1	2A	2791/2915 (95%)	522 (18%)	27 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	118/121 (97%)	33 (27%)	0
32	1a	1497/1521 (98%)	273 (18%)	0
32	2a	1501/1521 (98%)	335 (22%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1w	71/76 (93%)	32 (45%)	0
54	2w	71/76 (93%)	38 (53%)	0
55	1x	75/77 (97%)	14 (18%)	0
55	2x	75/77 (97%)	15 (20%)	0
57	1y	72/76 (94%)	35 (48%)	0
57	2y	72/76 (94%)	41 (56%)	0
All	All	9350/9620 (97%)	1850 (19%)	49 (0%)

5 of 1850 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	34	C
1	1A	45	C
1	1A	50	U
1	1A	55	G

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	277	C
1	2A	1026	U
1	2A	528	A
1	2A	827	U
1	2A	1275	A

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
32	PSU	1a	516	58,32	18,21,22	1.44	3 (16%)	21,30,33	1.95	5 (23%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	0.95	1 (4%)
32	5MC	2a	967	58,32	19,22,23	1.88	3 (15%)	26,32,35	1.17	3 (11%)
32	UR3	2a	1498	32	19,22,23	1.02	2 (10%)	26,32,35	1.73	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.10	2 (7%)
57	G7M	2y	46	57	20,26,27	1.37	2 (10%)	16,39,42	0.69	0
57	PSU	1y	39	57	18,21,22	1.34	2 (11%)	21,30,33	2.04	3 (14%)
54	U8U	1w	34	54,53	20,24,25	1.38	2 (10%)	22,34,37	1.34	4 (18%)
54	T6A	2w	37	54,53	26,34,35	0.98	2 (7%)	28,49,52	1.81	5 (17%)
1	OMG	1A	2251	55,58,1	19,26,27	0.94	1 (5%)	21,38,41	1.19	3 (14%)
32	M2G	1a	966	32	20,27,28	1.28	3 (15%)	19,40,43	0.96	1 (5%)
32	4OC	2a	1402	58,32	20,23,24	0.78	0	25,32,35	1.13	3 (12%)
54	5MU	2w	54	54	19,22,23	1.45	5 (26%)	27,32,35	1.67	5 (18%)
55	4SU	2x	8	55	18,21,22	2.25	5 (27%)	25,30,33	1.55	6 (24%)
54	A1B8A	1w	76	54	26,33,34	1.30	4 (15%)	23,46,49	1.50	1 (4%)
1	5MC	1A	1962	58,1	19,22,23	1.79	3 (15%)	26,32,35	1.18	3 (11%)
57	PSU	2y	55	57	18,21,22	1.42	2 (11%)	21,30,33	2.10	3 (14%)
1	PSU	1A	1917	1	18,21,22	1.37	3 (16%)	21,30,33	1.96	4 (19%)
55	PSU	1x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.13	4 (19%)
1	OMU	2A	2552	58,1	19,22,23	1.20	2 (10%)	25,31,34	1.77	5 (20%)
1	OMC	1A	1920	1	19,22,23	0.83	0	25,31,34	1.05	2 (8%)
32	M2G	2a	966	32	20,27,28	1.41	3 (15%)	19,40,43	1.01	1 (5%)
57	G7M	1y	46	57	20,26,27	1.35	2 (10%)	16,39,42	0.64	0
1	5MU	1A	1939	1	19,22,23	1.39	5 (26%)	27,32,35	2.17	7 (25%)
55	4SU	1x	8	55	18,21,22	2.28	5 (27%)	25,30,33	1.53	6 (24%)
32	G7M	2a	527	58,32	20,26,27	1.25	2 (10%)	16,39,42	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	2A	1939	1	19,22,23	1.40	5 (26%)	27,32,35	2.23	6 (22%)
32	MA6	1a	1519	32	19,26,27	1.05	2 (10%)	18,38,41	1.96	3 (16%)
55	5MU	1x	54	55	19,22,23	1.45	5 (26%)	27,32,35	1.89	6 (22%)
1	OMU	1A	2552	58,1	19,22,23	1.18	3 (15%)	25,31,34	1.85	5 (20%)
57	5MU	1y	54	57	19,22,23	1.36	5 (26%)	27,32,35	2.03	6 (22%)
1	5MC	2A	1962	58,1	19,22,23	1.58	3 (15%)	26,32,35	1.15	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.71	3 (15%)	26,32,35	1.27	3 (11%)
54	A1B8A	2w	76	54	26,33,34	1.22	3 (11%)	23,46,49	1.57	1 (4%)
57	T6A	2y	37	57,32	17,24,35	0.83	1 (5%)	16,35,52	1.25	2 (12%)
32	5MC	2a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.12	2 (7%)
57	U8U	1y	34	57	17,21,25	1.59	3 (17%)	21,30,37	1.46	3 (14%)
1	OMC	2A	1920	1	19,22,23	0.78	0	25,31,34	0.75	0
32	5MC	2a	1400	32	19,22,23	1.83	3 (15%)	26,32,35	1.24	4 (15%)
32	MA6	2a	1518	32	19,26,27	1.00	2 (10%)	18,38,41	1.96	3 (16%)
54	5MU	1w	54	54	19,22,23	1.39	5 (26%)	27,32,35	2.11	6 (22%)
56	FME	1z	1	56	8,9,10	1.03	0	8,9,11	1.24	2 (25%)
55	8AN	1x	76	58,55	17,24,25	1.18	2 (11%)	13,35,38	2.95	2 (15%)
54	PSU	2w	55	54	18,21,22	1.36	2 (11%)	21,30,33	1.99	4 (19%)
1	PSU	1A	2605	58,1	18,21,22	1.40	4 (22%)	21,30,33	2.10	3 (14%)
32	PSU	2a	516	58,32	18,21,22	1.41	3 (16%)	21,30,33	2.12	4 (19%)
57	5MU	2y	54	57	19,22,23	1.43	6 (31%)	27,32,35	2.11	6 (22%)
32	2MG	1a	1207	58,32	18,26,27	0.92	1 (5%)	16,38,41	1.46	4 (25%)
55	5MU	2x	54	55	19,22,23	1.36	4 (21%)	27,32,35	2.17	6 (22%)
54	U8U	2w	34	54,53	20,24,25	1.30	2 (10%)	22,34,37	1.07	2 (9%)
57	PSU	1y	55	57	18,21,22	1.40	2 (11%)	21,30,33	1.95	3 (14%)
32	5MC	1a	967	32	19,22,23	1.51	3 (15%)	26,32,35	1.14	2 (7%)
32	5MC	1a	1404	32	19,22,23	1.77	3 (15%)	26,32,35	1.13	2 (7%)
55	5MC	2x	32	55	19,22,23	1.70	3 (15%)	26,32,35	1.20	3 (11%)
1	2MA	2A	2503	58,1	18,25,26	0.69	0	20,37,40	1.93	3 (15%)
1	2MA	1A	2503	58,1	18,25,26	0.72	0	20,37,40	2.04	4 (20%)
57	T6A	1y	37	57	17,24,35	0.80	1 (5%)	16,35,52	1.30	2 (12%)
1	5MU	2A	1915	1	19,22,23	1.45	5 (26%)	27,32,35	2.07	6 (22%)
32	5MC	2a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.24	3 (11%)
55	PSU	2x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.07	4 (19%)
54	PSU	2w	39	54	18,21,22	1.31	2 (11%)	21,30,33	2.26	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
55	8AN	2x	76	58,55	17,24,25	1.15	2 (11%)	13,35,38	3.82	3 (23%)
56	FME	2z	1	56	8,9,10	0.99	0	8,9,11	1.04	1 (12%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.01	3 (14%)
32	2MG	2a	1207	32	18,26,27	0.94	1 (5%)	16,38,41	1.46	3 (18%)
57	U8U	2y	34	57,53	17,21,25	1.57	4 (23%)	21,30,37	1.54	3 (14%)
54	PSU	1w	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.91	4 (19%)
1	PSU	2A	2605	1	18,21,22	1.36	2 (11%)	21,30,33	1.85	4 (19%)
32	MA6	1a	1518	32	19,26,27	1.04	2 (10%)	18,38,41	1.88	3 (16%)
43	0TD	1l	92	43	8,9,10	4.39	1 (12%)	6,11,13	4.50	2 (33%)
54	T6A	1w	37	54	26,34,35	1.01	1 (3%)	28,49,52	1.86	4 (14%)
32	G7M	1a	527	58,32	20,26,27	1.13	1 (5%)	16,39,42	0.74	0
54	PSU	1w	55	54	18,21,22	1.39	2 (11%)	21,30,33	1.97	3 (14%)
1	5MU	1A	1915	1	19,22,23	1.37	5 (26%)	27,32,35	2.04	7 (25%)
54	G7M	1w	46	54	20,26,27	1.20	1 (5%)	16,39,42	0.81	0
54	G7M	2w	46	54	20,26,27	1.20	1 (5%)	16,39,42	0.88	0
55	5MC	1x	32	55	19,22,23	1.67	3 (15%)	26,32,35	1.25	3 (11%)
32	UR3	1a	1498	32	19,22,23	1.00	2 (10%)	26,32,35	1.78	4 (15%)
43	0TD	2l	92	43	8,9,10	4.46	1 (12%)	6,11,13	5.24	1 (16%)
32	MA6	2a	1519	32	19,26,27	1.00	2 (10%)	18,38,41	1.91	3 (16%)
1	5MC	1A	1942	1	19,22,23	1.67	3 (15%)	26,32,35	1.29	5 (19%)
1	OMG	2A	2251	55,1	19,26,27	0.89	1 (5%)	21,38,41	1.08	2 (9%)
57	PSU	2y	39	57	18,21,22	1.36	2 (11%)	21,30,33	1.95	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.98	3 (14%)
32	5MC	1a	1400	32	19,22,23	1.58	3 (15%)	26,32,35	1.13	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	1a	516	58,32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	2a	967	58,32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	G7M	2y	46	57	-	2/3/25/26	0/3/3/3
57	PSU	1y	39	57	-	0/7/25/26	0/2/2/2
54	U8U	1w	34	54,53	-	2/10/28/29	0/2/2/2
54	T6A	2w	37	54,53	-	4/19/41/42	0/3/3/3
1	OMG	1A	2251	55,58,1	-	0/5/27/28	0/3/3/3
32	M2G	1a	966	32	-	1/7/29/30	0/3/3/3
32	4OC	2a	1402	58,32	-	3/9/29/30	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
54	A1B8A	1w	76	54	-	2/16/38/39	0/3/3/3
1	5MC	1A	1962	58,1	-	1/7/25/26	0/2/2/2
57	PSU	2y	55	57	-	2/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	58,1	-	0/9/27/28	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
57	G7M	1y	46	57	-	1/3/25/26	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	58,32	-	3/3/25/26	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	58,1	-	0/9/27/28	0/2/2/2
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	58,1	-	4/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	A1B8A	2w	76	54	-	2/16/38/39	0/3/3/3
57	T6A	2y	37	57,32	-	0/3/25/42	0/3/3/3
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
57	U8U	1y	34	57	-	0/7/25/29	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	2a	1400	32	-	4/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
54	5MU	1w	54	54	-	1/7/25/26	0/2/2/2
56	FME	1z	1	56	-	4/7/9/11	-
55	8AN	1x	76	58,55	-	3/3/25/26	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2605	58,1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	58,32	-	0/7/25/26	0/2/2/2
57	5MU	2y	54	57	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	58,32	-	0/5/27/28	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	U8U	2w	34	54,53	-	2/10/28/29	0/2/2/2
57	PSU	1y	55	57	-	1/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	58,1	-	1/3/25/26	0/3/3/3
1	2MA	1A	2503	58,1	-	1/3/25/26	0/3/3/3
57	T6A	1y	37	57	-	1/3/25/42	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	58,55	-	0/3/25/26	0/3/3/3
56	FME	2z	1	56	-	2/7/9/11	-
1	PSU	2A	1917	1	-	2/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
57	U8U	2y	34	57,53	-	1/7/25/29	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
43	0TD	1l	92	43	-	3/7/12/14	-
54	T6A	1w	37	54	-	6/19/41/42	0/3/3/3
32	G7M	1a	527	58,32	-	2/3/25/26	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	2/3/25/26	0/3/3/3
54	G7M	2w	46	54	-	1/3/25/26	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	1/5/27/28	0/3/3/3
57	PSU	2y	39	57	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2

The worst 5 of 208 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.21	1.70	1.82
43	1l	92	0TD	CB-SB	-11.90	1.70	1.82
32	2a	967	5MC	C5-C4	7.05	1.49	1.44
32	2a	1400	5MC	C5-C4	6.88	1.49	1.44
1	1A	1962	5MC	C5-C4	6.79	1.49	1.44

The worst 5 of 272 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-12.58	79.76	102.36
43	1l	92	0TD	CSB-SB-CB	-10.57	83.37	102.36
55	2x	76	8AN	O4'-C1'-N9	9.13	120.85	108.75
55	1x	76	8AN	C4'-O4'-C1'	-7.79	102.79	109.92
55	2x	76	8AN	C4'-O4'-C1'	-7.50	103.06	109.92

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

51 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1402	4OC	2	0
32	2a	967	5MC	1	0
1	2A	1942	5MC	1	0
57	2y	46	G7M	1	0
57	1y	39	PSU	1	0
54	1w	34	U8U	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2w	37	T6A	1	0
1	1A	2251	OMG	1	0
32	2a	1402	4OC	3	0
54	2w	54	5MU	1	0
55	2x	8	4SU	1	0
54	1w	76	A1B8A	3	0
57	2y	55	PSU	2	0
1	1A	1917	PSU	1	0
1	2A	2552	OMU	2	0
1	1A	1939	5MU	2	0
55	1x	8	4SU	1	0
1	2A	1939	5MU	2	0
32	1a	1519	MA6	2	0
1	1A	2552	OMU	1	0
57	1y	54	5MU	2	0
54	2w	76	A1B8A	1	0
57	2y	37	T6A	1	0
32	2a	1404	5MC	1	0
1	2A	1920	OMC	1	0
32	2a	1400	5MC	1	0
32	2a	1518	MA6	3	0
54	1w	54	5MU	1	0
55	1x	76	8AN	2	0
32	2a	516	PSU	2	0
55	2x	54	5MU	1	0
54	2w	34	U8U	1	0
57	1y	55	PSU	2	0
32	1a	1404	5MC	1	0
55	2x	32	5MC	2	0
1	2A	2503	2MA	3	0
57	1y	37	T6A	4	0
55	2x	55	PSU	2	0
54	2w	39	PSU	2	0
1	1A	1911	PSU	1	0
55	2x	76	8AN	2	0
56	2z	1	FME	1	0
32	2a	1207	2MG	2	0
57	2y	34	U8U	1	0
32	1a	1518	MA6	2	0
54	1w	37	T6A	1	0
54	1w	55	PSU	2	0
54	2w	46	G7M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	2l	92	0TD	1	0
32	2a	1519	MA6	2	0
1	2A	2251	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2750 ligands modelled in this entry, 2748 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	SF4	1d	302	35	0,12,12	-	-	-		
61	SF4	2d	303	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	1d	302	35	-	-	0/6/5/5
61	SF4	2d	303	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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%)	-0.58	93 (3%)	49	43	18, 36, 91, 104	0
1	2A	2789/2915 (95%)	-0.04	84 (3%)	52	46	32, 58, 88, 103	0
2	1B	120/121 (99%)	-0.50	1 (0%)	82	79	29, 49, 62, 81	0
2	2B	120/121 (99%)	0.78	8 (6%)	25	20	61, 78, 85, 93	0
3	1D	275/276 (99%)	-0.35	1 (0%)	89	86	19, 37, 50, 71	0
3	2D	275/276 (99%)	0.15	4 (1%)	71	67	30, 50, 63, 80	0
4	1E	204/206 (99%)	-0.27	1 (0%)	87	84	17, 42, 58, 69	0
4	2E	204/206 (99%)	0.16	2 (0%)	79	75	36, 57, 69, 78	0
5	1F	203/210 (96%)	-0.28	0	100	100	18, 43, 66, 78	0
5	2F	203/210 (96%)	0.34	2 (0%)	79	75	37, 66, 77, 82	0
6	1G	181/182 (99%)	0.25	3 (1%)	69	64	39, 57, 70, 80	0
6	2G	181/182 (99%)	1.05	20 (11%)	12	9	64, 77, 82, 92	0
7	1H	174/180 (96%)	0.10	1 (0%)	85	83	38, 51, 64, 68	0
7	2H	174/180 (96%)	0.74	3 (1%)	69	64	67, 77, 84, 87	0
8	1I	146/148 (98%)	0.49	4 (2%)	56	50	44, 70, 79, 82	0
8	2I	146/148 (98%)	1.52	47 (32%)	1	1	52, 79, 87, 92	0
9	1N	140/140 (100%)	-0.21	0	100	100	24, 40, 56, 73	0
9	2N	140/140 (100%)	0.46	4 (2%)	54	48	44, 63, 75, 79	0
10	1O	122/122 (100%)	-0.23	1 (0%)	82	79	26, 41, 57, 63	0
10	2O	122/122 (100%)	0.25	0	100	100	44, 56, 68, 73	0
11	1P	149/150 (99%)	-0.15	0	100	100	20, 45, 64, 73	0
11	2P	149/150 (99%)	0.42	4 (2%)	56	50	38, 66, 77, 85	0
12	1Q	141/141 (100%)	-0.19	2 (1%)	73	68	23, 40, 54, 67	0
12	2Q	141/141 (100%)	0.69	5 (3%)	47	41	49, 64, 73, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.38	0 100 100	26, 35, 46, 55	0
13	2R	118/118 (100%)	0.06	2 (1%) 69 64	38, 52, 60, 66	0
14	1S	110/112 (98%)	-0.10	0 100 100	36, 48, 59, 64	0
14	2S	110/112 (98%)	1.10	17 (15%) 6 5	62, 72, 78, 82	0
15	1T	131/146 (89%)	0.01	2 (1%) 71 67	32, 46, 69, 74	0
15	2T	131/146 (89%)	0.30	1 (0%) 82 79	48, 59, 71, 75	0
16	1U	116/118 (98%)	-0.46	0 100 100	21, 32, 48, 55	0
16	2U	116/118 (98%)	0.20	0 100 100	45, 61, 73, 75	0
17	1V	101/101 (100%)	-0.34	0 100 100	21, 41, 57, 65	0
17	2V	101/101 (100%)	0.58	5 (4%) 35 30	45, 69, 75, 82	0
18	1W	112/113 (99%)	-0.46	0 100 100	24, 33, 51, 73	0
18	2W	112/113 (99%)	0.27	2 (1%) 67 62	35, 52, 64, 84	0
19	1X	95/96 (98%)	-0.28	1 (1%) 77 74	26, 38, 57, 64	0
19	2X	95/96 (98%)	0.37	1 (1%) 77 74	44, 58, 72, 78	0
20	1Y	107/110 (97%)	0.12	0 100 100	35, 49, 65, 76	0
20	2Y	107/110 (97%)	0.93	12 (11%) 11 9	60, 69, 78, 82	0
21	1Z	154/206 (74%)	0.61	14 (9%) 16 13	40, 61, 82, 94	0
21	2Z	160/206 (77%)	1.11	19 (11%) 10 8	64, 77, 86, 94	0
22	10	83/85 (97%)	-0.06	3 (3%) 46 40	27, 38, 62, 69	0
22	20	83/85 (97%)	0.92	8 (9%) 15 12	45, 64, 71, 84	0
23	11	97/98 (98%)	-0.07	1 (1%) 79 75	26, 45, 67, 71	0
23	21	97/98 (98%)	0.22	2 (2%) 63 58	40, 56, 70, 75	0
24	12	70/72 (97%)	-0.06	1 (1%) 73 68	35, 49, 57, 72	0
24	22	70/72 (97%)	0.64	0 100 100	59, 68, 75, 76	0
25	13	59/60 (98%)	-0.37	0 100 100	26, 37, 57, 64	0
25	23	59/60 (98%)	0.34	0 100 100	52, 63, 74, 77	0
26	14	69/71 (97%)	0.62	7 (10%) 14 12	55, 73, 85, 92	0
26	24	69/71 (97%)	1.15	7 (10%) 14 12	71, 82, 89, 94	0
27	15	59/60 (98%)	-0.47	1 (1%) 69 64	20, 33, 53, 66	0
27	25	59/60 (98%)	0.09	0 100 100	38, 51, 63, 77	0
28	16	53/54 (98%)	-0.35	0 100 100	32, 41, 53, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.56	1 (1%) 66 61	52, 62, 67, 73	0
29	17	48/49 (97%)	-0.43	0 100 100	21, 26, 52, 59	0
29	27	48/49 (97%)	-0.06	1 (2%) 63 58	35, 43, 60, 70	0
30	18	64/65 (98%)	-0.25	0 100 100	28, 34, 42, 52	0
30	28	64/65 (98%)	0.56	1 (1%) 70 65	45, 56, 62, 69	0
31	19	37/37 (100%)	-0.34	0 100 100	29, 40, 60, 60	0
31	29	37/37 (100%)	1.01	2 (5%) 32 27	58, 65, 73, 75	0
32	1a	1488/1521 (97%)	0.21	30 (2%) 64 59	33, 66, 88, 100	0
32	2a	1491/1521 (98%)	0.52	64 (4%) 40 34	53, 77, 92, 102	0
33	1b	231/256 (90%)	0.70	18 (7%) 20 17	61, 75, 83, 86	0
33	2b	231/256 (90%)	1.18	38 (16%) 5 4	71, 81, 87, 90	0
34	1c	206/239 (86%)	0.57	8 (3%) 44 38	57, 69, 77, 84	0
34	2c	206/239 (86%)	1.41	48 (23%) 2 2	71, 82, 86, 90	0
35	1d	208/209 (99%)	0.74	16 (7%) 21 17	54, 67, 76, 80	0
35	2d	208/209 (99%)	0.90	16 (7%) 21 17	61, 71, 78, 85	0
36	1e	148/162 (91%)	0.29	0 100 100	52, 62, 69, 79	0
36	2e	148/162 (91%)	1.00	15 (10%) 14 12	65, 75, 81, 88	0
37	1f	100/101 (99%)	0.37	2 (2%) 64 59	55, 65, 73, 76	0
37	2f	100/101 (99%)	0.42	2 (2%) 64 59	61, 71, 77, 79	0
38	1g	155/156 (99%)	0.51	8 (5%) 34 28	58, 69, 82, 87	0
38	2g	155/156 (99%)	1.07	22 (14%) 7 6	70, 78, 84, 87	0
39	1h	137/138 (99%)	0.47	2 (1%) 71 67	56, 65, 73, 76	0
39	2h	137/138 (99%)	1.01	9 (6%) 26 21	66, 74, 79, 83	0
40	1i	127/128 (99%)	0.91	7 (5%) 32 26	57, 73, 79, 82	0
40	2i	127/128 (99%)	1.34	22 (17%) 5 4	71, 80, 86, 88	0
41	1j	97/105 (92%)	0.92	5 (5%) 34 28	57, 74, 82, 85	0
41	2j	96/105 (91%)	1.39	21 (21%) 3 2	67, 81, 87, 89	0
42	1k	114/129 (88%)	0.66	4 (3%) 47 41	44, 66, 77, 82	0
42	2k	114/129 (88%)	0.77	4 (3%) 47 41	60, 73, 79, 82	0
43	1l	121/132 (91%)	0.37	5 (4%) 42 36	45, 58, 66, 72	0
43	2l	121/132 (91%)	0.59	7 (5%) 30 24	55, 69, 75, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.62	7 (5%) 30 25	56, 68, 77, 89	0
44	2m	122/126 (96%)	1.49	26 (21%) 3 2	70, 80, 86, 88	0
45	1n	60/61 (98%)	0.78	4 (6%) 25 20	58, 65, 71, 72	0
45	2n	60/61 (98%)	1.58	17 (28%) 1 1	70, 81, 85, 88	0
46	1o	88/89 (98%)	0.49	1 (1%) 77 74	49, 63, 73, 80	0
46	2o	88/89 (98%)	0.62	1 (1%) 77 74	62, 71, 79, 82	0
47	1p	82/88 (93%)	1.09	13 (15%) 6 5	58, 71, 76, 84	0
47	2p	82/88 (93%)	0.57	3 (3%) 45 39	53, 68, 74, 76	0
48	1q	99/105 (94%)	0.71	6 (6%) 28 23	56, 66, 74, 77	0
48	2q	99/105 (94%)	0.73	3 (3%) 52 46	60, 70, 77, 79	0
49	1r	68/88 (77%)	0.38	2 (2%) 54 48	53, 65, 74, 78	0
49	2r	68/88 (77%)	0.42	0 100 100	64, 71, 78, 81	0
50	1s	83/93 (89%)	0.58	2 (2%) 59 54	62, 71, 79, 83	0
50	2s	83/93 (89%)	1.61	24 (28%) 1 1	76, 83, 89, 91	0
51	1t	96/106 (90%)	0.86	7 (7%) 22 18	59, 68, 75, 79	0
51	2t	96/106 (90%)	0.47	4 (4%) 41 35	56, 68, 78, 82	0
52	1u	23/27 (85%)	1.04	2 (8%) 17 14	59, 67, 72, 75	0
52	2u	23/27 (85%)	2.01	11 (47%) 0 0	74, 77, 81, 81	0
53	1v	13/24 (54%)	1.53	5 (38%) 1 1	48, 77, 88, 91	0
53	2v	13/24 (54%)	2.05	4 (30%) 1 1	72, 87, 94, 96	0
54	1w	67/76 (88%)	1.57	19 (28%) 1 1	63, 95, 99, 102	0
54	2w	67/76 (88%)	1.99	32 (47%) 0 0	80, 96, 101, 104	0
55	1x	72/77 (93%)	0.50	2 (2%) 55 49	30, 63, 78, 84	0
55	2x	72/77 (93%)	0.92	7 (9%) 15 12	49, 79, 86, 93	0
56	1z	2/3 (66%)	0.54	0 100 100	39, 39, 39, 40	0
56	2z	2/3 (66%)	0.64	0 100 100	53, 53, 53, 58	0
57	1y	68/76 (89%)	1.64	20 (29%) 1 1	54, 95, 100, 102	0
57	2y	68/76 (89%)	1.74	22 (32%) 1 1	68, 96, 100, 102	0
All	All	20884/21754 (96%)	0.26	1018 (4%) 36 30	17, 63, 87, 104	0

The worst 5 of 1018 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	10.9
45	1n	2	ALA	7.0
44	2m	123	ALA	6.6
44	1m	123	ALA	6.1
21	2Z	174	VAL	5.8

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	0.27	0.17	93,100,111,117	0
57	G7M	2y	46	24/25	0.42	0.15	89,98,109,123	0
54	G7M	2w	46	24/25	0.44	0.15	88,97,107,115	0
54	G7M	1w	46	24/25	0.45	0.15	80,94,105,110	0
54	5MU	2w	54	21/22	0.52	0.18	83,96,102,106	0
54	PSU	1w	55	20/21	0.57	0.17	82,96,103,105	0
57	U8U	2y	34	20/24	0.57	0.24	93,100,106,118	0
57	G7M	1y	46	24/25	0.60	0.15	86,93,98,107	0
57	PSU	2y	55	20/21	0.61	0.14	83,95,103,115	0
57	5MU	2y	54	21/22	0.63	0.14	88,95,104,117	0
57	PSU	2y	39	20/21	0.64	0.15	89,92,102,108	0
57	T6A	1y	37	22/33	0.66	0.16	81,91,100,107	0
57	PSU	1y	39	20/21	0.67	0.14	84,92,101,107	0
57	U8U	1y	34	20/24	0.69	0.17	82,92,98,102	0
57	PSU	1y	55	20/21	0.70	0.14	91,94,102,104	0
57	T6A	2y	37	22/33	0.72	0.17	85,93,99,105	0
54	U8U	1w	34	23/24	0.75	0.17	64,83,93,99	0
1	5MU	2A	1915	21/22	0.76	0.18	79,84,89,96	0
54	T6A	2w	37	32/33	0.76	0.17	71,91,100,108	0
54	5MU	1w	54	21/22	0.76	0.13	80,89,93,94	0
57	5MU	1y	54	21/22	0.78	0.12	83,91,96,103	0
54	U8U	2w	34	23/24	0.81	0.16	82,87,92,96	0
54	T6A	1w	37	32/33	0.82	0.14	70,79,82,83	0
32	2MG	2a	1207	24/25	0.83	0.13	78,83,89,94	0
54	PSU	2w	39	20/21	0.83	0.16	82,93,96,96	0
32	PSU	2a	516	20/21	0.84	0.12	75,82,90,90	0
54	A1B8A	2w	76	31/32	0.84	0.16	52,68,78,82	0
55	4SU	2x	8	20/21	0.85	0.12	74,78,83,87	0
32	M2G	2a	966	25/26	0.86	0.17	59,70,87,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	PSU	1w	39	20/21	0.86	0.12	76,82,88,94	0
55	5MU	2x	54	21/22	0.87	0.13	76,79,84,94	0
55	PSU	2x	55	20/21	0.87	0.11	69,76,80,89	0
54	A1B8A	1w	76	31/32	0.87	0.14	36,52,62,70	0
32	5MC	2a	967	21/22	0.87	0.15	66,71,81,83	0
43	0TD	1l	92	10/11	0.88	0.13	48,54,58,66	0
43	0TD	2l	92	10/11	0.90	0.12	68,70,73,87	0
1	PSU	2A	1911	20/21	0.90	0.12	64,70,78,82	0
1	5MU	1A	1915	21/22	0.90	0.10	53,61,69,79	0
32	PSU	1a	516	20/21	0.91	0.09	58,64,70,77	0
1	PSU	2A	1917	20/21	0.91	0.12	62,75,79,81	0
55	5MU	1x	54	21/22	0.92	0.11	60,66,70,74	0
32	2MG	1a	1207	24/25	0.92	0.11	59,68,74,81	0
32	5MC	2a	1400	21/22	0.92	0.15	65,72,76,78	0
56	FME	2z	1	10/11	0.92	0.16	49,55,58,65	0
32	G7M	2a	527	24/25	0.93	0.10	60,68,72,74	0
32	4OC	2a	1402	22/23	0.93	0.11	55,66,69,74	0
55	PSU	1x	55	20/21	0.93	0.09	49,58,67,71	0
1	OMC	2A	1920	21/22	0.94	0.11	57,65,72,74	0
55	5MC	1x	32	21/22	0.94	0.13	48,52,62,62	0
32	5MC	2a	1407	21/22	0.94	0.10	56,61,62,66	0
56	FME	1z	1	10/11	0.94	0.15	37,45,49,51	0
55	4SU	1x	8	20/21	0.94	0.11	59,64,69,73	0
32	UR3	2a	1498	21/22	0.95	0.11	55,60,66,73	0
32	MA6	2a	1518	24/25	0.95	0.11	52,66,70,72	0
1	5MC	2A	1942	21/22	0.95	0.10	46,60,65,69	0
1	5MC	2A	1962	21/22	0.95	0.11	42,52,56,76	0
55	5MC	2x	32	21/22	0.95	0.12	63,72,77,83	0
32	G7M	1a	527	24/25	0.95	0.09	41,47,54,58	0
32	5MC	1a	967	21/22	0.95	0.09	56,61,66,69	0
55	8AN	2x	76	22/23	0.95	0.10	43,52,58,59	0
32	5MC	2a	1404	21/22	0.95	0.10	53,62,64,67	0
1	PSU	1A	1917	20/21	0.95	0.07	46,55,62,62	0
32	M2G	1a	966	25/26	0.96	0.10	44,58,64,67	0
1	OMG	2A	2251	24/25	0.96	0.09	36,41,47,49	0
1	OMU	2A	2552	21/22	0.96	0.09	33,45,50,51	0
1	PSU	2A	2605	20/21	0.96	0.09	31,41,47,47	0
32	5MC	1a	1400	21/22	0.96	0.10	47,50,55,61	0
32	5MC	1a	1404	21/22	0.96	0.09	35,43,48,52	0
32	MA6	1a	1519	24/25	0.96	0.09	36,43,47,50	0
32	MA6	2a	1519	24/25	0.96	0.12	54,65,72,74	0
1	5MC	1A	1942	21/22	0.96	0.09	38,44,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MA6	1a	1518	24/25	0.97	0.09	34,44,49,50	0
1	5MU	2A	1939	21/22	0.97	0.07	33,40,45,47	0
1	PSU	1A	1911	20/21	0.97	0.08	41,49,54,57	0
55	8AN	1x	76	22/23	0.97	0.08	24,34,42,44	0
32	4OC	1a	1402	22/23	0.97	0.09	43,48,53,57	0
1	2MA	2A	2503	23/24	0.97	0.08	26,37,41,47	0
1	OMC	1A	1920	21/22	0.97	0.07	34,45,50,52	0
32	5MC	1a	1407	21/22	0.97	0.07	33,42,47,48	0
1	PSU	1A	2605	20/21	0.98	0.07	21,28,34,34	0
1	5MU	1A	1939	21/22	0.98	0.05	22,29,31,35	0
1	5MC	1A	1962	21/22	0.98	0.06	22,31,36,45	0
1	OMG	1A	2251	24/25	0.98	0.05	21,26,29,31	0
32	UR3	1a	1498	21/22	0.98	0.07	33,42,44,45	0
1	2MA	1A	2503	23/24	0.98	0.06	16,23,27,27	0
1	OMU	1A	2552	21/22	0.98	0.06	23,28,32,35	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1798	1/1	0.55	0.17	81,81,81,81	0
58	MG	2A	3385	1/1	0.58	0.16	84,84,84,84	0
58	MG	2a	1756	1/1	0.62	0.18	82,82,82,82	0
58	MG	1B	229	1/1	0.63	0.20	74,74,74,74	0
58	MG	2A	3451	1/1	0.63	0.28	83,83,83,83	0
58	MG	2A	3437	1/1	0.64	0.29	77,77,77,77	0
58	MG	1a	1804	1/1	0.65	0.18	72,72,72,72	0
58	MG	1A	3260	1/1	0.65	0.20	85,85,85,85	0
58	MG	1a	1738	1/1	0.65	0.21	77,77,77,77	0
58	MG	1B	230	1/1	0.66	0.23	78,78,78,78	0
58	MG	2A	3755	1/1	0.66	0.26	59,59,59,59	0
58	MG	1A	3683	1/1	0.67	0.20	63,63,63,63	0
58	MG	2A	3113	1/1	0.67	0.30	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3171	1/1	0.68	0.20	80,80,80,80	0
58	MG	1A	3844	1/1	0.68	0.19	77,77,77,77	0
58	MG	2A	3669	1/1	0.68	0.18	77,77,77,77	0
58	MG	2A	3731	1/1	0.69	0.15	81,81,81,81	0
58	MG	2A	3608	1/1	0.69	0.20	63,63,63,63	0
58	MG	2A	3615	1/1	0.69	0.23	68,68,68,68	0
58	MG	2A	3175	1/1	0.69	0.23	68,68,68,68	0
58	MG	1A	3643	1/1	0.70	0.16	69,69,69,69	0
58	MG	2a	1789	1/1	0.70	0.20	70,70,70,70	0
58	MG	2a	1638	1/1	0.70	0.12	81,81,81,81	0
58	MG	1a	1809	1/1	0.71	0.18	72,72,72,72	0
58	MG	2G	201	1/1	0.71	0.23	75,75,75,75	0
58	MG	2A	3573	1/1	0.71	0.22	69,69,69,69	0
58	MG	1a	1733	1/1	0.72	0.17	85,85,85,85	0
58	MG	2A	3273	1/1	0.72	0.20	71,71,71,71	0
58	MG	2A	3332	1/1	0.73	0.25	72,72,72,72	0
58	MG	2A	3664	1/1	0.73	0.25	69,69,69,69	0
58	MG	1a	1802	1/1	0.73	0.24	81,81,81,81	0
58	MG	2a	1622	1/1	0.73	0.22	83,83,83,83	0
58	MG	2a	1607	1/1	0.74	0.36	67,67,67,67	0
58	MG	2A	3679	1/1	0.74	0.16	72,72,72,72	0
58	MG	2a	1805	1/1	0.74	0.20	68,68,68,68	0
58	MG	2A	3526	1/1	0.75	0.17	66,66,66,66	0
58	MG	2A	3704	1/1	0.75	0.20	69,69,69,69	0
58	MG	2a	1818	1/1	0.75	0.18	79,79,79,79	0
58	MG	2B	214	1/1	0.76	0.18	71,71,71,71	0
58	MG	1a	1731	1/1	0.76	0.18	66,66,66,66	0
58	MG	2a	1601	1/1	0.77	0.19	74,74,74,74	0
58	MG	1A	3772	1/1	0.77	0.14	20,20,20,20	0
58	MG	2A	3192	1/1	0.77	0.20	69,69,69,69	0
58	MG	1A	4083	1/1	0.77	0.16	58,58,58,58	0
58	MG	2a	1725	1/1	0.77	0.27	80,80,80,80	0
58	MG	1a	1760	1/1	0.77	0.12	67,67,67,67	0
58	MG	2A	3335	1/1	0.77	0.21	77,77,77,77	0
58	MG	2A	3833	1/1	0.77	0.20	65,65,65,65	0
58	MG	2A	3355	1/1	0.77	0.18	69,69,69,69	0
58	MG	2a	1812	1/1	0.77	0.18	83,83,83,83	0
58	MG	2a	1815	1/1	0.77	0.14	76,76,76,76	0
58	MG	1A	4089	1/1	0.77	0.17	45,45,45,45	0
58	MG	1A	3466	1/1	0.78	0.18	62,62,62,62	0
58	MG	1A	3882	1/1	0.78	0.13	23,23,23,23	0
58	MG	1x	109	1/1	0.78	0.34	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	2A	3327	1/1	0.78	0.16	71,71,71,71	0
58	MG	2A	3508	1/1	0.78	0.12	29,29,29,29	0
58	MG	2A	3690	1/1	0.78	0.12	70,70,70,70	0
58	MG	1A	4082	1/1	0.78	0.14	60,60,60,60	0
58	MG	1A	3267	1/1	0.78	0.20	62,62,62,62	0
58	MG	2a	1821	1/1	0.78	0.24	69,69,69,69	0
58	MG	2R	201	1/1	0.79	0.24	77,77,77,77	0
58	MG	1a	1755	1/1	0.79	0.12	60,60,60,60	0
58	MG	2A	3670	1/1	0.79	0.14	68,68,68,68	0
58	MG	1U	208	1/1	0.79	0.48	67,67,67,67	0
58	MG	1a	1622	1/1	0.79	0.20	66,66,66,66	0
58	MG	2a	1706	1/1	0.79	0.19	77,77,77,77	0
58	MG	1a	1697	1/1	0.79	0.17	66,66,66,66	0
58	MG	2A	3723	1/1	0.79	0.15	68,68,68,68	0
58	MG	1A	3752	1/1	0.79	0.13	65,65,65,65	0
58	MG	2A	3738	1/1	0.79	0.17	46,46,46,46	0
58	MG	1A	3468	1/1	0.79	0.13	56,56,56,56	0
58	MG	2A	3758	1/1	0.79	0.12	67,67,67,67	0
58	MG	1A	3687	1/1	0.79	0.13	64,64,64,64	0
58	MG	2A	3152	1/1	0.79	0.23	60,60,60,60	0
58	MG	2A	3380	1/1	0.79	0.29	76,76,76,76	0
58	MG	2j	201	1/1	0.79	0.20	71,71,71,71	0
58	MG	1A	3960	1/1	0.80	0.15	58,58,58,58	0
58	MG	2a	1655	1/1	0.80	0.17	80,80,80,80	0
58	MG	2A	3418	1/1	0.80	0.32	68,68,68,68	0
58	MG	2A	3653	1/1	0.80	0.14	65,65,65,65	0
58	MG	2A	3432	1/1	0.80	0.23	54,54,54,54	0
58	MG	1A	3957	1/1	0.80	0.10	46,46,46,46	0
58	MG	2A	3205	1/1	0.80	0.11	60,60,60,60	0
58	MG	2a	1800	1/1	0.80	0.17	86,86,86,86	0
58	MG	2A	3483	1/1	0.80	0.31	67,67,67,67	0
58	MG	2P	202	1/1	0.80	0.23	66,66,66,66	0
58	MG	2A	3097	1/1	0.80	0.15	72,72,72,72	0
58	MG	2A	3357	1/1	0.80	0.19	54,54,54,54	0
58	MG	2A	3705	1/1	0.80	0.18	59,59,59,59	0
58	MG	2A	3276	1/1	0.80	0.19	72,72,72,72	0
58	MG	2A	3024	1/1	0.81	0.15	61,61,61,61	0
58	MG	2A	3159	1/1	0.81	0.24	66,66,66,66	0
58	MG	2a	1733	1/1	0.81	0.22	70,70,70,70	0
58	MG	2a	1735	1/1	0.81	0.18	69,69,69,69	0
58	MG	1A	3326	1/1	0.81	0.11	65,65,65,65	0
58	MG	2A	3173	1/1	0.81	0.20	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3678	1/1	0.81	0.12	56,56,56,56	0
58	MG	2A	3106	1/1	0.81	0.30	72,72,72,72	0
58	MG	2A	3337	1/1	0.81	0.18	76,76,76,76	0
58	MG	1B	213	1/1	0.81	0.19	67,67,67,67	0
58	MG	2A	3115	1/1	0.81	0.22	62,62,62,62	0
58	MG	2A	3605	1/1	0.81	0.17	75,75,75,75	0
58	MG	2A	3256	1/1	0.81	0.14	58,58,58,58	0
58	MG	2A	3270	1/1	0.81	0.15	78,78,78,78	0
58	MG	2y	101	1/1	0.81	0.33	71,71,71,71	0
58	MG	2A	3773	1/1	0.82	0.10	46,46,46,46	0
58	MG	2A	3817	1/1	0.82	0.17	48,48,48,48	0
58	MG	1A	3878	1/1	0.82	0.12	61,61,61,61	0
58	MG	2B	208	1/1	0.82	0.10	62,62,62,62	0
58	MG	2A	3212	1/1	0.82	0.14	67,67,67,67	0
58	MG	2D	303	1/1	0.82	0.19	64,64,64,64	0
58	MG	2F	307	1/1	0.82	0.11	64,64,64,64	0
58	MG	2A	3502	1/1	0.82	0.16	55,55,55,55	0
58	MG	1B	234	1/1	0.82	0.16	66,66,66,66	0
58	MG	1A	3458	1/1	0.82	0.21	63,63,63,63	0
58	MG	20	104	1/1	0.82	0.11	55,55,55,55	0
58	MG	1A	3893	1/1	0.82	0.17	73,73,73,73	0
58	MG	2A	3600	1/1	0.82	0.17	55,55,55,55	0
58	MG	2A	3051	1/1	0.82	0.27	69,69,69,69	0
58	MG	2A	3291	1/1	0.82	0.14	59,59,59,59	0
58	MG	2A	3325	1/1	0.82	0.23	68,68,68,68	0
58	MG	2a	1704	1/1	0.82	0.14	55,55,55,55	0
58	MG	1a	1636	1/1	0.82	0.28	73,73,73,73	0
58	MG	1a	1683	1/1	0.82	0.28	68,68,68,68	0
58	MG	1A	3294	1/1	0.82	0.20	55,55,55,55	0
58	MG	1A	3707	1/1	0.82	0.11	29,29,29,29	0
58	MG	2A	3350	1/1	0.82	0.14	63,63,63,63	0
58	MG	2a	1757	1/1	0.82	0.09	89,89,89,89	0
58	MG	1A	3749	1/1	0.82	0.14	51,51,51,51	0
58	MG	1a	1737	1/1	0.82	0.24	62,62,62,62	0
58	MG	1A	3251	1/1	0.82	0.14	50,50,50,50	0
58	MG	1A	3536	1/1	0.82	0.12	59,59,59,59	0
58	MG	2A	3390	1/1	0.82	0.19	68,68,68,68	0
58	MG	2a	1814	1/1	0.82	0.20	63,63,63,63	0
58	MG	2A	3728	1/1	0.82	0.19	56,56,56,56	0
58	MG	1A	3809	1/1	0.82	0.14	51,51,51,51	0
58	MG	2A	3191	1/1	0.82	0.32	69,69,69,69	0
58	MG	1A	3383	1/1	0.82	0.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2x	103	1/1	0.82	0.19	69,69,69,69	0
58	MG	2A	3444	1/1	0.82	0.12	67,67,67,67	0
58	MG	2A	3300	1/1	0.83	0.22	59,59,59,59	0
58	MG	2A	3472	1/1	0.83	0.10	72,72,72,72	0
58	MG	1A	4019	1/1	0.83	0.15	75,75,75,75	0
58	MG	2a	1641	1/1	0.83	0.28	67,67,67,67	0
58	MG	1A	3801	1/1	0.83	0.14	53,53,53,53	0
58	MG	2a	1681	1/1	0.83	0.24	71,71,71,71	0
58	MG	2a	1700	1/1	0.83	0.13	75,75,75,75	0
58	MG	1w	101	1/1	0.83	0.15	77,77,77,77	0
58	MG	1w	103	1/1	0.83	0.17	87,87,87,87	0
58	MG	2a	1714	1/1	0.83	0.28	67,67,67,67	0
58	MG	2a	1715	1/1	0.83	0.12	63,63,63,63	0
58	MG	1E	314	1/1	0.83	0.30	50,50,50,50	0
58	MG	2A	3023	1/1	0.83	0.20	71,71,71,71	0
58	MG	1A	3329	1/1	0.83	0.13	52,52,52,52	0
58	MG	2A	3782	1/1	0.83	0.14	79,79,79,79	0
58	MG	2A	3044	1/1	0.83	0.20	66,66,66,66	0
58	MG	1A	3923	1/1	0.83	0.13	30,30,30,30	0
58	MG	2A	3646	1/1	0.83	0.13	77,77,77,77	0
58	MG	2A	3384	1/1	0.83	0.15	66,66,66,66	0
58	MG	2B	216	1/1	0.83	0.16	72,72,72,72	0
58	MG	2A	3052	1/1	0.83	0.22	67,67,67,67	0
58	MG	2A	3065	1/1	0.83	0.17	77,77,77,77	0
58	MG	2A	3075	1/1	0.83	0.17	72,72,72,72	0
58	MG	2A	3672	1/1	0.83	0.17	68,68,68,68	0
58	MG	1A	3626	1/1	0.83	0.16	48,48,48,48	0
58	MG	1a	1680	1/1	0.83	0.19	67,67,67,67	0
58	MG	2l	202	1/1	0.83	0.23	68,68,68,68	0
58	MG	2x	102	1/1	0.83	0.18	65,65,65,65	0
58	MG	28	101	1/1	0.83	0.26	64,64,64,64	0
58	MG	1A	3470	1/1	0.83	0.15	60,60,60,60	0
58	MG	20	103	1/1	0.84	0.16	59,59,59,59	0
58	MG	2A	3364	1/1	0.84	0.14	71,71,71,71	0
58	MG	2a	1742	1/1	0.84	0.26	77,77,77,77	0
58	MG	2a	1752	1/1	0.84	0.10	71,71,71,71	0
58	MG	2A	3089	1/1	0.84	0.14	58,58,58,58	0
58	MG	2A	3457	1/1	0.84	0.17	72,72,72,72	0
58	MG	1x	105	1/1	0.84	0.32	69,69,69,69	0
58	MG	2A	3634	1/1	0.84	0.15	41,41,41,41	0
58	MG	2A	3849	1/1	0.84	0.17	61,61,61,61	0
58	MG	1A	3992	1/1	0.84	0.10	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	2A	3313	1/1	0.84	0.13	59,59,59,59	0
58	MG	2A	3654	1/1	0.84	0.21	73,73,73,73	0
58	MG	2B	220	1/1	0.84	0.18	76,76,76,76	0
58	MG	2A	3729	1/1	0.84	0.16	66,66,66,66	0
58	MG	1a	1670	1/1	0.84	0.18	55,55,55,55	0
58	MG	2d	302	1/1	0.84	0.14	70,70,70,70	0
58	MG	2A	3197	1/1	0.84	0.16	66,66,66,66	0
58	MG	2k	201	1/1	0.84	0.12	64,64,64,64	0
58	MG	2A	3743	1/1	0.84	0.21	48,48,48,48	0
58	MG	2a	1717	1/1	0.84	0.20	76,76,76,76	0
58	MG	2a	1720	1/1	0.84	0.16	68,68,68,68	0
58	MG	2A	3359	1/1	0.84	0.12	75,75,75,75	0
58	MG	2A	3193	1/1	0.85	0.23	62,62,62,62	0
58	MG	2A	3530	1/1	0.85	0.22	63,63,63,63	0
58	MG	2A	3554	1/1	0.85	0.15	55,55,55,55	0
58	MG	2a	1674	1/1	0.85	0.22	67,67,67,67	0
58	MG	2A	3195	1/1	0.85	0.15	69,69,69,69	0
58	MG	2a	1684	1/1	0.85	0.22	62,62,62,62	0
58	MG	2A	3746	1/1	0.85	0.15	61,61,61,61	0
58	MG	2A	3582	1/1	0.85	0.19	81,81,81,81	0
58	MG	1a	1743	1/1	0.85	0.18	64,64,64,64	0
58	MG	1A	3810	1/1	0.85	0.14	46,46,46,46	0
58	MG	2A	3366	1/1	0.85	0.16	57,57,57,57	0
58	MG	2A	3792	1/1	0.85	0.10	73,73,73,73	0
58	MG	1a	1628	1/1	0.85	0.11	56,56,56,56	0
58	MG	1a	1776	1/1	0.85	0.11	66,66,66,66	0
58	MG	2A	3635	1/1	0.85	0.12	46,46,46,46	0
58	MG	2A	3862	1/1	0.85	0.18	62,62,62,62	0
58	MG	2B	203	1/1	0.85	0.20	63,63,63,63	0
58	MG	2B	204	1/1	0.85	0.16	70,70,70,70	0
58	MG	2B	206	1/1	0.85	0.17	58,58,58,58	0
58	MG	2A	3091	1/1	0.85	0.12	70,70,70,70	0
58	MG	2a	1781	1/1	0.85	0.14	63,63,63,63	0
58	MG	2a	1787	1/1	0.85	0.13	72,72,72,72	0
58	MG	2a	1788	1/1	0.85	0.15	65,65,65,65	0
58	MG	1B	222	1/1	0.85	0.17	58,58,58,58	0
58	MG	2A	3391	1/1	0.85	0.12	66,66,66,66	0
58	MG	1A	3245	1/1	0.85	0.12	59,59,59,59	0
58	MG	2A	3667	1/1	0.85	0.18	56,56,56,56	0
58	MG	1A	3956	1/1	0.85	0.10	45,45,45,45	0
58	MG	1A	3236	1/1	0.85	0.21	42,42,42,42	0
58	MG	1a	1687	1/1	0.85	0.31	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3388	1/1	0.85	0.17	61,61,61,61	0
58	MG	1G	203	1/1	0.85	0.10	68,68,68,68	0
58	MG	1P	206	1/1	0.85	0.24	55,55,55,55	0
58	MG	2A	3482	1/1	0.85	0.17	54,54,54,54	0
58	MG	1A	4094	1/1	0.85	0.17	53,53,53,53	0
58	MG	1W	207	1/1	0.85	0.19	32,32,32,32	0
58	MG	2t	201	1/1	0.85	0.19	48,48,48,48	0
58	MG	2w	101	1/1	0.85	0.27	84,84,84,84	0
58	MG	2a	1608	1/1	0.85	0.35	78,78,78,78	0
58	MG	1a	1739	1/1	0.85	0.15	62,62,62,62	0
58	MG	2a	1633	1/1	0.85	0.21	73,73,73,73	0
58	MG	1a	1768	1/1	0.86	0.14	64,64,64,64	0
58	MG	2A	3264	1/1	0.86	0.19	67,67,67,67	0
58	MG	2a	1630	1/1	0.86	0.17	62,62,62,62	0
58	MG	1A	3946	1/1	0.86	0.19	67,67,67,67	0
58	MG	2A	3434	1/1	0.86	0.20	59,59,59,59	0
58	MG	2A	3701	1/1	0.86	0.11	39,39,39,39	0
58	MG	2A	3703	1/1	0.86	0.17	63,63,63,63	0
58	MG	2A	3272	1/1	0.86	0.17	66,66,66,66	0
58	MG	1A	3191	1/1	0.86	0.18	53,53,53,53	0
58	MG	1A	3595	1/1	0.86	0.10	52,52,52,52	0
58	MG	1A	3833	1/1	0.86	0.13	46,46,46,46	0
58	MG	2a	1702	1/1	0.86	0.16	55,55,55,55	0
58	MG	2A	3292	1/1	0.86	0.30	73,73,73,73	0
58	MG	1b	301	1/1	0.86	0.20	81,81,81,81	0
58	MG	2A	3302	1/1	0.86	0.16	62,62,62,62	0
58	MG	2A	3739	1/1	0.86	0.14	72,72,72,72	0
58	MG	2A	3485	1/1	0.86	0.20	61,61,61,61	0
58	MG	2A	3495	1/1	0.86	0.15	64,64,64,64	0
58	MG	2A	3126	1/1	0.86	0.09	66,66,66,66	0
58	MG	1A	3599	1/1	0.86	0.22	73,73,73,73	0
58	MG	2a	1734	1/1	0.86	0.17	70,70,70,70	0
58	MG	2A	3763	1/1	0.86	0.20	74,74,74,74	0
58	MG	2A	3509	1/1	0.86	0.18	65,65,65,65	0
58	MG	2A	3153	1/1	0.86	0.14	62,62,62,62	0
58	MG	2a	1754	1/1	0.86	0.12	67,67,67,67	0
58	MG	1a	1714	1/1	0.86	0.24	58,58,58,58	0
58	MG	2A	3541	1/1	0.86	0.09	46,46,46,46	0
58	MG	2a	1766	1/1	0.86	0.17	79,79,79,79	0
58	MG	2A	3165	1/1	0.86	0.08	41,41,41,41	0
58	MG	2A	3561	1/1	0.86	0.09	35,35,35,35	0
58	MG	2A	3859	1/1	0.86	0.33	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	1a	1730	1/1	0.86	0.11	69,69,69,69	0
58	MG	2A	3348	1/1	0.86	0.17	59,59,59,59	0
58	MG	1A	3864	1/1	0.86	0.13	52,52,52,52	0
58	MG	1A	4061	1/1	0.86	0.14	45,45,45,45	0
58	MG	2a	1806	1/1	0.86	0.25	61,61,61,61	0
58	MG	1A	4078	1/1	0.86	0.12	49,49,49,49	0
58	MG	2A	3613	1/1	0.86	0.18	65,65,65,65	0
58	MG	2A	3358	1/1	0.86	0.11	70,70,70,70	0
58	MG	2A	3029	1/1	0.86	0.20	77,77,77,77	0
58	MG	2A	3362	1/1	0.86	0.17	65,65,65,65	0
58	MG	2a	1829	1/1	0.86	0.21	72,72,72,72	0
58	MG	1A	3610	1/1	0.86	0.12	35,35,35,35	0
58	MG	2A	3649	1/1	0.86	0.14	70,70,70,70	0
58	MG	1A	3621	1/1	0.86	0.12	33,33,33,33	0
58	MG	1A	3502	1/1	0.86	0.13	45,45,45,45	0
58	MG	2n	101	1/1	0.86	0.29	72,72,72,72	0
58	MG	2A	3657	1/1	0.86	0.13	64,64,64,64	0
58	MG	1A	3531	1/1	0.86	0.21	50,50,50,50	0
58	MG	2A	3206	1/1	0.86	0.17	66,66,66,66	0
58	MG	2A	3389	1/1	0.86	0.11	68,68,68,68	0
58	MG	1B	203	1/1	0.86	0.22	49,49,49,49	0
58	MG	1A	3889	1/1	0.87	0.12	34,34,34,34	0
58	MG	2A	3607	1/1	0.87	0.11	31,31,31,31	0
58	MG	2A	3103	1/1	0.87	0.20	58,58,58,58	0
58	MG	2A	3387	1/1	0.87	0.14	57,57,57,57	0
58	MG	1a	1631	1/1	0.87	0.32	59,59,59,59	0
58	MG	2a	1707	1/1	0.87	0.29	69,69,69,69	0
58	MG	2A	3804	1/1	0.87	0.13	55,55,55,55	0
58	MG	1A	3435	1/1	0.87	0.11	59,59,59,59	0
58	MG	1a	1664	1/1	0.87	0.17	59,59,59,59	0
58	MG	2A	3412	1/1	0.87	0.18	54,54,54,54	0
58	MG	1A	4093	1/1	0.87	0.11	69,69,69,69	0
58	MG	1A	3791	1/1	0.87	0.10	31,31,31,31	0
58	MG	2A	3864	1/1	0.87	0.16	64,64,64,64	0
58	MG	1A	3525	1/1	0.87	0.11	52,52,52,52	0
58	MG	1A	3951	1/1	0.87	0.18	65,65,65,65	0
58	MG	2a	1744	1/1	0.87	0.24	65,65,65,65	0
58	MG	2A	3317	1/1	0.87	0.18	52,52,52,52	0
58	MG	1x	101	1/1	0.87	0.32	62,62,62,62	0
58	MG	2B	210	1/1	0.87	0.14	71,71,71,71	0
58	MG	1a	1690	1/1	0.87	0.23	63,63,63,63	0
58	MG	1A	3244	1/1	0.87	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3334	1/1	0.87	0.25	70,70,70,70	0
58	MG	1A	3646	1/1	0.87	0.11	35,35,35,35	0
58	MG	2D	306	1/1	0.87	0.24	53,53,53,53	0
58	MG	1A	3824	1/1	0.87	0.08	35,35,35,35	0
58	MG	2A	3686	1/1	0.87	0.12	45,45,45,45	0
58	MG	2A	3338	1/1	0.87	0.11	73,73,73,73	0
58	MG	1A	3335	1/1	0.87	0.20	64,64,64,64	0
58	MG	1A	3543	1/1	0.87	0.09	62,62,62,62	0
58	MG	1A	4043	1/1	0.87	0.12	45,45,45,45	0
58	MG	1O	204	1/1	0.87	0.14	71,71,71,71	0
58	MG	2A	3721	1/1	0.87	0.12	69,69,69,69	0
58	MG	2a	1817	1/1	0.87	0.22	73,73,73,73	0
58	MG	1A	3187	1/1	0.87	0.10	52,52,52,52	0
58	MG	2A	3067	1/1	0.87	0.23	58,58,58,58	0
58	MG	1A	4076	1/1	0.87	0.21	47,47,47,47	0
58	MG	2a	1623	1/1	0.87	0.10	59,59,59,59	0
58	MG	2A	3232	1/1	0.87	0.43	54,54,54,54	0
58	MG	2A	3572	1/1	0.87	0.19	55,55,55,55	0
58	MG	2a	1637	1/1	0.87	0.36	67,67,67,67	0
58	MG	1A	3261	1/1	0.87	0.14	52,52,52,52	0
58	MG	2A	3740	1/1	0.87	0.20	60,60,60,60	0
58	MG	2a	1650	1/1	0.87	0.10	57,57,57,57	0
58	MG	2A	3576	1/1	0.87	0.10	55,55,55,55	0
58	MG	2A	3376	1/1	0.87	0.12	61,61,61,61	0
58	MG	2x	106	1/1	0.87	0.11	59,59,59,59	0
58	MG	1A	3472	1/1	0.87	0.31	64,64,64,64	0
58	MG	2B	218	1/1	0.88	0.16	76,76,76,76	0
58	MG	2A	3594	1/1	0.88	0.09	35,35,35,35	0
58	MG	1a	1774	1/1	0.88	0.11	54,54,54,54	0
58	MG	2A	3601	1/1	0.88	0.22	71,71,71,71	0
58	MG	1A	3913	1/1	0.88	0.08	30,30,30,30	0
58	MG	1A	3457	1/1	0.88	0.19	61,61,61,61	0
58	MG	1A	3584	1/1	0.88	0.10	34,34,34,34	0
58	MG	1A	3486	1/1	0.88	0.11	46,46,46,46	0
58	MG	1a	1642	1/1	0.88	0.19	65,65,65,65	0
58	MG	1B	211	1/1	0.88	0.09	44,44,44,44	0
58	MG	2A	3185	1/1	0.88	0.23	63,63,63,63	0
58	MG	1A	3208	1/1	0.88	0.17	63,63,63,63	0
58	MG	1A	3839	1/1	0.88	0.27	65,65,65,65	0
58	MG	1x	102	1/1	0.88	0.23	65,65,65,65	0
58	MG	1A	3507	1/1	0.88	0.11	59,59,59,59	0
58	MG	2A	3370	1/1	0.88	0.33	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3372	1/1	0.88	0.12	67,67,67,67	0
58	MG	1a	1684	1/1	0.88	0.10	62,62,62,62	0
58	MG	2A	3668	1/1	0.88	0.10	57,57,57,57	0
58	MG	2A	3198	1/1	0.88	0.26	64,64,64,64	0
58	MG	1A	3848	1/1	0.88	0.12	61,61,61,61	0
58	MG	2a	1642	1/1	0.88	0.24	69,69,69,69	0
58	MG	1A	3386	1/1	0.88	0.24	27,27,27,27	0
58	MG	2A	3676	1/1	0.88	0.16	59,59,59,59	0
58	MG	2a	1657	1/1	0.88	0.10	61,61,61,61	0
58	MG	2a	1663	1/1	0.88	0.15	84,84,84,84	0
58	MG	1a	1694	1/1	0.88	0.19	49,49,49,49	0
58	MG	2a	1677	1/1	0.88	0.22	63,63,63,63	0
58	MG	2A	3213	1/1	0.88	0.12	53,53,53,53	0
58	MG	2a	1682	1/1	0.88	0.11	75,75,75,75	0
58	MG	1E	311	1/1	0.88	0.08	29,29,29,29	0
58	MG	2A	3687	1/1	0.88	0.14	58,58,58,58	0
58	MG	2a	1701	1/1	0.88	0.17	73,73,73,73	0
58	MG	2A	3237	1/1	0.88	0.19	57,57,57,57	0
58	MG	2A	3395	1/1	0.88	0.11	65,65,65,65	0
58	MG	2A	3404	1/1	0.88	0.20	52,52,52,52	0
58	MG	2A	3243	1/1	0.88	0.14	60,60,60,60	0
58	MG	2a	1708	1/1	0.88	0.14	66,66,66,66	0
58	MG	2A	3247	1/1	0.88	0.12	64,64,64,64	0
58	MG	2A	3422	1/1	0.88	0.32	68,68,68,68	0
58	MG	1E	313	1/1	0.88	0.14	61,61,61,61	0
58	MG	1A	3167	1/1	0.88	0.10	38,38,38,38	0
58	MG	1A	3881	1/1	0.88	0.13	49,49,49,49	0
58	MG	2a	1728	1/1	0.88	0.15	61,61,61,61	0
58	MG	1A	3781	1/1	0.88	0.10	36,36,36,36	0
58	MG	2A	3733	1/1	0.88	0.12	77,77,77,77	0
58	MG	2A	3737	1/1	0.88	0.19	69,69,69,69	0
58	MG	2a	1737	1/1	0.88	0.09	66,66,66,66	0
58	MG	1A	3639	1/1	0.88	0.09	41,41,41,41	0
58	MG	1A	3367	1/1	0.88	0.15	47,47,47,47	0
58	MG	2a	1750	1/1	0.88	0.14	74,74,74,74	0
58	MG	2A	3280	1/1	0.88	0.19	67,67,67,67	0
58	MG	2A	3288	1/1	0.88	0.28	65,65,65,65	0
58	MG	1A	3897	1/1	0.88	0.10	35,35,35,35	0
58	MG	1Z	301	1/1	0.88	0.09	70,70,70,70	0
58	MG	2a	1761	1/1	0.88	0.21	65,65,65,65	0
58	MG	2A	3757	1/1	0.88	0.14	76,76,76,76	0
58	MG	2A	3295	1/1	0.88	0.09	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1784	1/1	0.88	0.16	86,86,86,86	0
58	MG	2A	3297	1/1	0.88	0.16	60,60,60,60	0
58	MG	2A	3098	1/1	0.88	0.14	77,77,77,77	0
58	MG	2A	3775	1/1	0.88	0.10	62,62,62,62	0
58	MG	2a	1794	1/1	0.88	0.20	66,66,66,66	0
58	MG	2A	3776	1/1	0.88	0.12	62,62,62,62	0
58	MG	1a	1747	1/1	0.88	0.07	49,49,49,49	0
58	MG	2a	1801	1/1	0.88	0.19	60,60,60,60	0
58	MG	2a	1802	1/1	0.88	0.26	68,68,68,68	0
58	MG	2A	3783	1/1	0.88	0.11	69,69,69,69	0
58	MG	2A	3510	1/1	0.88	0.10	44,44,44,44	0
58	MG	2A	3522	1/1	0.88	0.10	43,43,43,43	0
58	MG	2A	3809	1/1	0.88	0.09	37,37,37,37	0
58	MG	2A	3304	1/1	0.88	0.12	69,69,69,69	0
58	MG	1Z	302	1/1	0.88	0.13	55,55,55,55	0
58	MG	2A	3846	1/1	0.88	0.11	69,69,69,69	0
58	MG	2A	3540	1/1	0.88	0.12	50,50,50,50	0
58	MG	2a	1825	1/1	0.88	0.30	68,68,68,68	0
58	MG	2a	1826	1/1	0.88	0.14	58,58,58,58	0
58	MG	2A	3852	1/1	0.88	0.14	68,68,68,68	0
58	MG	2A	3110	1/1	0.88	0.08	72,72,72,72	0
58	MG	2A	3860	1/1	0.88	0.22	70,70,70,70	0
58	MG	2A	3324	1/1	0.88	0.12	51,51,51,51	0
58	MG	2l	201	1/1	0.88	0.09	66,66,66,66	0
58	MG	10	105	1/1	0.88	0.13	66,66,66,66	0
58	MG	2A	3564	1/1	0.88	0.16	55,55,55,55	0
58	MG	1a	1761	1/1	0.88	0.11	62,62,62,62	0
58	MG	2A	3329	1/1	0.88	0.25	72,72,72,72	0
58	MG	1a	1602	1/1	0.88	0.32	62,62,62,62	0
58	MG	2A	3578	1/1	0.88	0.19	60,60,60,60	0
58	MG	2x	105	1/1	0.88	0.26	68,68,68,68	0
58	MG	2A	3127	1/1	0.88	0.12	68,68,68,68	0
58	MG	2A	3585	1/1	0.88	0.09	60,60,60,60	0
58	MG	1A	3131	1/1	0.89	0.10	42,42,42,42	0
58	MG	1A	4047	1/1	0.89	0.07	17,17,17,17	0
58	MG	20	102	1/1	0.89	0.26	69,69,69,69	0
58	MG	1a	1677	1/1	0.89	0.21	52,52,52,52	0
58	MG	2A	3090	1/1	0.89	0.15	49,49,49,49	0
58	MG	1A	3590	1/1	0.89	0.24	59,59,59,59	0
58	MG	2A	3092	1/1	0.89	0.12	57,57,57,57	0
58	MG	1A	3265	1/1	0.89	0.21	66,66,66,66	0
58	MG	2A	3636	1/1	0.89	0.11	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	2a	1610	1/1	0.89	0.12	59,59,59,59	0
58	MG	2a	1612	1/1	0.89	0.12	64,64,64,64	0
58	MG	2a	1621	1/1	0.89	0.25	69,69,69,69	0
58	MG	2A	3642	1/1	0.89	0.10	51,51,51,51	0
58	MG	1A	3817	1/1	0.89	0.09	52,52,52,52	0
58	MG	2a	1624	1/1	0.89	0.20	56,56,56,56	0
58	MG	2a	1627	1/1	0.89	0.19	66,66,66,66	0
58	MG	1A	3350	1/1	0.89	0.22	59,59,59,59	0
58	MG	1A	3601	1/1	0.89	0.10	47,47,47,47	0
58	MG	1A	3253	1/1	0.89	0.09	44,44,44,44	0
58	MG	1a	1695	1/1	0.89	0.26	60,60,60,60	0
58	MG	2A	3662	1/1	0.89	0.14	64,64,64,64	0
58	MG	1A	3840	1/1	0.89	0.10	47,47,47,47	0
58	MG	2a	1644	1/1	0.89	0.14	56,56,56,56	0
58	MG	1a	1701	1/1	0.89	0.17	54,54,54,54	0
58	MG	2a	1653	1/1	0.89	0.16	63,63,63,63	0
58	MG	1A	3372	1/1	0.89	0.27	50,50,50,50	0
58	MG	2A	3136	1/1	0.89	0.13	52,52,52,52	0
58	MG	2A	3146	1/1	0.89	0.21	66,66,66,66	0
58	MG	2a	1665	1/1	0.89	0.13	63,63,63,63	0
58	MG	1A	3254	1/1	0.89	0.16	62,62,62,62	0
58	MG	1A	3480	1/1	0.89	0.13	51,51,51,51	0
58	MG	2A	3374	1/1	0.89	0.11	59,59,59,59	0
58	MG	1A	3866	1/1	0.89	0.14	52,52,52,52	0
58	MG	1A	3870	1/1	0.89	0.08	38,38,38,38	0
58	MG	1A	3306	1/1	0.89	0.10	52,52,52,52	0
58	MG	2A	3689	1/1	0.89	0.17	63,63,63,63	0
58	MG	1A	3496	1/1	0.89	0.12	53,53,53,53	0
58	MG	1A	3651	1/1	0.89	0.13	55,55,55,55	0
58	MG	1B	235	1/1	0.89	0.11	61,61,61,61	0
58	MG	1a	1754	1/1	0.89	0.12	76,76,76,76	0
58	MG	1E	302	1/1	0.89	0.14	36,36,36,36	0
58	MG	2A	3707	1/1	0.89	0.14	65,65,65,65	0
58	MG	2A	3716	1/1	0.89	0.12	60,60,60,60	0
58	MG	1A	3888	1/1	0.89	0.10	23,23,23,23	0
58	MG	1A	3321	1/1	0.89	0.13	47,47,47,47	0
58	MG	1A	3394	1/1	0.89	0.18	75,75,75,75	0
58	MG	1a	1773	1/1	0.89	0.10	37,37,37,37	0
58	MG	1A	3518	1/1	0.89	0.09	82,82,82,82	0
58	MG	2A	3423	1/1	0.89	0.23	52,52,52,52	0
58	MG	2A	3425	1/1	0.89	0.18	58,58,58,58	0
58	MG	1G	205	1/1	0.89	0.19	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	3433	1/1	0.89	0.21	56,56,56,56	0
58	MG	1a	1793	1/1	0.89	0.10	60,60,60,60	0
58	MG	1a	1795	1/1	0.89	0.24	69,69,69,69	0
58	MG	2A	3441	1/1	0.89	0.22	51,51,51,51	0
58	MG	2A	3216	1/1	0.89	0.29	73,73,73,73	0
58	MG	2A	3224	1/1	0.89	0.18	57,57,57,57	0
58	MG	1A	3905	1/1	0.89	0.09	51,51,51,51	0
58	MG	2a	1760	1/1	0.89	0.19	73,73,73,73	0
58	MG	2A	3470	1/1	0.89	0.11	53,53,53,53	0
58	MG	2A	3236	1/1	0.89	0.18	67,67,67,67	0
58	MG	2a	1772	1/1	0.89	0.09	85,85,85,85	0
58	MG	2a	1776	1/1	0.89	0.12	70,70,70,70	0
58	MG	1A	3405	1/1	0.89	0.18	43,43,43,43	0
58	MG	1A	3414	1/1	0.89	0.10	57,57,57,57	0
58	MG	1A	3934	1/1	0.89	0.14	51,51,51,51	0
58	MG	1t	201	1/1	0.89	0.18	57,57,57,57	0
58	MG	2A	3501	1/1	0.89	0.11	46,46,46,46	0
58	MG	2A	3260	1/1	0.89	0.16	56,56,56,56	0
58	MG	1A	3429	1/1	0.89	0.12	46,46,46,46	0
58	MG	1A	3539	1/1	0.89	0.12	59,59,59,59	0
58	MG	2A	3827	1/1	0.89	0.12	68,68,68,68	0
58	MG	1A	3783	1/1	0.89	0.14	54,54,54,54	0
58	MG	2A	3837	1/1	0.89	0.09	51,51,51,51	0
58	MG	2A	3841	1/1	0.89	0.12	54,54,54,54	0
58	MG	1a	1601	1/1	0.89	0.13	61,61,61,61	0
58	MG	1A	3785	1/1	0.89	0.10	62,62,62,62	0
58	MG	1a	1618	1/1	0.89	0.23	55,55,55,55	0
58	MG	2A	3853	1/1	0.89	0.11	51,51,51,51	0
58	MG	2A	3856	1/1	0.89	0.14	73,73,73,73	0
58	MG	1A	3958	1/1	0.89	0.08	23,23,23,23	0
58	MG	2A	3290	1/1	0.89	0.14	55,55,55,55	0
58	MG	1A	3202	1/1	0.89	0.09	47,47,47,47	0
58	MG	1A	3985	1/1	0.89	0.07	24,24,24,24	0
58	MG	2A	3563	1/1	0.89	0.09	40,40,40,40	0
58	MG	1a	1635	1/1	0.89	0.10	50,50,50,50	0
58	MG	1A	3798	1/1	0.89	0.09	20,20,20,20	0
58	MG	1a	1637	1/1	0.89	0.23	55,55,55,55	0
58	MG	2A	3574	1/1	0.89	0.16	60,60,60,60	0
58	MG	2A	3055	1/1	0.89	0.09	63,63,63,63	0
58	MG	2A	3058	1/1	0.89	0.21	58,58,58,58	0
58	MG	2v	101	1/1	0.89	0.13	63,63,63,63	0
58	MG	2v	102	1/1	0.89	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2v	103	1/1	0.89	0.48	72,72,72,72	0
58	MG	2v	104	1/1	0.89	0.17	67,67,67,67	0
58	MG	2A	3309	1/1	0.89	0.26	56,56,56,56	0
58	MG	2A	3063	1/1	0.89	0.10	46,46,46,46	0
58	MG	1A	3799	1/1	0.89	0.10	39,39,39,39	0
58	MG	2A	3598	1/1	0.89	0.15	57,57,57,57	0
58	MG	2A	3321	1/1	0.89	0.21	61,61,61,61	0
58	MG	2A	3066	1/1	0.89	0.15	52,52,52,52	0
58	MG	1A	3592	1/1	0.90	0.20	63,63,63,63	0
58	MG	1A	3059	1/1	0.90	0.10	36,36,36,36	0
58	MG	1a	1608	1/1	0.90	0.23	64,64,64,64	0
58	MG	1A	3369	1/1	0.90	0.24	53,53,53,53	0
58	MG	2A	3042	1/1	0.90	0.24	61,61,61,61	0
58	MG	2E	303	1/1	0.90	0.08	47,47,47,47	0
58	MG	1A	3971	1/1	0.90	0.11	58,58,58,58	0
58	MG	2A	3046	1/1	0.90	0.14	59,59,59,59	0
58	MG	2O	201	1/1	0.90	0.17	71,71,71,71	0
58	MG	2A	3580	1/1	0.90	0.12	49,49,49,49	0
58	MG	1A	3974	1/1	0.90	0.11	71,71,71,71	0
58	MG	2A	3301	1/1	0.90	0.14	60,60,60,60	0
58	MG	1A	3212	1/1	0.90	0.07	50,50,50,50	0
58	MG	2A	3303	1/1	0.90	0.08	63,63,63,63	0
58	MG	1A	3811	1/1	0.90	0.09	36,36,36,36	0
58	MG	1A	3995	1/1	0.90	0.09	25,25,25,25	0
58	MG	2A	3310	1/1	0.90	0.11	58,58,58,58	0
58	MG	1A	3815	1/1	0.90	0.18	58,58,58,58	0
58	MG	1a	1639	1/1	0.90	0.17	53,53,53,53	0
58	MG	2a	1611	1/1	0.90	0.18	66,66,66,66	0
58	MG	2A	3320	1/1	0.90	0.15	69,69,69,69	0
58	MG	2a	1616	1/1	0.90	0.12	65,65,65,65	0
58	MG	2a	1618	1/1	0.90	0.11	52,52,52,52	0
58	MG	1A	4020	1/1	0.90	0.11	53,53,53,53	0
58	MG	1a	1659	1/1	0.90	0.13	65,65,65,65	0
58	MG	1A	4027	1/1	0.90	0.11	46,46,46,46	0
58	MG	2A	3083	1/1	0.90	0.15	65,65,65,65	0
58	MG	2a	1625	1/1	0.90	0.12	64,64,64,64	0
58	MG	2A	3641	1/1	0.90	0.09	42,42,42,42	0
58	MG	1A	4030	1/1	0.90	0.10	63,63,63,63	0
58	MG	2a	1631	1/1	0.90	0.25	64,64,64,64	0
58	MG	2a	1632	1/1	0.90	0.08	74,74,74,74	0
58	MG	1a	1672	1/1	0.90	0.16	59,59,59,59	0
58	MG	1A	4034	1/1	0.90	0.13	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	1A	3375	1/1	0.90	0.11	39,39,39,39	0
58	MG	2a	1639	1/1	0.90	0.14	55,55,55,55	0
58	MG	1a	1681	1/1	0.90	0.12	48,48,48,48	0
58	MG	1A	3820	1/1	0.90	0.09	42,42,42,42	0
58	MG	2A	3344	1/1	0.90	0.18	72,72,72,72	0
58	MG	2a	1649	1/1	0.90	0.09	73,73,73,73	0
58	MG	1A	3380	1/1	0.90	0.10	45,45,45,45	0
58	MG	2A	3666	1/1	0.90	0.12	51,51,51,51	0
58	MG	1A	4068	1/1	0.90	0.08	44,44,44,44	0
58	MG	1A	3259	1/1	0.90	0.21	72,72,72,72	0
58	MG	2a	1658	1/1	0.90	0.10	62,62,62,62	0
58	MG	1A	3638	1/1	0.90	0.09	45,45,45,45	0
58	MG	2A	3114	1/1	0.90	0.20	63,63,63,63	0
58	MG	2a	1666	1/1	0.90	0.16	69,69,69,69	0
58	MG	1A	3292	1/1	0.90	0.23	56,56,56,56	0
58	MG	2A	3675	1/1	0.90	0.19	67,67,67,67	0
58	MG	2a	1680	1/1	0.90	0.26	59,59,59,59	0
58	MG	1A	3481	1/1	0.90	0.11	42,42,42,42	0
58	MG	2A	3363	1/1	0.90	0.24	63,63,63,63	0
58	MG	1A	3332	1/1	0.90	0.31	68,68,68,68	0
58	MG	2a	1687	1/1	0.90	0.19	67,67,67,67	0
58	MG	2A	3680	1/1	0.90	0.12	51,51,51,51	0
58	MG	2A	3684	1/1	0.90	0.09	57,57,57,57	0
58	MG	2A	3128	1/1	0.90	0.16	51,51,51,51	0
58	MG	2A	3368	1/1	0.90	0.19	61,61,61,61	0
58	MG	1A	3391	1/1	0.90	0.10	64,64,64,64	0
58	MG	2A	3371	1/1	0.90	0.24	63,63,63,63	0
58	MG	2A	3696	1/1	0.90	0.14	48,48,48,48	0
58	MG	2a	1711	1/1	0.90	0.08	71,71,71,71	0
58	MG	2A	3140	1/1	0.90	0.28	65,65,65,65	0
58	MG	1a	1718	1/1	0.90	0.30	66,66,66,66	0
58	MG	2a	1716	1/1	0.90	0.13	64,64,64,64	0
58	MG	1A	3661	1/1	0.90	0.07	25,25,25,25	0
58	MG	1A	3868	1/1	0.90	0.14	42,42,42,42	0
58	MG	2a	1724	1/1	0.90	0.14	76,76,76,76	0
58	MG	1B	208	1/1	0.90	0.11	63,63,63,63	0
58	MG	2A	3710	1/1	0.90	0.13	61,61,61,61	0
58	MG	2a	1731	1/1	0.90	0.24	47,47,47,47	0
58	MG	1B	210	1/1	0.90	0.10	50,50,50,50	0
58	MG	2A	3719	1/1	0.90	0.16	67,67,67,67	0
58	MG	2A	3386	1/1	0.90	0.09	52,52,52,52	0
58	MG	2A	3168	1/1	0.90	0.13	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1740	1/1	0.90	0.23	52,52,52,52	0
58	MG	2A	3726	1/1	0.90	0.10	49,49,49,49	0
58	MG	1A	3680	1/1	0.90	0.08	43,43,43,43	0
58	MG	2a	1749	1/1	0.90	0.13	71,71,71,71	0
58	MG	1A	3877	1/1	0.90	0.14	28,28,28,28	0
58	MG	1A	3023	1/1	0.90	0.26	51,51,51,51	0
58	MG	2A	3179	1/1	0.90	0.16	68,68,68,68	0
58	MG	2A	3401	1/1	0.90	0.29	58,58,58,58	0
58	MG	1B	225	1/1	0.90	0.09	57,57,57,57	0
58	MG	2A	3187	1/1	0.90	0.19	60,60,60,60	0
58	MG	2A	3190	1/1	0.90	0.33	69,69,69,69	0
58	MG	1A	3403	1/1	0.90	0.14	52,52,52,52	0
58	MG	2A	3745	1/1	0.90	0.23	64,64,64,64	0
58	MG	1A	3692	1/1	0.90	0.08	13,13,13,13	0
58	MG	1A	3404	1/1	0.90	0.13	51,51,51,51	0
58	MG	1A	3715	1/1	0.90	0.16	64,64,64,64	0
58	MG	1D	312	1/1	0.90	0.16	40,40,40,40	0
58	MG	1A	3891	1/1	0.90	0.08	29,29,29,29	0
58	MG	1A	3338	1/1	0.90	0.11	42,42,42,42	0
58	MG	2a	1790	1/1	0.90	0.11	59,59,59,59	0
58	MG	2a	1792	1/1	0.90	0.13	62,62,62,62	0
58	MG	1A	3894	1/1	0.90	0.08	37,37,37,37	0
58	MG	2a	1795	1/1	0.90	0.22	63,63,63,63	0
58	MG	1a	1788	1/1	0.90	0.10	70,70,70,70	0
58	MG	2A	3779	1/1	0.90	0.15	64,64,64,64	0
58	MG	2A	3447	1/1	0.90	0.16	65,65,65,65	0
58	MG	1a	1791	1/1	0.90	0.09	75,75,75,75	0
58	MG	2A	3454	1/1	0.90	0.10	65,65,65,65	0
58	MG	2A	3801	1/1	0.90	0.09	80,80,80,80	0
58	MG	1A	3407	1/1	0.90	0.15	46,46,46,46	0
58	MG	2A	3469	1/1	0.90	0.24	65,65,65,65	0
58	MG	2A	3812	1/1	0.90	0.09	53,53,53,53	0
58	MG	2A	3218	1/1	0.90	0.24	59,59,59,59	0
58	MG	2A	3826	1/1	0.90	0.22	69,69,69,69	0
58	MG	1A	3757	1/1	0.90	0.12	58,58,58,58	0
58	MG	1A	3348	1/1	0.90	0.14	50,50,50,50	0
58	MG	1A	3418	1/1	0.90	0.14	65,65,65,65	0
58	MG	2A	3484	1/1	0.90	0.14	66,66,66,66	0
58	MG	2A	3845	1/1	0.90	0.10	67,67,67,67	0
58	MG	2e	201	1/1	0.90	0.09	73,73,73,73	0
58	MG	1A	3927	1/1	0.90	0.15	47,47,47,47	0
58	MG	2A	3848	1/1	0.90	0.15	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	2A	3238	1/1	0.90	0.14	64,64,64,64	0
58	MG	2A	3241	1/1	0.90	0.10	48,48,48,48	0
58	MG	1A	3299	1/1	0.90	0.07	26,26,26,26	0
58	MG	1d	301	1/1	0.90	0.34	62,62,62,62	0
58	MG	2A	3253	1/1	0.90	0.21	73,73,73,73	0
58	MG	2A	3254	1/1	0.90	0.11	62,62,62,62	0
58	MG	1A	3939	1/1	0.90	0.10	26,26,26,26	0
58	MG	1Y	203	1/1	0.90	0.31	49,49,49,49	0
58	MG	1A	3544	1/1	0.90	0.08	62,62,62,62	0
58	MG	1A	3357	1/1	0.90	0.08	55,55,55,55	0
58	MG	1A	3448	1/1	0.90	0.13	61,61,61,61	0
58	MG	2A	3542	1/1	0.90	0.12	38,38,38,38	0
58	MG	1x	104	1/1	0.90	0.23	57,57,57,57	0
58	MG	14	101	1/1	0.90	0.17	69,69,69,69	0
58	MG	2B	209	1/1	0.91	0.10	67,67,67,67	0
58	MG	2A	3007	1/1	0.91	0.21	63,63,63,63	0
58	MG	1A	3393	1/1	0.91	0.25	69,69,69,69	0
58	MG	1A	3760	1/1	0.91	0.08	16,16,16,16	0
58	MG	1A	3887	1/1	0.91	0.07	39,39,39,39	0
58	MG	2B	219	1/1	0.91	0.19	77,77,77,77	0
58	MG	2A	3551	1/1	0.91	0.16	40,40,40,40	0
58	MG	2A	3035	1/1	0.91	0.06	31,31,31,31	0
58	MG	2A	3036	1/1	0.91	0.15	53,53,53,53	0
58	MG	2A	3287	1/1	0.91	0.09	56,56,56,56	0
58	MG	2E	307	1/1	0.91	0.18	63,63,63,63	0
58	MG	2F	303	1/1	0.91	0.07	40,40,40,40	0
58	MG	2F	304	1/1	0.91	0.13	66,66,66,66	0
58	MG	2A	3038	1/1	0.91	0.13	35,35,35,35	0
58	MG	2A	3568	1/1	0.91	0.09	47,47,47,47	0
58	MG	2A	3571	1/1	0.91	0.09	45,45,45,45	0
58	MG	2A	3039	1/1	0.91	0.21	58,58,58,58	0
58	MG	1A	3768	1/1	0.91	0.09	27,27,27,27	0
58	MG	2R	202	1/1	0.91	0.14	62,62,62,62	0
58	MG	2T	3501	1/1	0.91	0.24	65,65,65,65	0
58	MG	2W	201	1/1	0.91	0.18	60,60,60,60	0
58	MG	1A	3051	1/1	0.91	0.11	34,34,34,34	0
58	MG	2A	3045	1/1	0.91	0.08	75,75,75,75	0
58	MG	1a	1646	1/1	0.91	0.15	68,68,68,68	0
58	MG	27	103	1/1	0.91	0.08	44,44,44,44	0
58	MG	2A	3047	1/1	0.91	0.17	72,72,72,72	0
58	MG	1a	1651	1/1	0.91	0.12	46,46,46,46	0
58	MG	2a	1602	1/1	0.91	0.23	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1606	1/1	0.91	0.22	67,67,67,67	0
58	MG	1a	1656	1/1	0.91	0.13	62,62,62,62	0
58	MG	1A	3401	1/1	0.91	0.12	47,47,47,47	0
58	MG	2A	3596	1/1	0.91	0.10	58,58,58,58	0
58	MG	1a	1661	1/1	0.91	0.17	56,56,56,56	0
58	MG	2A	3599	1/1	0.91	0.12	60,60,60,60	0
58	MG	2A	3307	1/1	0.91	0.16	65,65,65,65	0
58	MG	2A	3308	1/1	0.91	0.13	57,57,57,57	0
58	MG	1A	3892	1/1	0.91	0.12	22,22,22,22	0
58	MG	1A	3288	1/1	0.91	0.12	57,57,57,57	0
58	MG	1A	3370	1/1	0.91	0.09	42,42,42,42	0
58	MG	2A	3316	1/1	0.91	0.09	49,49,49,49	0
58	MG	1a	1676	1/1	0.91	0.13	55,55,55,55	0
58	MG	2A	3624	1/1	0.91	0.11	55,55,55,55	0
58	MG	2a	1628	1/1	0.91	0.10	62,62,62,62	0
58	MG	2A	3632	1/1	0.91	0.13	54,54,54,54	0
58	MG	2A	3319	1/1	0.91	0.10	62,62,62,62	0
58	MG	1A	3477	1/1	0.91	0.11	42,42,42,42	0
58	MG	1A	3151	1/1	0.91	0.21	29,29,29,29	0
58	MG	1A	3052	1/1	0.91	0.09	46,46,46,46	0
58	MG	1A	3002	1/1	0.91	0.07	47,47,47,47	0
58	MG	1B	224	1/1	0.91	0.10	50,50,50,50	0
58	MG	1A	3488	1/1	0.91	0.10	40,40,40,40	0
58	MG	2A	3651	1/1	0.91	0.16	66,66,66,66	0
58	MG	2A	3331	1/1	0.91	0.12	59,59,59,59	0
58	MG	2a	1647	1/1	0.91	0.14	61,61,61,61	0
58	MG	1a	1688	1/1	0.91	0.14	51,51,51,51	0
58	MG	1A	3344	1/1	0.91	0.08	38,38,38,38	0
58	MG	2A	3660	1/1	0.91	0.09	66,66,66,66	0
58	MG	2A	3100	1/1	0.91	0.24	44,44,44,44	0
58	MG	2a	1656	1/1	0.91	0.14	85,85,85,85	0
58	MG	2A	3663	1/1	0.91	0.18	56,56,56,56	0
58	MG	2A	3102	1/1	0.91	0.25	67,67,67,67	0
58	MG	2a	1659	1/1	0.91	0.19	60,60,60,60	0
58	MG	2a	1660	1/1	0.91	0.20	78,78,78,78	0
58	MG	1A	3420	1/1	0.91	0.08	40,40,40,40	0
58	MG	1A	3945	1/1	0.91	0.11	58,58,58,58	0
58	MG	2A	3107	1/1	0.91	0.17	55,55,55,55	0
58	MG	2a	1672	1/1	0.91	0.11	56,56,56,56	0
58	MG	2A	3349	1/1	0.91	0.21	61,61,61,61	0
58	MG	1a	1696	1/1	0.91	0.27	59,59,59,59	0
58	MG	2a	1679	1/1	0.91	0.20	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	1A	3650	1/1	0.91	0.09	60,60,60,60	0
58	MG	2A	3673	1/1	0.91	0.08	64,64,64,64	0
58	MG	2A	3356	1/1	0.91	0.30	48,48,48,48	0
58	MG	1A	3506	1/1	0.91	0.14	57,57,57,57	0
58	MG	1a	1705	1/1	0.91	0.24	63,63,63,63	0
58	MG	2A	3124	1/1	0.91	0.26	66,66,66,66	0
58	MG	1a	1706	1/1	0.91	0.24	55,55,55,55	0
58	MG	1A	3653	1/1	0.91	0.09	40,40,40,40	0
58	MG	2A	3685	1/1	0.91	0.19	65,65,65,65	0
58	MG	1a	1717	1/1	0.91	0.09	60,60,60,60	0
58	MG	1E	307	1/1	0.91	0.30	59,59,59,59	0
58	MG	1A	3427	1/1	0.91	0.08	56,56,56,56	0
58	MG	1A	3428	1/1	0.91	0.07	53,53,53,53	0
58	MG	2a	1713	1/1	0.91	0.13	55,55,55,55	0
58	MG	2A	3692	1/1	0.91	0.09	67,67,67,67	0
58	MG	1A	3837	1/1	0.91	0.10	52,52,52,52	0
58	MG	1F	313	1/1	0.91	0.15	50,50,50,50	0
58	MG	1A	3838	1/1	0.91	0.17	61,61,61,61	0
58	MG	2a	1718	1/1	0.91	0.13	74,74,74,74	0
58	MG	1A	3061	1/1	0.91	0.21	43,43,43,43	0
58	MG	2A	3377	1/1	0.91	0.15	58,58,58,58	0
58	MG	1A	3977	1/1	0.91	0.08	67,67,67,67	0
58	MG	1A	3978	1/1	0.91	0.09	57,57,57,57	0
58	MG	2a	1729	1/1	0.91	0.17	61,61,61,61	0
58	MG	1S	201	1/1	0.91	0.25	41,41,41,41	0
58	MG	1A	3312	1/1	0.91	0.06	34,34,34,34	0
58	MG	2A	3178	1/1	0.91	0.11	44,44,44,44	0
58	MG	1a	1757	1/1	0.91	0.18	51,51,51,51	0
58	MG	1W	201	1/1	0.91	0.15	49,49,49,49	0
58	MG	1A	3440	1/1	0.91	0.18	46,46,46,46	0
58	MG	2A	3394	1/1	0.91	0.09	60,60,60,60	0
58	MG	1Y	202	1/1	0.91	0.15	66,66,66,66	0
58	MG	2A	3732	1/1	0.91	0.10	58,58,58,58	0
58	MG	1a	1772	1/1	0.91	0.10	66,66,66,66	0
58	MG	2A	3734	1/1	0.91	0.12	53,53,53,53	0
58	MG	2A	3735	1/1	0.91	0.12	54,54,54,54	0
58	MG	1A	3446	1/1	0.91	0.12	52,52,52,52	0
58	MG	2A	3407	1/1	0.91	0.15	41,41,41,41	0
58	MG	1A	4016	1/1	0.91	0.10	58,58,58,58	0
58	MG	2A	3417	1/1	0.91	0.19	49,49,49,49	0
58	MG	1A	3855	1/1	0.91	0.12	55,55,55,55	0
58	MG	2a	1768	1/1	0.91	0.08	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	2A	3420	1/1	0.91	0.25	64,64,64,64	0
58	MG	1A	3860	1/1	0.91	0.41	40,40,40,40	0
58	MG	2a	1778	1/1	0.91	0.11	52,52,52,52	0
58	MG	13	101	1/1	0.91	0.12	54,54,54,54	0
58	MG	2A	3756	1/1	0.91	0.10	63,63,63,63	0
58	MG	2A	3200	1/1	0.91	0.10	47,47,47,47	0
58	MG	2A	3428	1/1	0.91	0.20	62,62,62,62	0
58	MG	2A	3431	1/1	0.91	0.20	57,57,57,57	0
58	MG	2A	3204	1/1	0.91	0.12	58,58,58,58	0
58	MG	13	103	1/1	0.91	0.10	44,44,44,44	0
58	MG	1A	3862	1/1	0.91	0.11	52,52,52,52	0
58	MG	1A	3095	1/1	0.91	0.09	66,66,66,66	0
58	MG	1A	3728	1/1	0.91	0.16	56,56,56,56	0
58	MG	2A	3214	1/1	0.91	0.09	64,64,64,64	0
58	MG	2A	3786	1/1	0.91	0.10	55,55,55,55	0
58	MG	1a	1603	1/1	0.91	0.15	64,64,64,64	0
58	MG	2A	3794	1/1	0.91	0.21	67,67,67,67	0
58	MG	1a	1607	1/1	0.91	0.14	56,56,56,56	0
58	MG	2a	1811	1/1	0.91	0.07	70,70,70,70	0
58	MG	2A	3802	1/1	0.91	0.11	52,52,52,52	0
58	MG	1A	3743	1/1	0.91	0.09	19,19,19,19	0
58	MG	2A	3225	1/1	0.91	0.23	55,55,55,55	0
58	MG	2A	3460	1/1	0.91	0.10	71,71,71,71	0
58	MG	2A	3465	1/1	0.91	0.18	59,59,59,59	0
58	MG	2a	1819	1/1	0.91	0.17	55,55,55,55	0
58	MG	1a	1611	1/1	0.91	0.21	63,63,63,63	0
58	MG	1a	1613	1/1	0.91	0.13	61,61,61,61	0
58	MG	2A	3830	1/1	0.91	0.09	49,49,49,49	0
58	MG	1w	102	1/1	0.91	0.09	67,67,67,67	0
58	MG	2A	3481	1/1	0.91	0.23	54,54,54,54	0
58	MG	2A	3840	1/1	0.91	0.08	66,66,66,66	0
58	MG	2g	201	1/1	0.91	0.06	71,71,71,71	0
58	MG	2i	201	1/1	0.91	0.14	71,71,71,71	0
58	MG	1a	1615	1/1	0.91	0.11	60,60,60,60	0
58	MG	1a	1616	1/1	0.91	0.13	66,66,66,66	0
58	MG	1A	3456	1/1	0.91	0.07	45,45,45,45	0
58	MG	2A	3244	1/1	0.91	0.13	60,60,60,60	0
58	MG	2l	203	1/1	0.91	0.09	62,62,62,62	0
58	MG	1A	3751	1/1	0.91	0.11	35,35,35,35	0
58	MG	2A	3248	1/1	0.91	0.08	53,53,53,53	0
58	MG	2A	3250	1/1	0.91	0.10	50,50,50,50	0
58	MG	2A	3505	1/1	0.91	0.14	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	1A	4067	1/1	0.91	0.12	55,55,55,55	0
58	MG	1x	106	1/1	0.91	0.20	56,56,56,56	0
58	MG	1A	3392	1/1	0.91	0.17	51,51,51,51	0
58	MG	2A	3513	1/1	0.91	0.14	56,56,56,56	0
58	MG	2A	3514	1/1	0.91	0.11	46,46,46,46	0
58	MG	2A	3519	1/1	0.91	0.13	51,51,51,51	0
58	MG	2A	3258	1/1	0.91	0.15	57,57,57,57	0
58	MG	2A	3005	1/1	0.91	0.24	58,58,58,58	0
58	MG	2F	302	1/1	0.92	0.08	58,58,58,58	0
58	MG	1A	4056	1/1	0.92	0.12	46,46,46,46	0
58	MG	1A	3331	1/1	0.92	0.09	41,41,41,41	0
58	MG	1A	3450	1/1	0.92	0.10	56,56,56,56	0
58	MG	1a	1658	1/1	0.92	0.24	65,65,65,65	0
58	MG	2A	3314	1/1	0.92	0.07	49,49,49,49	0
58	MG	2A	3586	1/1	0.92	0.14	52,52,52,52	0
58	MG	2A	3588	1/1	0.92	0.08	47,47,47,47	0
58	MG	2A	3589	1/1	0.92	0.10	64,64,64,64	0
58	MG	1A	3714	1/1	0.92	0.07	63,63,63,63	0
58	MG	2U	201	1/1	0.92	0.28	50,50,50,50	0
58	MG	1A	4071	1/1	0.92	0.10	44,44,44,44	0
58	MG	1A	3266	1/1	0.92	0.28	52,52,52,52	0
58	MG	1a	1667	1/1	0.92	0.14	48,48,48,48	0
58	MG	1A	3867	1/1	0.92	0.07	39,39,39,39	0
58	MG	25	105	1/1	0.92	0.09	48,48,48,48	0
58	MG	2A	3322	1/1	0.92	0.23	55,55,55,55	0
58	MG	2A	3081	1/1	0.92	0.26	55,55,55,55	0
58	MG	1A	3720	1/1	0.92	0.22	58,58,58,58	0
58	MG	1A	3180	1/1	0.92	0.16	52,52,52,52	0
58	MG	2a	1603	1/1	0.92	0.08	68,68,68,68	0
58	MG	2A	3328	1/1	0.92	0.10	57,57,57,57	0
58	MG	1A	3546	1/1	0.92	0.38	40,40,40,40	0
58	MG	1A	3555	1/1	0.92	0.21	49,49,49,49	0
58	MG	2a	1609	1/1	0.92	0.17	73,73,73,73	0
58	MG	2A	3625	1/1	0.92	0.19	62,62,62,62	0
58	MG	1A	3569	1/1	0.92	0.14	48,48,48,48	0
58	MG	2A	3333	1/1	0.92	0.12	55,55,55,55	0
58	MG	1A	4097	1/1	0.92	0.17	47,47,47,47	0
58	MG	1A	3283	1/1	0.92	0.25	45,45,45,45	0
58	MG	2A	3638	1/1	0.92	0.12	57,57,57,57	0
58	MG	1A	3460	1/1	0.92	0.12	59,59,59,59	0
58	MG	1A	3758	1/1	0.92	0.14	47,47,47,47	0
58	MG	2A	3643	1/1	0.92	0.14	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	1A	3185	1/1	0.92	0.07	37,37,37,37	0
58	MG	2A	3345	1/1	0.92	0.11	53,53,53,53	0
58	MG	2A	3347	1/1	0.92	0.14	61,61,61,61	0
58	MG	2A	3652	1/1	0.92	0.10	75,75,75,75	0
58	MG	1a	1693	1/1	0.92	0.21	55,55,55,55	0
58	MG	1A	3593	1/1	0.92	0.17	48,48,48,48	0
58	MG	1A	3769	1/1	0.92	0.11	36,36,36,36	0
58	MG	2A	3353	1/1	0.92	0.11	61,61,61,61	0
58	MG	1B	223	1/1	0.92	0.16	51,51,51,51	0
58	MG	1A	3114	1/1	0.92	0.06	37,37,37,37	0
58	MG	2a	1640	1/1	0.92	0.15	76,76,76,76	0
58	MG	1a	1699	1/1	0.92	0.10	58,58,58,58	0
58	MG	1A	3776	1/1	0.92	0.08	33,33,33,33	0
58	MG	1A	3895	1/1	0.92	0.17	37,37,37,37	0
58	MG	2A	3361	1/1	0.92	0.14	63,63,63,63	0
58	MG	1A	3777	1/1	0.92	0.07	60,60,60,60	0
58	MG	1a	1713	1/1	0.92	0.23	64,64,64,64	0
58	MG	2A	3129	1/1	0.92	0.10	67,67,67,67	0
58	MG	2A	3132	1/1	0.92	0.08	55,55,55,55	0
58	MG	1B	231	1/1	0.92	0.08	61,61,61,61	0
58	MG	1A	3596	1/1	0.92	0.17	55,55,55,55	0
58	MG	2A	3142	1/1	0.92	0.13	52,52,52,52	0
58	MG	1A	3907	1/1	0.92	0.07	46,46,46,46	0
58	MG	1a	1726	1/1	0.92	0.09	44,44,44,44	0
58	MG	2A	3683	1/1	0.92	0.09	67,67,67,67	0
58	MG	2A	3375	1/1	0.92	0.21	66,66,66,66	0
58	MG	1A	3129	1/1	0.92	0.07	56,56,56,56	0
58	MG	1A	3354	1/1	0.92	0.16	53,53,53,53	0
58	MG	1A	3475	1/1	0.92	0.13	42,42,42,42	0
58	MG	1A	3355	1/1	0.92	0.10	63,63,63,63	0
58	MG	2a	1678	1/1	0.92	0.17	62,62,62,62	0
58	MG	2A	3170	1/1	0.92	0.12	59,59,59,59	0
58	MG	2A	3691	1/1	0.92	0.07	66,66,66,66	0
58	MG	1A	3479	1/1	0.92	0.29	54,54,54,54	0
58	MG	1A	3940	1/1	0.92	0.09	22,22,22,22	0
58	MG	1a	1742	1/1	0.92	0.09	70,70,70,70	0
58	MG	2A	3702	1/1	0.92	0.11	45,45,45,45	0
58	MG	2a	1693	1/1	0.92	0.20	70,70,70,70	0
58	MG	2a	1698	1/1	0.92	0.30	58,58,58,58	0
58	MG	1A	3942	1/1	0.92	0.14	66,66,66,66	0
58	MG	1A	3072	1/1	0.92	0.06	15,15,15,15	0
58	MG	2A	3393	1/1	0.92	0.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3411	1/1	0.92	0.12	47,47,47,47	0
58	MG	2A	3709	1/1	0.92	0.14	51,51,51,51	0
58	MG	1A	3640	1/1	0.92	0.11	57,57,57,57	0
58	MG	1A	3641	1/1	0.92	0.06	22,22,22,22	0
58	MG	2a	1709	1/1	0.92	0.07	73,73,73,73	0
58	MG	2a	1710	1/1	0.92	0.12	75,75,75,75	0
58	MG	1A	3813	1/1	0.92	0.07	45,45,45,45	0
58	MG	1S	202	1/1	0.92	0.12	46,46,46,46	0
58	MG	1a	1762	1/1	0.92	0.12	61,61,61,61	0
58	MG	2A	3725	1/1	0.92	0.16	53,53,53,53	0
58	MG	2A	3415	1/1	0.92	0.17	63,63,63,63	0
58	MG	2A	3416	1/1	0.92	0.25	59,59,59,59	0
58	MG	2A	3194	1/1	0.92	0.11	55,55,55,55	0
58	MG	2a	1719	1/1	0.92	0.18	63,63,63,63	0
58	MG	1a	1767	1/1	0.92	0.10	55,55,55,55	0
58	MG	2a	1722	1/1	0.92	0.18	64,64,64,64	0
58	MG	2a	1723	1/1	0.92	0.16	64,64,64,64	0
58	MG	2A	3196	1/1	0.92	0.23	65,65,65,65	0
58	MG	1A	3814	1/1	0.92	0.18	48,48,48,48	0
58	MG	1A	3305	1/1	0.92	0.22	53,53,53,53	0
58	MG	1A	3964	1/1	0.92	0.10	30,30,30,30	0
58	MG	1A	3087	1/1	0.92	0.22	36,36,36,36	0
58	MG	2A	3429	1/1	0.92	0.14	39,39,39,39	0
58	MG	2A	3430	1/1	0.92	0.27	60,60,60,60	0
58	MG	1A	3310	1/1	0.92	0.08	49,49,49,49	0
58	MG	1a	1780	1/1	0.92	0.12	47,47,47,47	0
58	MG	2a	1738	1/1	0.92	0.08	48,48,48,48	0
58	MG	1A	3045	1/1	0.92	0.09	37,37,37,37	0
58	MG	2a	1741	1/1	0.92	0.18	61,61,61,61	0
58	MG	1A	3313	1/1	0.92	0.09	53,53,53,53	0
58	MG	2a	1743	1/1	0.92	0.09	60,60,60,60	0
58	MG	2A	3435	1/1	0.92	0.22	55,55,55,55	0
58	MG	2a	1747	1/1	0.92	0.09	72,72,72,72	0
58	MG	1a	1792	1/1	0.92	0.14	60,60,60,60	0
58	MG	1A	3980	1/1	0.92	0.09	20,20,20,20	0
58	MG	2a	1751	1/1	0.92	0.24	70,70,70,70	0
58	MG	1A	3376	1/1	0.92	0.09	49,49,49,49	0
58	MG	1A	3676	1/1	0.92	0.12	18,18,18,18	0
58	MG	2A	3765	1/1	0.92	0.14	64,64,64,64	0
58	MG	13	104	1/1	0.92	0.10	28,28,28,28	0
58	MG	2a	1758	1/1	0.92	0.07	65,65,65,65	0
58	MG	1A	3678	1/1	0.92	0.06	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	16	101	1/1	0.92	0.20	43,43,43,43	0
58	MG	2A	3778	1/1	0.92	0.09	51,51,51,51	0
58	MG	2a	1767	1/1	0.92	0.10	69,69,69,69	0
58	MG	2A	3459	1/1	0.92	0.11	67,67,67,67	0
58	MG	2A	3780	1/1	0.92	0.10	56,56,56,56	0
58	MG	2a	1773	1/1	0.92	0.20	70,70,70,70	0
58	MG	18	109	1/1	0.92	0.12	49,49,49,49	0
58	MG	2A	3464	1/1	0.92	0.22	51,51,51,51	0
58	MG	2A	3785	1/1	0.92	0.10	46,46,46,46	0
58	MG	1f	201	1/1	0.92	0.14	49,49,49,49	0
58	MG	2A	3467	1/1	0.92	0.16	56,56,56,56	0
58	MG	1n	101	1/1	0.92	0.14	57,57,57,57	0
58	MG	2A	3242	1/1	0.92	0.31	51,51,51,51	0
58	MG	1A	3997	1/1	0.92	0.11	65,65,65,65	0
58	MG	2A	3473	1/1	0.92	0.14	57,57,57,57	0
58	MG	1v	101	1/1	0.92	0.20	75,75,75,75	0
58	MG	2A	3811	1/1	0.92	0.11	51,51,51,51	0
58	MG	2a	1797	1/1	0.92	0.14	69,69,69,69	0
58	MG	1A	3998	1/1	0.92	0.11	72,72,72,72	0
58	MG	2A	3814	1/1	0.92	0.08	60,60,60,60	0
58	MG	1A	4011	1/1	0.92	0.12	56,56,56,56	0
58	MG	1A	3168	1/1	0.92	0.17	57,57,57,57	0
58	MG	1A	4018	1/1	0.92	0.10	61,61,61,61	0
58	MG	2A	3486	1/1	0.92	0.09	59,59,59,59	0
58	MG	2a	1810	1/1	0.92	0.11	64,64,64,64	0
58	MG	1A	3262	1/1	0.92	0.18	59,59,59,59	0
58	MG	1A	3847	1/1	0.92	0.09	46,46,46,46	0
58	MG	1A	4021	1/1	0.92	0.10	45,45,45,45	0
58	MG	2A	3504	1/1	0.92	0.15	58,58,58,58	0
58	MG	1A	3685	1/1	0.92	0.08	42,42,42,42	0
58	MG	2A	3263	1/1	0.92	0.21	59,59,59,59	0
58	MG	1A	3854	1/1	0.92	0.14	66,66,66,66	0
58	MG	2A	3001	1/1	0.92	0.28	53,53,53,53	0
58	MG	2A	3271	1/1	0.92	0.10	61,61,61,61	0
58	MG	1a	1620	1/1	0.92	0.16	52,52,52,52	0
58	MG	1A	3241	1/1	0.92	0.19	50,50,50,50	0
58	MG	2A	3013	1/1	0.92	0.08	49,49,49,49	0
58	MG	2A	3525	1/1	0.92	0.11	68,68,68,68	0
58	MG	1a	1623	1/1	0.92	0.12	47,47,47,47	0
58	MG	1a	1626	1/1	0.92	0.22	64,64,64,64	0
58	MG	2B	202	1/1	0.92	0.07	65,65,65,65	0
58	MG	2A	3534	1/1	0.92	0.09	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	1a	1627	1/1	0.92	0.19	52,52,52,52	0
58	MG	1A	4035	1/1	0.92	0.07	50,50,50,50	0
58	MG	1a	1630	1/1	0.92	0.20	60,60,60,60	0
58	MG	2A	3547	1/1	0.92	0.08	37,37,37,37	0
58	MG	1A	4039	1/1	0.92	0.10	27,27,27,27	0
58	MG	1a	1632	1/1	0.92	0.22	63,63,63,63	0
58	MG	2A	3041	1/1	0.92	0.23	55,55,55,55	0
58	MG	2B	217	1/1	0.92	0.10	62,62,62,62	0
58	MG	1A	3856	1/1	0.92	0.08	27,27,27,27	0
58	MG	1A	4045	1/1	0.92	0.08	52,52,52,52	0
58	MG	1A	3859	1/1	0.92	0.11	62,62,62,62	0
58	MG	1A	4049	1/1	0.92	0.14	57,57,57,57	0
58	MG	1A	4051	1/1	0.92	0.09	58,58,58,58	0
58	MG	2A	3306	1/1	0.92	0.10	51,51,51,51	0
58	MG	2A	3048	1/1	0.92	0.08	46,46,46,46	0
58	MG	1A	3198	1/1	0.93	0.10	32,32,32,32	0
58	MG	2A	3549	1/1	0.93	0.10	44,44,44,44	0
58	MG	2E	302	1/1	0.93	0.13	58,58,58,58	0
58	MG	1a	1647	1/1	0.93	0.25	54,54,54,54	0
58	MG	2A	3552	1/1	0.93	0.09	41,41,41,41	0
58	MG	2A	3296	1/1	0.93	0.13	56,56,56,56	0
58	MG	1A	4096	1/1	0.93	0.20	56,56,56,56	0
58	MG	2A	3298	1/1	0.93	0.14	51,51,51,51	0
58	MG	1a	1653	1/1	0.93	0.07	46,46,46,46	0
58	MG	1a	1655	1/1	0.93	0.11	60,60,60,60	0
58	MG	2A	3570	1/1	0.93	0.06	41,41,41,41	0
58	MG	2O	202	1/1	0.93	0.10	55,55,55,55	0
58	MG	2P	201	1/1	0.93	0.10	50,50,50,50	0
58	MG	1A	3803	1/1	0.93	0.10	64,64,64,64	0
58	MG	1A	3909	1/1	0.93	0.20	39,39,39,39	0
58	MG	1B	205	1/1	0.93	0.21	61,61,61,61	0
58	MG	1A	3808	1/1	0.93	0.35	28,28,28,28	0
58	MG	1A	3918	1/1	0.93	0.07	58,58,58,58	0
58	MG	2U	202	1/1	0.93	0.09	60,60,60,60	0
58	MG	1A	3300	1/1	0.93	0.11	37,37,37,37	0
58	MG	2Z	301	1/1	0.93	0.13	78,78,78,78	0
58	MG	2A	3054	1/1	0.93	0.27	60,60,60,60	0
58	MG	1a	1668	1/1	0.93	0.15	51,51,51,51	0
58	MG	2A	3057	1/1	0.93	0.16	72,72,72,72	0
58	MG	25	101	1/1	0.93	0.25	62,62,62,62	0
58	MG	1B	212	1/1	0.93	0.17	64,64,64,64	0
58	MG	2A	3315	1/1	0.93	0.18	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	2A	3060	1/1	0.93	0.15	55,55,55,55	0
58	MG	1A	3537	1/1	0.93	0.15	52,52,52,52	0
58	MG	1a	1674	1/1	0.93	0.17	56,56,56,56	0
58	MG	1A	3656	1/1	0.93	0.10	39,39,39,39	0
58	MG	1A	3812	1/1	0.93	0.10	42,42,42,42	0
58	MG	2A	3073	1/1	0.93	0.08	43,43,43,43	0
58	MG	2A	3323	1/1	0.93	0.15	57,57,57,57	0
58	MG	2A	3603	1/1	0.93	0.09	57,57,57,57	0
58	MG	2A	3604	1/1	0.93	0.15	60,60,60,60	0
58	MG	1a	1679	1/1	0.93	0.14	59,59,59,59	0
58	MG	2A	3606	1/1	0.93	0.08	23,23,23,23	0
58	MG	2a	1614	1/1	0.93	0.22	74,74,74,74	0
58	MG	2A	3080	1/1	0.93	0.09	40,40,40,40	0
58	MG	1A	3349	1/1	0.93	0.13	52,52,52,52	0
58	MG	1A	3665	1/1	0.93	0.06	35,35,35,35	0
58	MG	1B	226	1/1	0.93	0.07	48,48,48,48	0
58	MG	2A	3616	1/1	0.93	0.09	33,33,33,33	0
58	MG	1A	3667	1/1	0.93	0.08	19,19,19,19	0
58	MG	1A	3540	1/1	0.93	0.14	53,53,53,53	0
58	MG	2A	3631	1/1	0.93	0.08	42,42,42,42	0
58	MG	1A	3301	1/1	0.93	0.31	51,51,51,51	0
58	MG	1a	1689	1/1	0.93	0.30	51,51,51,51	0
58	MG	1B	233	1/1	0.93	0.08	46,46,46,46	0
58	MG	1a	1692	1/1	0.93	0.27	47,47,47,47	0
58	MG	1A	3057	1/1	0.93	0.07	41,41,41,41	0
58	MG	2A	3340	1/1	0.93	0.09	54,54,54,54	0
58	MG	1A	3205	1/1	0.93	0.12	53,53,53,53	0
58	MG	1A	3836	1/1	0.93	0.08	36,36,36,36	0
58	MG	1A	3551	1/1	0.93	0.13	24,24,24,24	0
58	MG	1A	3308	1/1	0.93	0.13	47,47,47,47	0
58	MG	1A	3968	1/1	0.93	0.07	68,68,68,68	0
58	MG	1A	3969	1/1	0.93	0.10	60,60,60,60	0
58	MG	2A	3352	1/1	0.93	0.19	62,62,62,62	0
58	MG	2a	1648	1/1	0.93	0.09	60,60,60,60	0
58	MG	1a	1702	1/1	0.93	0.14	53,53,53,53	0
58	MG	2A	3354	1/1	0.93	0.09	46,46,46,46	0
58	MG	1A	3564	1/1	0.93	0.14	36,36,36,36	0
58	MG	2A	3125	1/1	0.93	0.14	50,50,50,50	0
58	MG	1E	316	1/1	0.93	0.07	36,36,36,36	0
58	MG	1a	1708	1/1	0.93	0.47	69,69,69,69	0
58	MG	1A	3972	1/1	0.93	0.08	40,40,40,40	0
58	MG	1G	201	1/1	0.93	0.10	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	3130	1/1	0.93	0.08	47,47,47,47	0
58	MG	2a	1662	1/1	0.93	0.16	69,69,69,69	0
58	MG	1a	1715	1/1	0.93	0.17	53,53,53,53	0
58	MG	2A	3133	1/1	0.93	0.12	80,80,80,80	0
58	MG	2A	3134	1/1	0.93	0.08	40,40,40,40	0
58	MG	2a	1668	1/1	0.93	0.08	67,67,67,67	0
58	MG	2a	1670	1/1	0.93	0.25	66,66,66,66	0
58	MG	2A	3367	1/1	0.93	0.09	54,54,54,54	0
58	MG	1A	3699	1/1	0.93	0.09	36,36,36,36	0
58	MG	2a	1675	1/1	0.93	0.27	63,63,63,63	0
58	MG	2A	3137	1/1	0.93	0.19	58,58,58,58	0
58	MG	1A	3841	1/1	0.93	0.06	38,38,38,38	0
58	MG	1a	1725	1/1	0.93	0.07	46,46,46,46	0
58	MG	1O	201	1/1	0.93	0.08	54,54,54,54	0
58	MG	2A	3147	1/1	0.93	0.12	48,48,48,48	0
58	MG	2A	3148	1/1	0.93	0.23	52,52,52,52	0
58	MG	1A	3360	1/1	0.93	0.10	37,37,37,37	0
58	MG	2a	1685	1/1	0.93	0.29	68,68,68,68	0
58	MG	2A	3378	1/1	0.93	0.16	62,62,62,62	0
58	MG	2a	1688	1/1	0.93	0.13	60,60,60,60	0
58	MG	1A	3712	1/1	0.93	0.13	52,52,52,52	0
58	MG	2a	1694	1/1	0.93	0.20	62,62,62,62	0
58	MG	2A	3381	1/1	0.93	0.07	50,50,50,50	0
58	MG	2A	3156	1/1	0.93	0.21	56,56,56,56	0
58	MG	1Q	207	1/1	0.93	0.09	32,32,32,32	0
58	MG	1R	202	1/1	0.93	0.10	49,49,49,49	0
58	MG	2A	3694	1/1	0.93	0.08	19,19,19,19	0
58	MG	1R	204	1/1	0.93	0.11	44,44,44,44	0
58	MG	2A	3388	1/1	0.93	0.12	68,68,68,68	0
58	MG	1A	3473	1/1	0.93	0.14	46,46,46,46	0
58	MG	1a	1741	1/1	0.93	0.10	61,61,61,61	0
58	MG	2A	3172	1/1	0.93	0.16	56,56,56,56	0
58	MG	2A	3392	1/1	0.93	0.22	68,68,68,68	0
58	MG	1A	3987	1/1	0.93	0.08	40,40,40,40	0
58	MG	1U	204	1/1	0.93	0.25	37,37,37,37	0
58	MG	1A	3586	1/1	0.93	0.06	42,42,42,42	0
58	MG	1V	209	1/1	0.93	0.10	55,55,55,55	0
58	MG	1A	3073	1/1	0.93	0.26	53,53,53,53	0
58	MG	2A	3720	1/1	0.93	0.12	56,56,56,56	0
58	MG	1A	3724	1/1	0.93	0.11	63,63,63,63	0
58	MG	2A	3411	1/1	0.93	0.12	41,41,41,41	0
58	MG	2a	1721	1/1	0.93	0.17	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	1A	3727	1/1	0.93	0.07	68,68,68,68	0
58	MG	1A	3170	1/1	0.93	0.19	39,39,39,39	0
58	MG	1A	3416	1/1	0.93	0.18	48,48,48,48	0
58	MG	1A	3863	1/1	0.93	0.10	54,54,54,54	0
58	MG	1A	3213	1/1	0.93	0.13	50,50,50,50	0
58	MG	10	108	1/1	0.93	0.14	52,52,52,52	0
58	MG	2a	1730	1/1	0.93	0.11	66,66,66,66	0
58	MG	11	104	1/1	0.93	0.10	63,63,63,63	0
58	MG	1A	3225	1/1	0.93	0.07	48,48,48,48	0
58	MG	1A	3230	1/1	0.93	0.09	45,45,45,45	0
58	MG	2A	3736	1/1	0.93	0.07	61,61,61,61	0
58	MG	2A	3426	1/1	0.93	0.11	71,71,71,71	0
58	MG	1A	3025	1/1	0.93	0.07	43,43,43,43	0
58	MG	2a	1739	1/1	0.93	0.35	59,59,59,59	0
58	MG	1a	1782	1/1	0.93	0.06	50,50,50,50	0
58	MG	1a	1783	1/1	0.93	0.07	63,63,63,63	0
58	MG	1A	3608	1/1	0.93	0.07	29,29,29,29	0
58	MG	2A	3744	1/1	0.93	0.16	51,51,51,51	0
58	MG	15	106	1/1	0.93	0.09	46,46,46,46	0
58	MG	1A	3872	1/1	0.93	0.27	44,44,44,44	0
58	MG	2A	3753	1/1	0.93	0.10	40,40,40,40	0
58	MG	18	102	1/1	0.93	0.15	37,37,37,37	0
58	MG	18	105	1/1	0.93	0.17	40,40,40,40	0
58	MG	18	106	1/1	0.93	0.14	56,56,56,56	0
58	MG	1A	3875	1/1	0.93	0.28	51,51,51,51	0
58	MG	1a	1808	1/1	0.93	0.20	56,56,56,56	0
58	MG	2A	3227	1/1	0.93	0.14	57,57,57,57	0
58	MG	2A	3770	1/1	0.93	0.13	58,58,58,58	0
58	MG	2a	1759	1/1	0.93	0.08	71,71,71,71	0
58	MG	2A	3231	1/1	0.93	0.17	41,41,41,41	0
58	MG	2A	3774	1/1	0.93	0.13	61,61,61,61	0
58	MG	2a	1765	1/1	0.93	0.06	68,68,68,68	0
58	MG	1A	3182	1/1	0.93	0.09	53,53,53,53	0
58	MG	1A	4040	1/1	0.93	0.06	39,39,39,39	0
58	MG	1A	3617	1/1	0.93	0.12	11,11,11,11	0
58	MG	1A	3620	1/1	0.93	0.09	65,65,65,65	0
58	MG	2A	3240	1/1	0.93	0.09	38,38,38,38	0
58	MG	2a	1775	1/1	0.93	0.13	61,61,61,61	0
58	MG	1A	3149	1/1	0.93	0.32	34,34,34,34	0
58	MG	2A	3466	1/1	0.93	0.16	50,50,50,50	0
58	MG	1A	3883	1/1	0.93	0.07	28,28,28,28	0
58	MG	1A	3053	1/1	0.93	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1785	1/1	0.93	0.11	65,65,65,65	0
58	MG	2A	3791	1/1	0.93	0.11	71,71,71,71	0
58	MG	1a	1614	1/1	0.93	0.19	54,54,54,54	0
58	MG	2A	3245	1/1	0.93	0.12	50,50,50,50	0
58	MG	2A	3800	1/1	0.93	0.11	60,60,60,60	0
58	MG	1A	4053	1/1	0.93	0.18	36,36,36,36	0
58	MG	2A	3475	1/1	0.93	0.14	60,60,60,60	0
58	MG	1A	3630	1/1	0.93	0.06	28,28,28,28	0
58	MG	2A	3808	1/1	0.93	0.14	35,35,35,35	0
58	MG	1A	3162	1/1	0.93	0.11	47,47,47,47	0
58	MG	2a	1799	1/1	0.93	0.13	71,71,71,71	0
58	MG	2A	3251	1/1	0.93	0.22	62,62,62,62	0
58	MG	1A	4062	1/1	0.93	0.09	23,23,23,23	0
58	MG	1A	3516	1/1	0.93	0.11	49,49,49,49	0
58	MG	2a	1803	1/1	0.93	0.12	53,53,53,53	0
58	MG	1A	3390	1/1	0.93	0.23	36,36,36,36	0
58	MG	2A	3819	1/1	0.93	0.17	63,63,63,63	0
58	MG	2a	1808	1/1	0.93	0.12	74,74,74,74	0
58	MG	2A	3487	1/1	0.93	0.10	51,51,51,51	0
58	MG	2A	3494	1/1	0.93	0.10	62,62,62,62	0
58	MG	2A	3257	1/1	0.93	0.14	48,48,48,48	0
58	MG	2A	3500	1/1	0.93	0.13	63,63,63,63	0
58	MG	1A	4069	1/1	0.93	0.09	45,45,45,45	0
58	MG	2a	1816	1/1	0.93	0.15	68,68,68,68	0
58	MG	1x	107	1/1	0.93	0.24	67,67,67,67	0
58	MG	2A	3503	1/1	0.93	0.13	40,40,40,40	0
58	MG	1A	3519	1/1	0.93	0.06	50,50,50,50	0
58	MG	1x	110	1/1	0.93	0.21	63,63,63,63	0
58	MG	2A	3507	1/1	0.93	0.18	57,57,57,57	0
58	MG	2A	3268	1/1	0.93	0.20	65,65,65,65	0
58	MG	2a	1828	1/1	0.93	0.11	71,71,71,71	0
58	MG	1A	4073	1/1	0.93	0.08	32,32,32,32	0
58	MG	1A	3793	1/1	0.93	0.10	39,39,39,39	0
58	MG	1A	3523	1/1	0.93	0.22	36,36,36,36	0
58	MG	2f	202	1/1	0.93	0.10	67,67,67,67	0
58	MG	2A	3008	1/1	0.93	0.13	55,55,55,55	0
58	MG	2A	3515	1/1	0.93	0.11	60,60,60,60	0
58	MG	2A	3518	1/1	0.93	0.08	49,49,49,49	0
58	MG	2A	3275	1/1	0.93	0.24	55,55,55,55	0
58	MG	2A	3520	1/1	0.93	0.10	33,33,33,33	0
58	MG	2A	3521	1/1	0.93	0.13	58,58,58,58	0
58	MG	1A	4081	1/1	0.93	0.09	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	3524	1/1	0.93	0.08	40,40,40,40	0
58	MG	2q	201	1/1	0.93	0.08	72,72,72,72	0
58	MG	2A	3277	1/1	0.93	0.10	58,58,58,58	0
58	MG	1A	3339	1/1	0.93	0.08	52,52,52,52	0
58	MG	2A	3529	1/1	0.93	0.10	57,57,57,57	0
58	MG	2B	211	1/1	0.93	0.13	57,57,57,57	0
58	MG	2B	213	1/1	0.93	0.20	62,62,62,62	0
58	MG	2A	3286	1/1	0.93	0.08	47,47,47,47	0
58	MG	1A	3898	1/1	0.93	0.07	54,54,54,54	0
58	MG	2A	3537	1/1	0.93	0.08	35,35,35,35	0
58	MG	1A	4084	1/1	0.93	0.17	56,56,56,56	0
58	MG	1A	3902	1/1	0.93	0.13	44,44,44,44	0
58	MG	1A	3903	1/1	0.93	0.22	29,29,29,29	0
59	K	1A	3556	1/1	0.93	0.20	72,72,72,72	0
58	MG	2A	3810	1/1	0.94	0.11	59,59,59,59	0
58	MG	1A	4055	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	3829	1/1	0.94	0.09	35,35,35,35	0
58	MG	1A	3597	1/1	0.94	0.15	32,32,32,32	0
58	MG	1a	1669	1/1	0.94	0.18	63,63,63,63	0
58	MG	2A	3424	1/1	0.94	0.28	58,58,58,58	0
58	MG	2A	3820	1/1	0.94	0.13	44,44,44,44	0
58	MG	1A	3433	1/1	0.94	0.14	44,44,44,44	0
58	MG	2A	3131	1/1	0.94	0.09	44,44,44,44	0
58	MG	2A	3427	1/1	0.94	0.15	46,46,46,46	0
58	MG	2A	3831	1/1	0.94	0.08	73,73,73,73	0
58	MG	1a	1671	1/1	0.94	0.26	68,68,68,68	0
58	MG	2A	3835	1/1	0.94	0.08	45,45,45,45	0
58	MG	1A	3064	1/1	0.94	0.11	49,49,49,49	0
58	MG	1A	3605	1/1	0.94	0.07	46,46,46,46	0
58	MG	1a	1675	1/1	0.94	0.16	48,48,48,48	0
58	MG	1A	3606	1/1	0.94	0.12	24,24,24,24	0
58	MG	1A	3439	1/1	0.94	0.20	42,42,42,42	0
58	MG	1A	3242	1/1	0.94	0.06	45,45,45,45	0
58	MG	2A	3145	1/1	0.94	0.16	43,43,43,43	0
58	MG	1A	4074	1/1	0.94	0.12	54,54,54,54	0
58	MG	1A	3441	1/1	0.94	0.12	37,37,37,37	0
58	MG	1A	3445	1/1	0.94	0.06	52,52,52,52	0
58	MG	2A	3857	1/1	0.94	0.12	53,53,53,53	0
58	MG	1A	4079	1/1	0.94	0.11	55,55,55,55	0
58	MG	2A	3449	1/1	0.94	0.15	50,50,50,50	0
58	MG	2A	3861	1/1	0.94	0.10	54,54,54,54	0
58	MG	1a	1686	1/1	0.94	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3452	1/1	0.94	0.10	48,48,48,48	0
58	MG	2B	201	1/1	0.94	0.13	63,63,63,63	0
58	MG	1A	4080	1/1	0.94	0.16	66,66,66,66	0
58	MG	2A	3456	1/1	0.94	0.45	45,45,45,45	0
58	MG	2A	3157	1/1	0.94	0.14	43,43,43,43	0
58	MG	1A	3243	1/1	0.94	0.15	57,57,57,57	0
58	MG	2A	3161	1/1	0.94	0.17	68,68,68,68	0
58	MG	2A	3462	1/1	0.94	0.14	71,71,71,71	0
58	MG	2A	3163	1/1	0.94	0.20	66,66,66,66	0
58	MG	1A	3853	1/1	0.94	0.16	45,45,45,45	0
58	MG	2A	3166	1/1	0.94	0.11	51,51,51,51	0
58	MG	2A	3167	1/1	0.94	0.11	47,47,47,47	0
58	MG	2B	215	1/1	0.94	0.12	63,63,63,63	0
58	MG	1A	3624	1/1	0.94	0.09	43,43,43,43	0
58	MG	1a	1691	1/1	0.94	0.23	60,60,60,60	0
58	MG	1A	3337	1/1	0.94	0.07	45,45,45,45	0
58	MG	1A	4086	1/1	0.94	0.16	50,50,50,50	0
58	MG	1A	3157	1/1	0.94	0.06	51,51,51,51	0
58	MG	1A	4092	1/1	0.94	0.15	55,55,55,55	0
58	MG	2A	3176	1/1	0.94	0.12	73,73,73,73	0
58	MG	2D	307	1/1	0.94	0.09	53,53,53,53	0
58	MG	2E	301	1/1	0.94	0.17	63,63,63,63	0
58	MG	1A	3634	1/1	0.94	0.11	46,46,46,46	0
58	MG	1A	3451	1/1	0.94	0.10	50,50,50,50	0
58	MG	2E	306	1/1	0.94	0.07	30,30,30,30	0
58	MG	2A	3181	1/1	0.94	0.11	47,47,47,47	0
58	MG	2F	301	1/1	0.94	0.20	60,60,60,60	0
58	MG	2A	3182	1/1	0.94	0.18	52,52,52,52	0
58	MG	1a	1698	1/1	0.94	0.19	50,50,50,50	0
58	MG	2A	3488	1/1	0.94	0.15	58,58,58,58	0
58	MG	2F	305	1/1	0.94	0.20	47,47,47,47	0
58	MG	2A	3489	1/1	0.94	0.32	57,57,57,57	0
58	MG	1A	3050	1/1	0.94	0.11	38,38,38,38	0
58	MG	1a	1700	1/1	0.94	0.08	54,54,54,54	0
58	MG	2A	3498	1/1	0.94	0.09	63,63,63,63	0
58	MG	1A	3248	1/1	0.94	0.06	54,54,54,54	0
58	MG	1A	3163	1/1	0.94	0.24	61,61,61,61	0
58	MG	1a	1703	1/1	0.94	0.18	62,62,62,62	0
58	MG	1a	1704	1/1	0.94	0.13	55,55,55,55	0
58	MG	2T	3500	1/1	0.94	0.08	63,63,63,63	0
58	MG	1B	204	1/1	0.94	0.05	35,35,35,35	0
58	MG	1A	3865	1/1	0.94	0.07	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1B	206	1/1	0.94	0.06	40,40,40,40	0
58	MG	1a	1710	1/1	0.94	0.12	52,52,52,52	0
58	MG	2Y	201	1/1	0.94	0.18	48,48,48,48	0
58	MG	2A	3199	1/1	0.94	0.21	56,56,56,56	0
58	MG	1a	1711	1/1	0.94	0.12	46,46,46,46	0
58	MG	2A	3201	1/1	0.94	0.28	67,67,67,67	0
58	MG	1A	3164	1/1	0.94	0.13	48,48,48,48	0
58	MG	23	101	1/1	0.94	0.09	46,46,46,46	0
58	MG	1A	3645	1/1	0.94	0.10	28,28,28,28	0
58	MG	1A	3465	1/1	0.94	0.15	49,49,49,49	0
58	MG	1A	3869	1/1	0.94	0.27	32,32,32,32	0
58	MG	1A	3021	1/1	0.94	0.08	39,39,39,39	0
58	MG	1a	1724	1/1	0.94	0.09	58,58,58,58	0
58	MG	1B	215	1/1	0.94	0.10	53,53,53,53	0
58	MG	1A	3871	1/1	0.94	0.23	38,38,38,38	0
58	MG	2a	1605	1/1	0.94	0.14	58,58,58,58	0
58	MG	2A	3220	1/1	0.94	0.13	48,48,48,48	0
58	MG	1A	3352	1/1	0.94	0.16	37,37,37,37	0
58	MG	2A	3528	1/1	0.94	0.18	58,58,58,58	0
58	MG	1A	3258	1/1	0.94	0.20	50,50,50,50	0
58	MG	1A	3654	1/1	0.94	0.11	40,40,40,40	0
58	MG	2A	3531	1/1	0.94	0.14	42,42,42,42	0
58	MG	1a	1734	1/1	0.94	0.16	51,51,51,51	0
58	MG	1A	3081	1/1	0.94	0.16	36,36,36,36	0
58	MG	2A	3539	1/1	0.94	0.12	39,39,39,39	0
58	MG	2a	1617	1/1	0.94	0.16	49,49,49,49	0
58	MG	2A	3235	1/1	0.94	0.10	41,41,41,41	0
58	MG	2a	1619	1/1	0.94	0.06	43,43,43,43	0
58	MG	1A	3001	1/1	0.94	0.06	39,39,39,39	0
58	MG	1A	3663	1/1	0.94	0.05	23,23,23,23	0
58	MG	1a	1740	1/1	0.94	0.09	56,56,56,56	0
58	MG	1A	3358	1/1	0.94	0.08	47,47,47,47	0
58	MG	1A	3094	1/1	0.94	0.10	43,43,43,43	0
58	MG	2a	1626	1/1	0.94	0.09	65,65,65,65	0
58	MG	1A	3670	1/1	0.94	0.08	27,27,27,27	0
58	MG	1A	3673	1/1	0.94	0.07	20,20,20,20	0
58	MG	2a	1629	1/1	0.94	0.12	64,64,64,64	0
58	MG	1A	3890	1/1	0.94	0.06	25,25,25,25	0
58	MG	1A	3363	1/1	0.94	0.22	42,42,42,42	0
58	MG	2A	3246	1/1	0.94	0.11	62,62,62,62	0
58	MG	2A	3567	1/1	0.94	0.09	64,64,64,64	0
58	MG	2a	1635	1/1	0.94	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1636	1/1	0.94	0.26	59,59,59,59	0
58	MG	1A	3004	1/1	0.94	0.05	24,24,24,24	0
58	MG	1a	1759	1/1	0.94	0.09	56,56,56,56	0
58	MG	2A	3249	1/1	0.94	0.06	63,63,63,63	0
58	MG	1E	310	1/1	0.94	0.10	48,48,48,48	0
58	MG	1A	3101	1/1	0.94	0.09	36,36,36,36	0
58	MG	1A	3483	1/1	0.94	0.14	50,50,50,50	0
58	MG	1a	1763	1/1	0.94	0.09	64,64,64,64	0
58	MG	2A	3255	1/1	0.94	0.07	68,68,68,68	0
58	MG	1A	3104	1/1	0.94	0.11	29,29,29,29	0
58	MG	1A	3487	1/1	0.94	0.08	47,47,47,47	0
58	MG	2A	3583	1/1	0.94	0.06	52,52,52,52	0
58	MG	2a	1651	1/1	0.94	0.05	51,51,51,51	0
58	MG	2a	1652	1/1	0.94	0.27	66,66,66,66	0
58	MG	2A	3584	1/1	0.94	0.08	63,63,63,63	0
58	MG	1a	1769	1/1	0.94	0.12	60,60,60,60	0
58	MG	1F	309	1/1	0.94	0.09	40,40,40,40	0
58	MG	1A	3040	1/1	0.94	0.07	30,30,30,30	0
58	MG	1A	3697	1/1	0.94	0.10	41,41,41,41	0
58	MG	2A	3266	1/1	0.94	0.16	54,54,54,54	0
58	MG	1A	3489	1/1	0.94	0.18	47,47,47,47	0
58	MG	2A	3269	1/1	0.94	0.10	62,62,62,62	0
58	MG	1A	3705	1/1	0.94	0.13	37,37,37,37	0
58	MG	2a	1664	1/1	0.94	0.08	62,62,62,62	0
58	MG	1A	3270	1/1	0.94	0.19	39,39,39,39	0
58	MG	1A	3711	1/1	0.94	0.12	56,56,56,56	0
58	MG	1a	1785	1/1	0.94	0.09	63,63,63,63	0
58	MG	1A	3500	1/1	0.94	0.09	58,58,58,58	0
58	MG	1a	1790	1/1	0.94	0.07	73,73,73,73	0
58	MG	2a	1673	1/1	0.94	0.11	66,66,66,66	0
58	MG	1Q	204	1/1	0.94	0.13	60,60,60,60	0
58	MG	1Q	206	1/1	0.94	0.09	51,51,51,51	0
58	MG	2A	3285	1/1	0.94	0.07	61,61,61,61	0
58	MG	2A	3609	1/1	0.94	0.07	50,50,50,50	0
58	MG	2A	3610	1/1	0.94	0.10	43,43,43,43	0
58	MG	1A	3271	1/1	0.94	0.07	46,46,46,46	0
58	MG	1a	1794	1/1	0.94	0.13	65,65,65,65	0
58	MG	1A	3922	1/1	0.94	0.07	45,45,45,45	0
58	MG	2a	1683	1/1	0.94	0.08	61,61,61,61	0
58	MG	2A	3617	1/1	0.94	0.11	44,44,44,44	0
58	MG	2A	3623	1/1	0.94	0.07	37,37,37,37	0
58	MG	2a	1686	1/1	0.94	0.18	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	1a	1796	1/1	0.94	0.09	68,68,68,68	0
58	MG	1a	1797	1/1	0.94	0.06	47,47,47,47	0
58	MG	2a	1689	1/1	0.94	0.23	60,60,60,60	0
58	MG	2a	1690	1/1	0.94	0.15	64,64,64,64	0
58	MG	2a	1691	1/1	0.94	0.27	60,60,60,60	0
58	MG	2A	3627	1/1	0.94	0.15	53,53,53,53	0
58	MG	1A	3505	1/1	0.94	0.07	46,46,46,46	0
58	MG	2a	1695	1/1	0.94	0.11	76,76,76,76	0
58	MG	2A	3293	1/1	0.94	0.24	56,56,56,56	0
58	MG	2a	1699	1/1	0.94	0.14	57,57,57,57	0
58	MG	1a	1803	1/1	0.94	0.23	58,58,58,58	0
58	MG	1A	3924	1/1	0.94	0.06	40,40,40,40	0
58	MG	1a	1805	1/1	0.94	0.14	53,53,53,53	0
58	MG	1A	3926	1/1	0.94	0.10	45,45,45,45	0
58	MG	1T	202	1/1	0.94	0.10	41,41,41,41	0
58	MG	1U	203	1/1	0.94	0.07	57,57,57,57	0
58	MG	1A	3379	1/1	0.94	0.20	38,38,38,38	0
58	MG	2A	3644	1/1	0.94	0.24	53,53,53,53	0
58	MG	1e	202	1/1	0.94	0.10	54,54,54,54	0
58	MG	1A	3280	1/1	0.94	0.39	33,33,33,33	0
58	MG	1l	202	1/1	0.94	0.06	55,55,55,55	0
58	MG	1A	3508	1/1	0.94	0.12	63,63,63,63	0
58	MG	1A	3281	1/1	0.94	0.07	42,42,42,42	0
58	MG	1A	3941	1/1	0.94	0.08	51,51,51,51	0
58	MG	1A	3734	1/1	0.94	0.11	61,61,61,61	0
58	MG	2A	3659	1/1	0.94	0.13	50,50,50,50	0
58	MG	2A	3311	1/1	0.94	0.11	62,62,62,62	0
58	MG	2A	3312	1/1	0.94	0.11	68,68,68,68	0
58	MG	1A	3943	1/1	0.94	0.07	51,51,51,51	0
58	MG	1A	3735	1/1	0.94	0.17	57,57,57,57	0
58	MG	1A	3517	1/1	0.94	0.17	60,60,60,60	0
58	MG	1A	3747	1/1	0.94	0.17	62,62,62,62	0
58	MG	10	106	1/1	0.94	0.10	64,64,64,64	0
58	MG	1A	3954	1/1	0.94	0.07	44,44,44,44	0
58	MG	1l	101	1/1	0.94	0.30	47,47,47,47	0
58	MG	2A	3671	1/1	0.94	0.10	47,47,47,47	0
58	MG	1A	3955	1/1	0.94	0.05	34,34,34,34	0
58	MG	2a	1732	1/1	0.94	0.26	59,59,59,59	0
58	MG	1A	3194	1/1	0.94	0.28	36,36,36,36	0
58	MG	1A	3195	1/1	0.94	0.21	47,47,47,47	0
58	MG	1x	111	1/1	0.94	0.21	55,55,55,55	0
58	MG	2a	1736	1/1	0.94	0.26	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	3115	1/1	0.94	0.08	40,40,40,40	0
58	MG	1A	3524	1/1	0.94	0.18	47,47,47,47	0
58	MG	15	103	1/1	0.94	0.17	30,30,30,30	0
58	MG	2A	3681	1/1	0.94	0.06	68,68,68,68	0
58	MG	1A	3962	1/1	0.94	0.07	16,16,16,16	0
58	MG	1A	3119	1/1	0.94	0.08	33,33,33,33	0
58	MG	2A	3014	1/1	0.94	0.08	45,45,45,45	0
58	MG	2A	3016	1/1	0.94	0.10	74,74,74,74	0
58	MG	2a	1745	1/1	0.94	0.09	77,77,77,77	0
58	MG	17	102	1/1	0.94	0.10	45,45,45,45	0
58	MG	18	101	1/1	0.94	0.13	47,47,47,47	0
58	MG	1A	3965	1/1	0.94	0.12	54,54,54,54	0
58	MG	2A	3033	1/1	0.94	0.20	51,51,51,51	0
58	MG	1A	3296	1/1	0.94	0.30	60,60,60,60	0
58	MG	2A	3341	1/1	0.94	0.16	68,68,68,68	0
58	MG	2A	3695	1/1	0.94	0.10	65,65,65,65	0
58	MG	1A	3763	1/1	0.94	0.07	20,20,20,20	0
58	MG	18	108	1/1	0.94	0.12	48,48,48,48	0
58	MG	2A	3346	1/1	0.94	0.07	55,55,55,55	0
58	MG	1A	3970	1/1	0.94	0.09	62,62,62,62	0
58	MG	1A	3767	1/1	0.94	0.08	25,25,25,25	0
58	MG	2a	1762	1/1	0.94	0.07	56,56,56,56	0
58	MG	1A	3532	1/1	0.94	0.19	57,57,57,57	0
58	MG	2A	3706	1/1	0.94	0.13	53,53,53,53	0
58	MG	2A	3043	1/1	0.94	0.14	67,67,67,67	0
58	MG	2A	3351	1/1	0.94	0.17	64,64,64,64	0
58	MG	2a	1770	1/1	0.94	0.07	79,79,79,79	0
58	MG	1A	3120	1/1	0.94	0.10	33,33,33,33	0
58	MG	1a	1604	1/1	0.94	0.13	64,64,64,64	0
58	MG	1A	3207	1/1	0.94	0.10	52,52,52,52	0
58	MG	1A	3774	1/1	0.94	0.09	20,20,20,20	0
58	MG	1A	3397	1/1	0.94	0.20	31,31,31,31	0
58	MG	1A	3981	1/1	0.94	0.08	39,39,39,39	0
58	MG	1A	3017	1/1	0.94	0.17	34,34,34,34	0
58	MG	1A	3986	1/1	0.94	0.23	41,41,41,41	0
58	MG	2A	3727	1/1	0.94	0.18	48,48,48,48	0
58	MG	1A	3047	1/1	0.94	0.09	19,19,19,19	0
58	MG	1A	3135	1/1	0.94	0.11	31,31,31,31	0
58	MG	1A	3219	1/1	0.94	0.10	42,42,42,42	0
58	MG	2a	1791	1/1	0.94	0.23	71,71,71,71	0
58	MG	1a	1621	1/1	0.94	0.05	46,46,46,46	0
58	MG	2A	3061	1/1	0.94	0.14	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	3062	1/1	0.94	0.07	41,41,41,41	0
58	MG	2a	1796	1/1	0.94	0.12	53,53,53,53	0
58	MG	1A	3222	1/1	0.94	0.16	47,47,47,47	0
58	MG	1A	3552	1/1	0.94	0.27	29,29,29,29	0
58	MG	1A	3794	1/1	0.94	0.11	52,52,52,52	0
58	MG	1A	3554	1/1	0.94	0.14	54,54,54,54	0
58	MG	2A	3373	1/1	0.94	0.11	52,52,52,52	0
58	MG	1A	3223	1/1	0.94	0.12	43,43,43,43	0
58	MG	2A	3741	1/1	0.94	0.06	42,42,42,42	0
58	MG	1A	3142	1/1	0.94	0.09	43,43,43,43	0
58	MG	2A	3078	1/1	0.94	0.11	50,50,50,50	0
58	MG	1A	3319	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	3571	1/1	0.94	0.07	39,39,39,39	0
58	MG	2A	3748	1/1	0.94	0.08	63,63,63,63	0
58	MG	2A	3751	1/1	0.94	0.07	51,51,51,51	0
58	MG	2A	3379	1/1	0.94	0.20	46,46,46,46	0
58	MG	1A	3582	1/1	0.94	0.12	54,54,54,54	0
58	MG	2A	3085	1/1	0.94	0.14	55,55,55,55	0
58	MG	2A	3383	1/1	0.94	0.28	58,58,58,58	0
58	MG	1A	3583	1/1	0.94	0.08	38,38,38,38	0
58	MG	2A	3762	1/1	0.94	0.08	53,53,53,53	0
58	MG	1A	4032	1/1	0.94	0.09	33,33,33,33	0
58	MG	2a	1822	1/1	0.94	0.23	64,64,64,64	0
58	MG	2a	1824	1/1	0.94	0.16	61,61,61,61	0
58	MG	1A	3227	1/1	0.94	0.11	28,28,28,28	0
58	MG	2A	3768	1/1	0.94	0.07	51,51,51,51	0
58	MG	1A	3585	1/1	0.94	0.12	35,35,35,35	0
58	MG	2A	3093	1/1	0.94	0.06	42,42,42,42	0
58	MG	2d	301	1/1	0.94	0.40	60,60,60,60	0
58	MG	1a	1643	1/1	0.94	0.13	50,50,50,50	0
58	MG	1A	3419	1/1	0.94	0.08	40,40,40,40	0
58	MG	1A	3322	1/1	0.94	0.12	56,56,56,56	0
58	MG	1A	4042	1/1	0.94	0.07	37,37,37,37	0
58	MG	1A	3324	1/1	0.94	0.11	45,45,45,45	0
58	MG	2A	3105	1/1	0.94	0.12	54,54,54,54	0
58	MG	2A	3781	1/1	0.94	0.14	74,74,74,74	0
58	MG	1a	1654	1/1	0.94	0.15	60,60,60,60	0
58	MG	2A	3396	1/1	0.94	0.08	52,52,52,52	0
58	MG	1A	3147	1/1	0.94	0.09	30,30,30,30	0
58	MG	1A	3062	1/1	0.94	0.21	40,40,40,40	0
58	MG	2A	3789	1/1	0.94	0.08	52,52,52,52	0
58	MG	1a	1657	1/1	0.94	0.10	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	3410	1/1	0.94	0.10	42,42,42,42	0
58	MG	1A	3823	1/1	0.94	0.08	23,23,23,23	0
58	MG	2A	3795	1/1	0.94	0.09	40,40,40,40	0
58	MG	1A	3432	1/1	0.94	0.13	39,39,39,39	0
58	MG	2A	3413	1/1	0.94	0.28	52,52,52,52	0
58	MG	2x	101	1/1	0.94	0.08	56,56,56,56	0
58	MG	2A	3414	1/1	0.94	0.14	54,54,54,54	0
58	MG	2A	3119	1/1	0.94	0.18	57,57,57,57	0
58	MG	2A	3806	1/1	0.94	0.07	37,37,37,37	0
58	MG	2A	3807	1/1	0.94	0.08	52,52,52,52	0
58	MG	1A	3827	1/1	0.94	0.08	37,37,37,37	0
58	MG	1a	1663	1/1	0.94	0.11	54,54,54,54	0
58	MG	2A	3446	1/1	0.95	0.28	48,48,48,48	0
58	MG	2A	3828	1/1	0.95	0.07	56,56,56,56	0
58	MG	1B	228	1/1	0.95	0.08	46,46,46,46	0
58	MG	2A	3164	1/1	0.95	0.09	53,53,53,53	0
58	MG	1A	3425	1/1	0.95	0.12	50,50,50,50	0
58	MG	2A	3834	1/1	0.95	0.13	55,55,55,55	0
58	MG	1A	3900	1/1	0.95	0.08	44,44,44,44	0
58	MG	2A	3453	1/1	0.95	0.07	42,42,42,42	0
58	MG	1A	3158	1/1	0.95	0.12	27,27,27,27	0
58	MG	2A	3455	1/1	0.95	0.17	45,45,45,45	0
58	MG	2A	3843	1/1	0.95	0.09	52,52,52,52	0
58	MG	1a	1707	1/1	0.95	0.18	41,41,41,41	0
58	MG	1A	3713	1/1	0.95	0.14	52,52,52,52	0
58	MG	2A	3847	1/1	0.95	0.06	66,66,66,66	0
58	MG	1A	3272	1/1	0.95	0.26	47,47,47,47	0
58	MG	1A	3274	1/1	0.95	0.09	41,41,41,41	0
58	MG	2A	3851	1/1	0.95	0.10	51,51,51,51	0
58	MG	1A	3542	1/1	0.95	0.09	61,61,61,61	0
58	MG	2A	3174	1/1	0.95	0.13	47,47,47,47	0
58	MG	1A	3346	1/1	0.95	0.07	39,39,39,39	0
58	MG	1E	304	1/1	0.95	0.12	35,35,35,35	0
58	MG	1A	3915	1/1	0.95	0.16	28,28,28,28	0
58	MG	2A	3468	1/1	0.95	0.14	48,48,48,48	0
58	MG	1E	308	1/1	0.95	0.08	40,40,40,40	0
58	MG	1a	1720	1/1	0.95	0.10	49,49,49,49	0
58	MG	2A	3471	1/1	0.95	0.09	37,37,37,37	0
58	MG	1a	1721	1/1	0.95	0.17	54,54,54,54	0
58	MG	1A	3278	1/1	0.95	0.14	28,28,28,28	0
58	MG	1A	3919	1/1	0.95	0.07	31,31,31,31	0
58	MG	2A	3476	1/1	0.95	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2B	205	1/1	0.95	0.08	48,48,48,48	0
58	MG	2A	3477	1/1	0.95	0.06	61,61,61,61	0
58	MG	2B	207	1/1	0.95	0.07	62,62,62,62	0
58	MG	2A	3480	1/1	0.95	0.12	37,37,37,37	0
58	MG	1A	3920	1/1	0.95	0.07	46,46,46,46	0
58	MG	1A	3921	1/1	0.95	0.12	69,69,69,69	0
58	MG	1E	315	1/1	0.95	0.05	45,45,45,45	0
58	MG	2B	212	1/1	0.95	0.25	62,62,62,62	0
58	MG	1a	1732	1/1	0.95	0.08	52,52,52,52	0
58	MG	1A	3545	1/1	0.95	0.18	60,60,60,60	0
58	MG	1F	303	1/1	0.95	0.12	29,29,29,29	0
58	MG	1A	3434	1/1	0.95	0.10	52,52,52,52	0
58	MG	1F	310	1/1	0.95	0.14	47,47,47,47	0
58	MG	1F	311	1/1	0.95	0.17	40,40,40,40	0
58	MG	2A	3493	1/1	0.95	0.18	44,44,44,44	0
58	MG	1A	3016	1/1	0.95	0.14	61,61,61,61	0
58	MG	1A	3736	1/1	0.95	0.07	42,42,42,42	0
58	MG	1A	3737	1/1	0.95	0.07	64,64,64,64	0
58	MG	1G	204	1/1	0.95	0.12	52,52,52,52	0
58	MG	1A	3111	1/1	0.95	0.17	39,39,39,39	0
58	MG	1a	1749	1/1	0.95	0.14	53,53,53,53	0
58	MG	2A	3207	1/1	0.95	0.08	55,55,55,55	0
58	MG	2E	304	1/1	0.95	0.08	61,61,61,61	0
58	MG	2A	3208	1/1	0.95	0.08	42,42,42,42	0
58	MG	1a	1752	1/1	0.95	0.09	48,48,48,48	0
58	MG	1a	1753	1/1	0.95	0.19	58,58,58,58	0
58	MG	1H	201	1/1	0.95	0.09	36,36,36,36	0
58	MG	2A	3215	1/1	0.95	0.10	67,67,67,67	0
58	MG	1I	201	1/1	0.95	0.08	59,59,59,59	0
58	MG	2A	3217	1/1	0.95	0.14	44,44,44,44	0
58	MG	2F	306	1/1	0.95	0.34	50,50,50,50	0
58	MG	1N	201	1/1	0.95	0.08	39,39,39,39	0
58	MG	2A	3219	1/1	0.95	0.15	46,46,46,46	0
58	MG	2A	3516	1/1	0.95	0.07	42,42,42,42	0
58	MG	1A	3076	1/1	0.95	0.22	51,51,51,51	0
58	MG	2A	3222	1/1	0.95	0.17	50,50,50,50	0
58	MG	2A	3223	1/1	0.95	0.20	52,52,52,52	0
58	MG	2Q	201	1/1	0.95	0.08	56,56,56,56	0
58	MG	1O	202	1/1	0.95	0.17	55,55,55,55	0
58	MG	1A	3748	1/1	0.95	0.07	49,49,49,49	0
58	MG	1P	204	1/1	0.95	0.36	57,57,57,57	0
58	MG	2A	3228	1/1	0.95	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2T	3502	1/1	0.95	0.10	52,52,52,52	0
58	MG	2A	3229	1/1	0.95	0.07	67,67,67,67	0
58	MG	2A	3527	1/1	0.95	0.07	39,39,39,39	0
58	MG	2A	3230	1/1	0.95	0.07	31,31,31,31	0
58	MG	1A	3353	1/1	0.95	0.18	54,54,54,54	0
58	MG	1a	1765	1/1	0.95	0.07	60,60,60,60	0
58	MG	1Q	202	1/1	0.95	0.09	33,33,33,33	0
58	MG	2A	3532	1/1	0.95	0.14	52,52,52,52	0
58	MG	1Q	203	1/1	0.95	0.06	38,38,38,38	0
58	MG	1A	3557	1/1	0.95	0.08	41,41,41,41	0
58	MG	2A	3538	1/1	0.95	0.08	49,49,49,49	0
58	MG	25	102	1/1	0.95	0.20	39,39,39,39	0
58	MG	1a	1771	1/1	0.95	0.09	66,66,66,66	0
58	MG	2A	3239	1/1	0.95	0.10	63,63,63,63	0
58	MG	1A	3563	1/1	0.95	0.23	58,58,58,58	0
58	MG	1A	3442	1/1	0.95	0.28	44,44,44,44	0
58	MG	1A	3286	1/1	0.95	0.12	52,52,52,52	0
58	MG	1a	1775	1/1	0.95	0.12	58,58,58,58	0
58	MG	2A	3550	1/1	0.95	0.12	46,46,46,46	0
58	MG	1A	3950	1/1	0.95	0.07	45,45,45,45	0
58	MG	1a	1779	1/1	0.95	0.09	69,69,69,69	0
58	MG	2A	3553	1/1	0.95	0.07	29,29,29,29	0
58	MG	1A	3570	1/1	0.95	0.20	32,32,32,32	0
58	MG	2A	3560	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3953	1/1	0.95	0.06	43,43,43,43	0
58	MG	1S	203	1/1	0.95	0.11	61,61,61,61	0
58	MG	1A	3761	1/1	0.95	0.13	45,45,45,45	0
58	MG	2A	3565	1/1	0.95	0.16	54,54,54,54	0
58	MG	2A	3566	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3027	1/1	0.95	0.20	27,27,27,27	0
58	MG	1A	3764	1/1	0.95	0.06	25,25,25,25	0
58	MG	1U	205	1/1	0.95	0.09	31,31,31,31	0
58	MG	1U	206	1/1	0.95	0.32	30,30,30,30	0
58	MG	1A	3573	1/1	0.95	0.14	40,40,40,40	0
58	MG	1V	208	1/1	0.95	0.08	51,51,51,51	0
58	MG	1A	3577	1/1	0.95	0.08	45,45,45,45	0
58	MG	1A	3959	1/1	0.95	0.10	49,49,49,49	0
58	MG	2A	3577	1/1	0.95	0.10	53,53,53,53	0
58	MG	1W	202	1/1	0.95	0.13	53,53,53,53	0
58	MG	2A	3262	1/1	0.95	0.28	58,58,58,58	0
58	MG	1a	1798	1/1	0.95	0.08	66,66,66,66	0
58	MG	1A	3580	1/1	0.95	0.12	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3356	1/1	0.95	0.09	43,43,43,43	0
58	MG	1A	3449	1/1	0.95	0.12	47,47,47,47	0
58	MG	2a	1634	1/1	0.95	0.14	64,64,64,64	0
58	MG	1A	3116	1/1	0.95	0.07	41,41,41,41	0
58	MG	1a	1807	1/1	0.95	0.07	51,51,51,51	0
58	MG	1A	3967	1/1	0.95	0.07	53,53,53,53	0
58	MG	2A	3591	1/1	0.95	0.13	53,53,53,53	0
58	MG	2A	3592	1/1	0.95	0.14	53,53,53,53	0
58	MG	2A	3593	1/1	0.95	0.10	58,58,58,58	0
58	MG	1A	3085	1/1	0.95	0.14	31,31,31,31	0
58	MG	2A	3595	1/1	0.95	0.14	62,62,62,62	0
58	MG	1A	3453	1/1	0.95	0.09	41,41,41,41	0
58	MG	2a	1646	1/1	0.95	0.08	61,61,61,61	0
58	MG	2A	3597	1/1	0.95	0.13	53,53,53,53	0
58	MG	1A	3588	1/1	0.95	0.12	50,50,50,50	0
58	MG	10	109	1/1	0.95	0.07	46,46,46,46	0
58	MG	1A	3240	1/1	0.95	0.20	34,34,34,34	0
58	MG	1l	201	1/1	0.95	0.05	76,76,76,76	0
58	MG	2A	3602	1/1	0.95	0.11	54,54,54,54	0
58	MG	2A	3281	1/1	0.95	0.08	47,47,47,47	0
58	MG	2a	1654	1/1	0.95	0.06	58,58,58,58	0
58	MG	2A	3282	1/1	0.95	0.07	44,44,44,44	0
58	MG	2A	3284	1/1	0.95	0.11	71,71,71,71	0
58	MG	1A	3788	1/1	0.95	0.08	58,58,58,58	0
58	MG	1l	105	1/1	0.95	0.07	42,42,42,42	0
58	MG	1n	102	1/1	0.95	0.26	59,59,59,59	0
58	MG	1p	101	1/1	0.95	0.11	51,51,51,51	0
58	MG	2a	1661	1/1	0.95	0.12	70,70,70,70	0
58	MG	2A	3289	1/1	0.95	0.12	58,58,58,58	0
58	MG	2A	3612	1/1	0.95	0.15	37,37,37,37	0
58	MG	1A	3591	1/1	0.95	0.12	53,53,53,53	0
58	MG	13	102	1/1	0.95	0.07	34,34,34,34	0
58	MG	1A	3361	1/1	0.95	0.12	36,36,36,36	0
58	MG	1A	3297	1/1	0.95	0.11	35,35,35,35	0
58	MG	2A	3619	1/1	0.95	0.07	40,40,40,40	0
58	MG	2A	3621	1/1	0.95	0.13	38,38,38,38	0
58	MG	2A	3294	1/1	0.95	0.09	61,61,61,61	0
58	MG	1A	3795	1/1	0.95	0.06	23,23,23,23	0
58	MG	1A	3594	1/1	0.95	0.16	52,52,52,52	0
58	MG	15	105	1/1	0.95	0.16	38,38,38,38	0
58	MG	1A	3982	1/1	0.95	0.11	35,35,35,35	0
58	MG	2A	3299	1/1	0.95	0.15	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	3459	1/1	0.95	0.09	31,31,31,31	0
58	MG	1A	3179	1/1	0.95	0.13	23,23,23,23	0
58	MG	1A	3461	1/1	0.95	0.15	37,37,37,37	0
58	MG	1A	3598	1/1	0.95	0.11	37,37,37,37	0
58	MG	2A	3639	1/1	0.95	0.15	54,54,54,54	0
58	MG	1A	3993	1/1	0.95	0.05	16,16,16,16	0
58	MG	1A	3464	1/1	0.95	0.08	54,54,54,54	0
58	MG	18	107	1/1	0.95	0.10	58,58,58,58	0
58	MG	2A	3002	1/1	0.95	0.27	49,49,49,49	0
58	MG	1A	3368	1/1	0.95	0.12	53,53,53,53	0
58	MG	1A	3033	1/1	0.95	0.17	30,30,30,30	0
58	MG	2A	3650	1/1	0.95	0.18	60,60,60,60	0
58	MG	2a	1692	1/1	0.95	0.12	82,82,82,82	0
58	MG	1A	4000	1/1	0.95	0.14	39,39,39,39	0
58	MG	1A	4002	1/1	0.95	0.07	24,24,24,24	0
58	MG	1A	3467	1/1	0.95	0.20	47,47,47,47	0
58	MG	2a	1696	1/1	0.95	0.18	60,60,60,60	0
58	MG	2A	3015	1/1	0.95	0.09	48,48,48,48	0
58	MG	1A	4015	1/1	0.95	0.13	58,58,58,58	0
58	MG	2A	3658	1/1	0.95	0.05	48,48,48,48	0
58	MG	2A	3020	1/1	0.95	0.08	56,56,56,56	0
58	MG	1a	1605	1/1	0.95	0.10	47,47,47,47	0
58	MG	2a	1703	1/1	0.95	0.12	59,59,59,59	0
58	MG	1a	1606	1/1	0.95	0.12	65,65,65,65	0
58	MG	2A	3025	1/1	0.95	0.10	52,52,52,52	0
58	MG	2A	3026	1/1	0.95	0.16	46,46,46,46	0
58	MG	2A	3028	1/1	0.95	0.13	58,58,58,58	0
58	MG	1A	3181	1/1	0.95	0.10	48,48,48,48	0
58	MG	2A	3030	1/1	0.95	0.12	44,44,44,44	0
58	MG	1A	3304	1/1	0.95	0.23	56,56,56,56	0
58	MG	1A	3373	1/1	0.95	0.07	37,37,37,37	0
58	MG	1A	3124	1/1	0.95	0.27	32,32,32,32	0
58	MG	1A	3183	1/1	0.95	0.14	67,67,67,67	0
58	MG	1A	4022	1/1	0.95	0.07	49,49,49,49	0
58	MG	1A	3307	1/1	0.95	0.09	57,57,57,57	0
58	MG	1A	3128	1/1	0.95	0.11	33,33,33,33	0
58	MG	2A	3677	1/1	0.95	0.11	54,54,54,54	0
58	MG	1A	4031	1/1	0.95	0.12	38,38,38,38	0
58	MG	1A	3826	1/1	0.95	0.06	33,33,33,33	0
58	MG	2A	3336	1/1	0.95	0.17	59,59,59,59	0
58	MG	1A	3309	1/1	0.95	0.13	45,45,45,45	0
58	MG	1A	3828	1/1	0.95	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1624	1/1	0.95	0.27	54,54,54,54	0
58	MG	2a	1726	1/1	0.95	0.25	63,63,63,63	0
58	MG	2a	1727	1/1	0.95	0.17	62,62,62,62	0
58	MG	1A	4036	1/1	0.95	0.06	37,37,37,37	0
58	MG	2A	3342	1/1	0.95	0.11	55,55,55,55	0
58	MG	2A	3343	1/1	0.95	0.20	52,52,52,52	0
58	MG	2A	3688	1/1	0.95	0.06	69,69,69,69	0
58	MG	2A	3050	1/1	0.95	0.11	47,47,47,47	0
58	MG	1A	3632	1/1	0.95	0.06	30,30,30,30	0
58	MG	1A	3088	1/1	0.95	0.09	38,38,38,38	0
58	MG	1A	3835	1/1	0.95	0.09	51,51,51,51	0
58	MG	2A	3693	1/1	0.95	0.07	51,51,51,51	0
58	MG	1A	3636	1/1	0.95	0.06	20,20,20,20	0
58	MG	1A	3090	1/1	0.95	0.08	39,39,39,39	0
58	MG	1a	1634	1/1	0.95	0.28	74,74,74,74	0
58	MG	2A	3697	1/1	0.95	0.27	61,61,61,61	0
58	MG	2A	3698	1/1	0.95	0.11	55,55,55,55	0
58	MG	2A	3699	1/1	0.95	0.12	44,44,44,44	0
58	MG	1A	3484	1/1	0.95	0.22	52,52,52,52	0
58	MG	1A	4048	1/1	0.95	0.11	53,53,53,53	0
58	MG	1A	3389	1/1	0.95	0.28	46,46,46,46	0
58	MG	2a	1746	1/1	0.95	0.17	63,63,63,63	0
58	MG	1A	4050	1/1	0.95	0.06	39,39,39,39	0
58	MG	1a	1640	1/1	0.95	0.17	56,56,56,56	0
58	MG	1A	3091	1/1	0.95	0.10	36,36,36,36	0
58	MG	1A	3315	1/1	0.95	0.06	26,26,26,26	0
58	MG	2A	3068	1/1	0.95	0.18	52,52,52,52	0
58	MG	2A	3070	1/1	0.95	0.05	34,34,34,34	0
58	MG	2A	3711	1/1	0.95	0.10	54,54,54,54	0
58	MG	2A	3712	1/1	0.95	0.08	48,48,48,48	0
58	MG	2A	3714	1/1	0.95	0.08	40,40,40,40	0
58	MG	2A	3072	1/1	0.95	0.10	46,46,46,46	0
58	MG	2A	3718	1/1	0.95	0.15	58,58,58,58	0
58	MG	1A	3843	1/1	0.95	0.07	40,40,40,40	0
58	MG	1A	3644	1/1	0.95	0.06	61,61,61,61	0
58	MG	2a	1763	1/1	0.95	0.15	55,55,55,55	0
58	MG	2a	1764	1/1	0.95	0.09	51,51,51,51	0
58	MG	2A	3076	1/1	0.95	0.10	48,48,48,48	0
58	MG	1a	1650	1/1	0.95	0.10	50,50,50,50	0
58	MG	1A	4058	1/1	0.95	0.09	43,43,43,43	0
58	MG	1a	1652	1/1	0.95	0.19	56,56,56,56	0
58	MG	2a	1769	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	2A	3082	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3256	1/1	0.95	0.07	39,39,39,39	0
58	MG	1A	3495	1/1	0.95	0.23	45,45,45,45	0
58	MG	1A	3648	1/1	0.95	0.06	26,26,26,26	0
58	MG	1A	3649	1/1	0.95	0.05	29,29,29,29	0
58	MG	2a	1777	1/1	0.95	0.14	64,64,64,64	0
58	MG	1A	3137	1/1	0.95	0.33	34,34,34,34	0
58	MG	1A	3499	1/1	0.95	0.13	57,57,57,57	0
58	MG	2a	1783	1/1	0.95	0.19	58,58,58,58	0
58	MG	1A	3858	1/1	0.95	0.10	36,36,36,36	0
58	MG	2A	3094	1/1	0.95	0.14	52,52,52,52	0
58	MG	1A	3092	1/1	0.95	0.10	47,47,47,47	0
58	MG	1A	3006	1/1	0.95	0.11	40,40,40,40	0
58	MG	2A	3099	1/1	0.95	0.11	55,55,55,55	0
58	MG	1A	3861	1/1	0.95	0.06	45,45,45,45	0
58	MG	2A	3101	1/1	0.95	0.23	59,59,59,59	0
58	MG	1a	1665	1/1	0.95	0.21	56,56,56,56	0
58	MG	1A	3399	1/1	0.95	0.13	40,40,40,40	0
58	MG	2A	3104	1/1	0.95	0.10	34,34,34,34	0
58	MG	1A	3657	1/1	0.95	0.06	31,31,31,31	0
58	MG	2A	3747	1/1	0.95	0.10	53,53,53,53	0
58	MG	1A	3148	1/1	0.95	0.18	43,43,43,43	0
58	MG	1A	3327	1/1	0.95	0.23	48,48,48,48	0
58	MG	2A	3108	1/1	0.95	0.11	62,62,62,62	0
58	MG	1A	3664	1/1	0.95	0.09	46,46,46,46	0
58	MG	2A	3111	1/1	0.95	0.12	51,51,51,51	0
58	MG	1A	3328	1/1	0.95	0.21	52,52,52,52	0
58	MG	2a	1804	1/1	0.95	0.24	53,53,53,53	0
58	MG	1a	1673	1/1	0.95	0.14	48,48,48,48	0
58	MG	2A	3760	1/1	0.95	0.07	51,51,51,51	0
58	MG	1A	3206	1/1	0.95	0.07	33,33,33,33	0
58	MG	2a	1809	1/1	0.95	0.18	63,63,63,63	0
58	MG	2A	3399	1/1	0.95	0.17	39,39,39,39	0
58	MG	2A	3400	1/1	0.95	0.10	39,39,39,39	0
58	MG	1A	4087	1/1	0.95	0.10	47,47,47,47	0
58	MG	2A	3403	1/1	0.95	0.19	49,49,49,49	0
58	MG	2A	3120	1/1	0.95	0.08	42,42,42,42	0
58	MG	2A	3123	1/1	0.95	0.08	48,48,48,48	0
58	MG	2A	3409	1/1	0.95	0.09	37,37,37,37	0
58	MG	1A	3024	1/1	0.95	0.06	38,38,38,38	0
58	MG	1A	4090	1/1	0.95	0.13	58,58,58,58	0
58	MG	1a	1678	1/1	0.95	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	1A	3671	1/1	0.95	0.09	40,40,40,40	0
58	MG	2a	1823	1/1	0.95	0.18	59,59,59,59	0
58	MG	1A	3100	1/1	0.95	0.17	49,49,49,49	0
58	MG	1A	3333	1/1	0.95	0.06	48,48,48,48	0
58	MG	1A	3873	1/1	0.95	0.19	34,34,34,34	0
58	MG	2a	1827	1/1	0.95	0.14	63,63,63,63	0
58	MG	1A	3520	1/1	0.95	0.09	45,45,45,45	0
58	MG	1B	201	1/1	0.95	0.06	42,42,42,42	0
58	MG	2a	1830	1/1	0.95	0.11	65,65,65,65	0
58	MG	1A	3521	1/1	0.95	0.07	44,44,44,44	0
58	MG	2A	3421	1/1	0.95	0.17	47,47,47,47	0
58	MG	1A	3334	1/1	0.95	0.11	56,56,56,56	0
58	MG	2A	3793	1/1	0.95	0.07	60,60,60,60	0
58	MG	2A	3135	1/1	0.95	0.10	57,57,57,57	0
58	MG	1A	3152	1/1	0.95	0.23	40,40,40,40	0
58	MG	2A	3797	1/1	0.95	0.13	65,65,65,65	0
58	MG	2A	3798	1/1	0.95	0.06	43,43,43,43	0
58	MG	1A	3336	1/1	0.95	0.06	57,57,57,57	0
58	MG	1A	3691	1/1	0.95	0.08	17,17,17,17	0
58	MG	1A	3527	1/1	0.95	0.11	44,44,44,44	0
58	MG	2l	204	1/1	0.95	0.05	61,61,61,61	0
58	MG	2A	3803	1/1	0.95	0.06	41,41,41,41	0
58	MG	1A	3528	1/1	0.95	0.19	49,49,49,49	0
58	MG	2q	202	1/1	0.95	0.09	65,65,65,65	0
58	MG	1A	3698	1/1	0.95	0.06	28,28,28,28	0
58	MG	1A	3529	1/1	0.95	0.21	38,38,38,38	0
58	MG	1A	3700	1/1	0.95	0.07	28,28,28,28	0
58	MG	1B	221	1/1	0.95	0.10	60,60,60,60	0
58	MG	1A	3701	1/1	0.95	0.04	25,25,25,25	0
58	MG	2A	3155	1/1	0.95	0.16	57,57,57,57	0
58	MG	1A	3055	1/1	0.95	0.14	37,37,37,37	0
58	MG	1A	3422	1/1	0.95	0.10	40,40,40,40	0
58	MG	2A	3440	1/1	0.95	0.07	47,47,47,47	0
58	MG	2x	104	1/1	0.95	0.26	55,55,55,55	0
58	MG	1A	3709	1/1	0.95	0.14	37,37,37,37	0
58	MG	2A	3442	1/1	0.95	0.06	54,54,54,54	0
58	MG	2A	3823	1/1	0.95	0.09	60,60,60,60	0
58	MG	1A	3710	1/1	0.95	0.08	42,42,42,42	0
58	MG	1A	4095	1/1	0.96	0.16	37,37,37,37	0
58	MG	1A	3579	1/1	0.96	0.07	34,34,34,34	0
58	MG	2A	3562	1/1	0.96	0.11	45,45,45,45	0
58	MG	1A	3381	1/1	0.96	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1644	1/1	0.96	0.18	38,38,38,38	0
58	MG	1A	3904	1/1	0.96	0.11	53,53,53,53	0
58	MG	1A	3320	1/1	0.96	0.16	46,46,46,46	0
58	MG	1A	3742	1/1	0.96	0.05	54,54,54,54	0
58	MG	1A	3067	1/1	0.96	0.13	45,45,45,45	0
58	MG	1A	3469	1/1	0.96	0.10	40,40,40,40	0
58	MG	1A	3914	1/1	0.96	0.06	27,27,27,27	0
58	MG	1B	209	1/1	0.96	0.13	48,48,48,48	0
58	MG	1A	3138	1/1	0.96	0.10	41,41,41,41	0
58	MG	2A	3049	1/1	0.96	0.12	33,33,33,33	0
58	MG	1A	3916	1/1	0.96	0.11	49,49,49,49	0
58	MG	1A	3917	1/1	0.96	0.06	39,39,39,39	0
58	MG	1A	3471	1/1	0.96	0.20	51,51,51,51	0
58	MG	2A	3579	1/1	0.96	0.11	55,55,55,55	0
58	MG	2A	3053	1/1	0.96	0.12	66,66,66,66	0
58	MG	2A	3305	1/1	0.96	0.31	60,60,60,60	0
58	MG	1A	3323	1/1	0.96	0.13	51,51,51,51	0
58	MG	1a	1660	1/1	0.96	0.12	67,67,67,67	0
58	MG	2A	3056	1/1	0.96	0.09	48,48,48,48	0
58	MG	1B	219	1/1	0.96	0.09	38,38,38,38	0
58	MG	2P	203	1/1	0.96	0.08	55,55,55,55	0
58	MG	1A	3210	1/1	0.96	0.11	41,41,41,41	0
58	MG	2A	3059	1/1	0.96	0.15	49,49,49,49	0
58	MG	1A	3754	1/1	0.96	0.09	44,44,44,44	0
58	MG	1A	3264	1/1	0.96	0.21	45,45,45,45	0
58	MG	1a	1666	1/1	0.96	0.23	63,63,63,63	0
58	MG	1A	3476	1/1	0.96	0.11	41,41,41,41	0
58	MG	2A	3064	1/1	0.96	0.10	68,68,68,68	0
58	MG	1A	3759	1/1	0.96	0.08	43,43,43,43	0
58	MG	2V	201	1/1	0.96	0.23	52,52,52,52	0
58	MG	2A	3318	1/1	0.96	0.07	51,51,51,51	0
58	MG	1A	3169	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3044	1/1	0.96	0.05	30,30,30,30	0
58	MG	1A	3215	1/1	0.96	0.15	40,40,40,40	0
58	MG	2A	3069	1/1	0.96	0.06	43,43,43,43	0
58	MG	1A	3395	1/1	0.96	0.25	43,43,43,43	0
58	MG	2A	3071	1/1	0.96	0.13	50,50,50,50	0
58	MG	23	102	1/1	0.96	0.07	57,57,57,57	0
58	MG	23	103	1/1	0.96	0.08	59,59,59,59	0
58	MG	1A	3482	1/1	0.96	0.09	46,46,46,46	0
58	MG	1A	3330	1/1	0.96	0.13	43,43,43,43	0
58	MG	2A	3074	1/1	0.96	0.10	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	27	102	1/1	0.96	0.07	53,53,53,53	0
58	MG	1A	3269	1/1	0.96	0.12	44,44,44,44	0
58	MG	2A	3330	1/1	0.96	0.10	43,43,43,43	0
58	MG	1A	3600	1/1	0.96	0.11	37,37,37,37	0
58	MG	1B	236	1/1	0.96	0.10	44,44,44,44	0
58	MG	1D	302	1/1	0.96	0.18	36,36,36,36	0
58	MG	2a	1604	1/1	0.96	0.10	52,52,52,52	0
58	MG	1D	308	1/1	0.96	0.06	37,37,37,37	0
58	MG	1D	310	1/1	0.96	0.27	27,27,27,27	0
58	MG	1D	311	1/1	0.96	0.08	42,42,42,42	0
58	MG	1A	3216	1/1	0.96	0.10	40,40,40,40	0
58	MG	2A	3618	1/1	0.96	0.15	51,51,51,51	0
58	MG	2A	3086	1/1	0.96	0.07	47,47,47,47	0
58	MG	2A	3620	1/1	0.96	0.11	51,51,51,51	0
58	MG	2A	3087	1/1	0.96	0.06	44,44,44,44	0
58	MG	2a	1613	1/1	0.96	0.10	46,46,46,46	0
58	MG	1E	301	1/1	0.96	0.28	37,37,37,37	0
58	MG	1A	3602	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3949	1/1	0.96	0.06	49,49,49,49	0
58	MG	1E	306	1/1	0.96	0.14	29,29,29,29	0
58	MG	2A	3628	1/1	0.96	0.18	54,54,54,54	0
58	MG	2a	1620	1/1	0.96	0.07	62,62,62,62	0
58	MG	1A	3603	1/1	0.96	0.08	24,24,24,24	0
58	MG	1A	3217	1/1	0.96	0.13	38,38,38,38	0
58	MG	2A	3095	1/1	0.96	0.13	50,50,50,50	0
58	MG	2A	3096	1/1	0.96	0.07	31,31,31,31	0
58	MG	1A	3176	1/1	0.96	0.04	26,26,26,26	0
58	MG	1A	3220	1/1	0.96	0.07	45,45,45,45	0
58	MG	1A	3786	1/1	0.96	0.08	43,43,43,43	0
58	MG	2A	3640	1/1	0.96	0.10	32,32,32,32	0
58	MG	1A	3609	1/1	0.96	0.06	41,41,41,41	0
58	MG	1A	3790	1/1	0.96	0.06	34,34,34,34	0
58	MG	1A	3490	1/1	0.96	0.06	47,47,47,47	0
58	MG	1F	301	1/1	0.96	0.15	40,40,40,40	0
58	MG	1A	3792	1/1	0.96	0.09	58,58,58,58	0
58	MG	1F	307	1/1	0.96	0.15	25,25,25,25	0
58	MG	1A	3493	1/1	0.96	0.18	36,36,36,36	0
58	MG	1A	3619	1/1	0.96	0.07	30,30,30,30	0
58	MG	2A	3360	1/1	0.96	0.10	46,46,46,46	0
58	MG	1A	3963	1/1	0.96	0.08	47,47,47,47	0
58	MG	2A	3109	1/1	0.96	0.16	50,50,50,50	0
58	MG	2A	3655	1/1	0.96	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3656	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3177	1/1	0.96	0.04	22,22,22,22	0
58	MG	2a	1643	1/1	0.96	0.28	63,63,63,63	0
58	MG	1A	3408	1/1	0.96	0.09	46,46,46,46	0
58	MG	2a	1645	1/1	0.96	0.08	66,66,66,66	0
58	MG	1A	3497	1/1	0.96	0.04	28,28,28,28	0
58	MG	1A	3498	1/1	0.96	0.07	39,39,39,39	0
58	MG	1A	3627	1/1	0.96	0.05	21,21,21,21	0
58	MG	2A	3118	1/1	0.96	0.17	48,48,48,48	0
58	MG	1A	3629	1/1	0.96	0.07	31,31,31,31	0
58	MG	1A	3409	1/1	0.96	0.06	35,35,35,35	0
58	MG	2A	3121	1/1	0.96	0.07	49,49,49,49	0
58	MG	2A	3122	1/1	0.96	0.09	69,69,69,69	0
58	MG	1A	3026	1/1	0.96	0.19	69,69,69,69	0
58	MG	1N	202	1/1	0.96	0.05	35,35,35,35	0
58	MG	1N	204	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3973	1/1	0.96	0.05	59,59,59,59	0
58	MG	1a	1716	1/1	0.96	0.13	67,67,67,67	0
58	MG	2A	3674	1/1	0.96	0.12	53,53,53,53	0
58	MG	1A	3501	1/1	0.96	0.10	46,46,46,46	0
58	MG	1A	3976	1/1	0.96	0.09	58,58,58,58	0
58	MG	2A	3382	1/1	0.96	0.08	59,59,59,59	0
58	MG	1P	202	1/1	0.96	0.17	28,28,28,28	0
58	MG	1A	3412	1/1	0.96	0.15	44,44,44,44	0
58	MG	1A	3413	1/1	0.96	0.05	50,50,50,50	0
58	MG	1A	3015	1/1	0.96	0.10	49,49,49,49	0
58	MG	2a	1667	1/1	0.96	0.12	44,44,44,44	0
58	MG	1A	3415	1/1	0.96	0.33	44,44,44,44	0
58	MG	2a	1669	1/1	0.96	0.07	56,56,56,56	0
58	MG	1a	1727	1/1	0.96	0.11	33,33,33,33	0
58	MG	1a	1729	1/1	0.96	0.08	51,51,51,51	0
58	MG	1A	3079	1/1	0.96	0.07	57,57,57,57	0
58	MG	2A	3138	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3509	1/1	0.96	0.14	37,37,37,37	0
58	MG	1A	3511	1/1	0.96	0.23	26,26,26,26	0
58	MG	2A	3144	1/1	0.96	0.11	47,47,47,47	0
58	MG	1A	3514	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3988	1/1	0.96	0.07	43,43,43,43	0
58	MG	1A	3515	1/1	0.96	0.06	49,49,49,49	0
58	MG	1A	3340	1/1	0.96	0.18	48,48,48,48	0
58	MG	2A	3150	1/1	0.96	0.09	61,61,61,61	0
58	MG	2A	3402	1/1	0.96	0.18	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	3994	1/1	0.96	0.09	27,27,27,27	0
58	MG	1A	3341	1/1	0.96	0.18	36,36,36,36	0
58	MG	2A	3405	1/1	0.96	0.13	48,48,48,48	0
58	MG	1A	3996	1/1	0.96	0.06	34,34,34,34	0
58	MG	2A	3408	1/1	0.96	0.22	51,51,51,51	0
58	MG	1A	3150	1/1	0.96	0.21	37,37,37,37	0
58	MG	1A	3231	1/1	0.96	0.05	50,50,50,50	0
58	MG	1a	1745	1/1	0.96	0.12	44,44,44,44	0
58	MG	2A	3160	1/1	0.96	0.08	63,63,63,63	0
58	MG	1a	1746	1/1	0.96	0.14	47,47,47,47	0
58	MG	1A	3999	1/1	0.96	0.06	61,61,61,61	0
58	MG	1A	3834	1/1	0.96	0.09	48,48,48,48	0
58	MG	1V	202	1/1	0.96	0.23	28,28,28,28	0
58	MG	1V	206	1/1	0.96	0.17	43,43,43,43	0
58	MG	2A	3713	1/1	0.96	0.15	59,59,59,59	0
58	MG	1A	3347	1/1	0.96	0.08	34,34,34,34	0
58	MG	2A	3419	1/1	0.96	0.22	45,45,45,45	0
58	MG	1A	4004	1/1	0.96	0.06	35,35,35,35	0
58	MG	1a	1756	1/1	0.96	0.05	47,47,47,47	0
58	MG	1A	4005	1/1	0.96	0.07	25,25,25,25	0
58	MG	1a	1758	1/1	0.96	0.12	63,63,63,63	0
58	MG	1A	3426	1/1	0.96	0.17	57,57,57,57	0
58	MG	1A	4012	1/1	0.96	0.15	68,68,68,68	0
58	MG	1X	101	1/1	0.96	0.34	34,34,34,34	0
58	MG	1X	102	1/1	0.96	0.09	39,39,39,39	0
58	MG	1A	3290	1/1	0.96	0.13	36,36,36,36	0
58	MG	1A	3291	1/1	0.96	0.07	37,37,37,37	0
58	MG	2A	3180	1/1	0.96	0.05	59,59,59,59	0
58	MG	1A	4017	1/1	0.96	0.06	51,51,51,51	0
58	MG	1A	3659	1/1	0.96	0.08	28,28,28,28	0
58	MG	2A	3183	1/1	0.96	0.11	57,57,57,57	0
58	MG	10	101	1/1	0.96	0.08	34,34,34,34	0
58	MG	2A	3186	1/1	0.96	0.14	67,67,67,67	0
58	MG	2A	3436	1/1	0.96	0.12	41,41,41,41	0
58	MG	10	102	1/1	0.96	0.10	44,44,44,44	0
58	MG	10	104	1/1	0.96	0.12	36,36,36,36	0
58	MG	1A	3660	1/1	0.96	0.05	29,29,29,29	0
58	MG	1A	3232	1/1	0.96	0.15	41,41,41,41	0
58	MG	2A	3443	1/1	0.96	0.12	58,58,58,58	0
58	MG	10	107	1/1	0.96	0.07	39,39,39,39	0
58	MG	2A	3445	1/1	0.96	0.11	52,52,52,52	0
58	MG	1A	3526	1/1	0.96	0.16	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1777	1/1	0.96	0.10	49,49,49,49	0
58	MG	1a	1778	1/1	0.96	0.06	46,46,46,46	0
58	MG	2A	3750	1/1	0.96	0.08	54,54,54,54	0
58	MG	1A	3430	1/1	0.96	0.05	42,42,42,42	0
58	MG	2A	3752	1/1	0.96	0.12	57,57,57,57	0
58	MG	1A	3846	1/1	0.96	0.11	44,44,44,44	0
58	MG	11	102	1/1	0.96	0.08	43,43,43,43	0
58	MG	11	103	1/1	0.96	0.06	48,48,48,48	0
58	MG	1A	4029	1/1	0.96	0.07	47,47,47,47	0
58	MG	2A	3202	1/1	0.96	0.14	50,50,50,50	0
58	MG	2A	3759	1/1	0.96	0.14	56,56,56,56	0
58	MG	2A	3203	1/1	0.96	0.12	55,55,55,55	0
58	MG	2A	3458	1/1	0.96	0.07	57,57,57,57	0
58	MG	1A	3431	1/1	0.96	0.10	39,39,39,39	0
58	MG	2A	3764	1/1	0.96	0.09	57,57,57,57	0
58	MG	1A	3351	1/1	0.96	0.11	55,55,55,55	0
58	MG	2A	3767	1/1	0.96	0.12	59,59,59,59	0
58	MG	1A	3530	1/1	0.96	0.12	39,39,39,39	0
58	MG	2A	3769	1/1	0.96	0.07	48,48,48,48	0
58	MG	1A	4033	1/1	0.96	0.07	29,29,29,29	0
58	MG	2A	3771	1/1	0.96	0.05	69,69,69,69	0
58	MG	1A	3049	1/1	0.96	0.05	23,23,23,23	0
58	MG	2a	1753	1/1	0.96	0.07	56,56,56,56	0
58	MG	2A	3209	1/1	0.96	0.08	47,47,47,47	0
58	MG	13	105	1/1	0.96	0.05	31,31,31,31	0
58	MG	1A	3238	1/1	0.96	0.10	36,36,36,36	0
58	MG	2A	3777	1/1	0.96	0.06	48,48,48,48	0
58	MG	15	101	1/1	0.96	0.30	35,35,35,35	0
58	MG	15	102	1/1	0.96	0.14	33,33,33,33	0
58	MG	1A	3534	1/1	0.96	0.09	25,25,25,25	0
58	MG	1A	3857	1/1	0.96	0.11	22,22,22,22	0
58	MG	1A	3127	1/1	0.96	0.15	45,45,45,45	0
58	MG	1A	3153	1/1	0.96	0.07	30,30,30,30	0
58	MG	2A	3784	1/1	0.96	0.11	48,48,48,48	0
58	MG	16	102	1/1	0.96	0.06	54,54,54,54	0
58	MG	2A	3221	1/1	0.96	0.20	60,60,60,60	0
58	MG	2A	3787	1/1	0.96	0.10	52,52,52,52	0
58	MG	2A	3479	1/1	0.96	0.10	43,43,43,43	0
58	MG	2A	3790	1/1	0.96	0.08	58,58,58,58	0
58	MG	2a	1771	1/1	0.96	0.10	63,63,63,63	0
58	MG	1A	3682	1/1	0.96	0.04	27,27,27,27	0
58	MG	17	104	1/1	0.96	0.06	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	17	105	1/1	0.96	0.07	28,28,28,28	0
58	MG	1a	1810	1/1	0.96	0.14	56,56,56,56	0
58	MG	17	106	1/1	0.96	0.11	54,54,54,54	0
58	MG	2A	3796	1/1	0.96	0.10	52,52,52,52	0
58	MG	2a	1780	1/1	0.96	0.10	56,56,56,56	0
58	MG	1A	3189	1/1	0.96	0.09	35,35,35,35	0
58	MG	2a	1782	1/1	0.96	0.11	56,56,56,56	0
58	MG	1A	3019	1/1	0.96	0.07	40,40,40,40	0
58	MG	2A	3799	1/1	0.96	0.07	47,47,47,47	0
58	MG	18	103	1/1	0.96	0.07	35,35,35,35	0
58	MG	2a	1786	1/1	0.96	0.08	54,54,54,54	0
58	MG	1A	3541	1/1	0.96	0.06	40,40,40,40	0
58	MG	1A	3690	1/1	0.96	0.06	35,35,35,35	0
58	MG	2A	3491	1/1	0.96	0.13	49,49,49,49	0
58	MG	1m	3001	1/1	0.96	0.05	59,59,59,59	0
58	MG	1A	3103	1/1	0.96	0.12	28,28,28,28	0
58	MG	1A	3161	1/1	0.96	0.37	35,35,35,35	0
58	MG	2a	1793	1/1	0.96	0.06	65,65,65,65	0
58	MG	1A	3694	1/1	0.96	0.08	69,69,69,69	0
58	MG	2A	3499	1/1	0.96	0.07	63,63,63,63	0
58	MG	1A	3246	1/1	0.96	0.05	46,46,46,46	0
58	MG	1A	3447	1/1	0.96	0.21	35,35,35,35	0
58	MG	1A	3196	1/1	0.96	0.04	30,30,30,30	0
58	MG	1A	3365	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3197	1/1	0.96	0.21	32,32,32,32	0
58	MG	1A	4063	1/1	0.96	0.05	36,36,36,36	0
58	MG	2A	3506	1/1	0.96	0.10	28,28,28,28	0
58	MG	2A	3821	1/1	0.96	0.08	51,51,51,51	0
58	MG	2A	3822	1/1	0.96	0.10	47,47,47,47	0
58	MG	1A	3703	1/1	0.96	0.06	17,17,17,17	0
58	MG	2A	3824	1/1	0.96	0.07	46,46,46,46	0
58	MG	1x	103	1/1	0.96	0.18	53,53,53,53	0
58	MG	1A	3039	1/1	0.96	0.07	49,49,49,49	0
58	MG	1A	3009	1/1	0.96	0.07	28,28,28,28	0
58	MG	2A	3512	1/1	0.96	0.09	64,64,64,64	0
58	MG	1a	1612	1/1	0.96	0.10	26,26,26,26	0
58	MG	2a	1813	1/1	0.96	0.05	63,63,63,63	0
58	MG	2A	3832	1/1	0.96	0.15	59,59,59,59	0
58	MG	1A	4070	1/1	0.96	0.06	32,32,32,32	0
58	MG	1x	108	1/1	0.96	0.06	26,26,26,26	0
58	MG	1A	3311	1/1	0.96	0.21	44,44,44,44	0
58	MG	1A	3879	1/1	0.96	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	3838	1/1	0.96	0.07	40,40,40,40	0
58	MG	2a	1820	1/1	0.96	0.14	61,61,61,61	0
58	MG	1A	3562	1/1	0.96	0.08	57,57,57,57	0
58	MG	1a	1617	1/1	0.96	0.05	52,52,52,52	0
58	MG	2A	3842	1/1	0.96	0.07	46,46,46,46	0
58	MG	1A	3371	1/1	0.96	0.29	47,47,47,47	0
58	MG	2A	3844	1/1	0.96	0.09	45,45,45,45	0
58	MG	1A	3255	1/1	0.96	0.09	22,22,22,22	0
58	MG	2A	3523	1/1	0.96	0.05	47,47,47,47	0
58	MG	2A	3259	1/1	0.96	0.09	53,53,53,53	0
58	MG	2A	3006	1/1	0.96	0.23	55,55,55,55	0
58	MG	1A	3884	1/1	0.96	0.12	30,30,30,30	0
58	MG	1A	3203	1/1	0.96	0.14	21,21,21,21	0
58	MG	2A	3009	1/1	0.96	0.07	52,52,52,52	0
58	MG	2A	3010	1/1	0.96	0.09	61,61,61,61	0
58	MG	1A	3314	1/1	0.96	0.17	53,53,53,53	0
58	MG	1A	3136	1/1	0.96	0.14	22,22,22,22	0
58	MG	2A	3858	1/1	0.96	0.08	53,53,53,53	0
58	MG	1A	3717	1/1	0.96	0.07	49,49,49,49	0
58	MG	2A	3533	1/1	0.96	0.20	60,60,60,60	0
58	MG	1A	3719	1/1	0.96	0.06	47,47,47,47	0
58	MG	2A	3536	1/1	0.96	0.09	55,55,55,55	0
58	MG	2A	3863	1/1	0.96	0.08	58,58,58,58	0
58	MG	2A	3017	1/1	0.96	0.07	40,40,40,40	0
58	MG	2A	3018	1/1	0.96	0.17	49,49,49,49	0
58	MG	1A	4085	1/1	0.96	0.11	39,39,39,39	0
58	MG	1A	3572	1/1	0.96	0.05	35,35,35,35	0
58	MG	1A	3316	1/1	0.96	0.21	31,31,31,31	0
58	MG	2A	3278	1/1	0.96	0.08	60,60,60,60	0
58	MG	2A	3543	1/1	0.96	0.07	52,52,52,52	0
58	MG	2A	3544	1/1	0.96	0.06	37,37,37,37	0
58	MG	1A	4088	1/1	0.96	0.06	47,47,47,47	0
58	MG	1A	3725	1/1	0.96	0.06	33,33,33,33	0
58	MG	1A	3574	1/1	0.96	0.11	40,40,40,40	0
58	MG	1A	3575	1/1	0.96	0.12	45,45,45,45	0
58	MG	1A	3729	1/1	0.96	0.08	63,63,63,63	0
58	MG	2A	3031	1/1	0.96	0.08	48,48,48,48	0
58	MG	1A	3165	1/1	0.96	0.16	35,35,35,35	0
58	MG	2A	3556	1/1	0.96	0.06	41,41,41,41	0
58	MG	2A	3557	1/1	0.96	0.07	36,36,36,36	0
58	MG	2A	3558	1/1	0.96	0.08	62,62,62,62	0
59	K	2A	3448	1/1	0.96	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	ZN	14	102	1/1	0.96	0.10	112,112,112,112	0
58	MG	1A	3398	1/1	0.97	0.09	31,31,31,31	0
58	MG	1A	3071	1/1	0.97	0.15	28,28,28,28	0
58	MG	1A	3400	1/1	0.97	0.06	36,36,36,36	0
58	MG	1B	207	1/1	0.97	0.15	46,46,46,46	0
58	MG	2A	3326	1/1	0.97	0.07	36,36,36,36	0
58	MG	1A	3204	1/1	0.97	0.10	27,27,27,27	0
58	MG	1A	3263	1/1	0.97	0.23	46,46,46,46	0
58	MG	2Q	202	1/1	0.97	0.06	45,45,45,45	0
58	MG	1A	3730	1/1	0.97	0.07	47,47,47,47	0
58	MG	1A	3005	1/1	0.97	0.05	26,26,26,26	0
58	MG	1A	3901	1/1	0.97	0.10	33,33,33,33	0
58	MG	2A	3611	1/1	0.97	0.08	36,36,36,36	0
58	MG	1a	1662	1/1	0.97	0.05	47,47,47,47	0
58	MG	1A	3107	1/1	0.97	0.21	31,31,31,31	0
58	MG	2A	3614	1/1	0.97	0.08	45,45,45,45	0
58	MG	1B	214	1/1	0.97	0.19	51,51,51,51	0
58	MG	2V	202	1/1	0.97	0.05	51,51,51,51	0
58	MG	1A	3406	1/1	0.97	0.09	42,42,42,42	0
58	MG	2X	101	1/1	0.97	0.07	64,64,64,64	0
58	MG	1B	218	1/1	0.97	0.05	40,40,40,40	0
58	MG	1A	3034	1/1	0.97	0.06	45,45,45,45	0
58	MG	20	101	1/1	0.97	0.16	64,64,64,64	0
58	MG	1B	220	1/1	0.97	0.08	31,31,31,31	0
58	MG	2A	3339	1/1	0.97	0.05	51,51,51,51	0
58	MG	2A	3077	1/1	0.97	0.09	37,37,37,37	0
58	MG	2A	3622	1/1	0.97	0.10	51,51,51,51	0
58	MG	1A	3738	1/1	0.97	0.09	58,58,58,58	0
58	MG	2A	3079	1/1	0.97	0.07	24,24,24,24	0
58	MG	1A	3739	1/1	0.97	0.07	37,37,37,37	0
58	MG	2A	3626	1/1	0.97	0.07	41,41,41,41	0
58	MG	25	103	1/1	0.97	0.08	47,47,47,47	0
58	MG	1A	3908	1/1	0.97	0.10	33,33,33,33	0
58	MG	27	101	1/1	0.97	0.16	51,51,51,51	0
58	MG	1A	3741	1/1	0.97	0.07	47,47,47,47	0
58	MG	2A	3629	1/1	0.97	0.07	37,37,37,37	0
58	MG	1A	3910	1/1	0.97	0.14	32,32,32,32	0
58	MG	2A	3084	1/1	0.97	0.06	43,43,43,43	0
58	MG	2A	3633	1/1	0.97	0.08	52,52,52,52	0
58	MG	1A	3912	1/1	0.97	0.03	26,26,26,26	0
58	MG	1B	227	1/1	0.97	0.06	39,39,39,39	0
58	MG	1A	3154	1/1	0.97	0.10	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	2A	3088	1/1	0.97	0.06	50,50,50,50	0
58	MG	1A	3268	1/1	0.97	0.23	40,40,40,40	0
58	MG	1A	3745	1/1	0.97	0.06	42,42,42,42	0
58	MG	1A	3491	1/1	0.97	0.12	46,46,46,46	0
58	MG	1A	3492	1/1	0.97	0.10	36,36,36,36	0
58	MG	1A	3209	1/1	0.97	0.06	36,36,36,36	0
58	MG	1a	1682	1/1	0.97	0.05	48,48,48,48	0
58	MG	2A	3645	1/1	0.97	0.06	51,51,51,51	0
58	MG	1A	3494	1/1	0.97	0.09	45,45,45,45	0
58	MG	2a	1615	1/1	0.97	0.07	67,67,67,67	0
58	MG	1A	3112	1/1	0.97	0.10	32,32,32,32	0
58	MG	1a	1685	1/1	0.97	0.12	55,55,55,55	0
58	MG	1A	3753	1/1	0.97	0.04	38,38,38,38	0
58	MG	1D	303	1/1	0.97	0.14	40,40,40,40	0
58	MG	1A	3113	1/1	0.97	0.08	33,33,33,33	0
58	MG	1D	309	1/1	0.97	0.04	32,32,32,32	0
58	MG	1A	3755	1/1	0.97	0.07	32,32,32,32	0
58	MG	1A	3756	1/1	0.97	0.07	33,33,33,33	0
58	MG	1A	3925	1/1	0.97	0.07	49,49,49,49	0
58	MG	1D	313	1/1	0.97	0.10	31,31,31,31	0
58	MG	1A	3010	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	3273	1/1	0.97	0.05	44,44,44,44	0
58	MG	1A	3928	1/1	0.97	0.04	17,17,17,17	0
58	MG	1A	3932	1/1	0.97	0.04	33,33,33,33	0
58	MG	1A	3933	1/1	0.97	0.05	34,34,34,34	0
58	MG	1A	3018	1/1	0.97	0.14	39,39,39,39	0
58	MG	1A	3417	1/1	0.97	0.10	37,37,37,37	0
58	MG	1A	3607	1/1	0.97	0.07	46,46,46,46	0
58	MG	1A	3342	1/1	0.97	0.22	37,37,37,37	0
58	MG	2A	3116	1/1	0.97	0.25	56,56,56,56	0
58	MG	1A	3276	1/1	0.97	0.09	29,29,29,29	0
58	MG	1A	3765	1/1	0.97	0.06	29,29,29,29	0
58	MG	1A	3766	1/1	0.97	0.07	39,39,39,39	0
58	MG	1A	3503	1/1	0.97	0.05	36,36,36,36	0
58	MG	1F	302	1/1	0.97	0.18	32,32,32,32	0
58	MG	1A	3947	1/1	0.97	0.07	57,57,57,57	0
58	MG	1a	1709	1/1	0.97	0.13	45,45,45,45	0
58	MG	1F	304	1/1	0.97	0.07	51,51,51,51	0
58	MG	1A	3948	1/1	0.97	0.09	47,47,47,47	0
58	MG	1a	1712	1/1	0.97	0.20	55,55,55,55	0
58	MG	1F	308	1/1	0.97	0.17	29,29,29,29	0
58	MG	2A	3682	1/1	0.97	0.13	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3616	1/1	0.97	0.04	36,36,36,36	0
58	MG	1A	3345	1/1	0.97	0.16	33,33,33,33	0
58	MG	1A	3770	1/1	0.97	0.13	25,25,25,25	0
58	MG	1F	312	1/1	0.97	0.05	48,48,48,48	0
58	MG	1A	3952	1/1	0.97	0.07	55,55,55,55	0
58	MG	1a	1719	1/1	0.97	0.10	52,52,52,52	0
58	MG	1A	3771	1/1	0.97	0.05	23,23,23,23	0
58	MG	1G	202	1/1	0.97	0.20	50,50,50,50	0
58	MG	1a	1722	1/1	0.97	0.08	45,45,45,45	0
58	MG	1a	1723	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	3421	1/1	0.97	0.13	42,42,42,42	0
58	MG	1A	3773	1/1	0.97	0.04	45,45,45,45	0
58	MG	2A	3143	1/1	0.97	0.17	41,41,41,41	0
58	MG	1A	3277	1/1	0.97	0.32	44,44,44,44	0
58	MG	1A	3423	1/1	0.97	0.06	42,42,42,42	0
58	MG	1A	3424	1/1	0.97	0.10	43,43,43,43	0
58	MG	1A	3779	1/1	0.97	0.06	21,21,21,21	0
58	MG	1A	3780	1/1	0.97	0.06	29,29,29,29	0
58	MG	1A	3510	1/1	0.97	0.29	31,31,31,31	0
58	MG	1A	3782	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3041	1/1	0.97	0.16	28,28,28,28	0
58	MG	1a	1735	1/1	0.97	0.10	45,45,45,45	0
58	MG	1O	203	1/1	0.97	0.07	52,52,52,52	0
58	MG	2a	1671	1/1	0.97	0.11	53,53,53,53	0
58	MG	1A	3784	1/1	0.97	0.05	17,17,17,17	0
58	MG	2A	3158	1/1	0.97	0.11	47,47,47,47	0
58	MG	1P	201	1/1	0.97	0.14	23,23,23,23	0
58	MG	1A	3628	1/1	0.97	0.07	53,53,53,53	0
58	MG	2a	1676	1/1	0.97	0.09	51,51,51,51	0
58	MG	1A	3513	1/1	0.97	0.10	24,24,24,24	0
58	MG	1P	205	1/1	0.97	0.04	33,33,33,33	0
58	MG	1A	3787	1/1	0.97	0.03	23,23,23,23	0
58	MG	2A	3715	1/1	0.97	0.10	50,50,50,50	0
58	MG	1Q	201	1/1	0.97	0.23	32,32,32,32	0
58	MG	1A	3082	1/1	0.97	0.21	32,32,32,32	0
58	MG	1A	3083	1/1	0.97	0.12	35,35,35,35	0
58	MG	1A	3633	1/1	0.97	0.05	20,20,20,20	0
58	MG	1a	1750	1/1	0.97	0.08	59,59,59,59	0
58	MG	1a	1751	1/1	0.97	0.05	54,54,54,54	0
58	MG	1A	3166	1/1	0.97	0.06	39,39,39,39	0
58	MG	1A	3122	1/1	0.97	0.12	29,29,29,29	0
58	MG	1A	3637	1/1	0.97	0.07	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	1A	3287	1/1	0.97	0.06	45,45,45,45	0
58	MG	1A	3797	1/1	0.97	0.07	16,16,16,16	0
58	MG	1A	3979	1/1	0.97	0.12	46,46,46,46	0
58	MG	1A	3123	1/1	0.97	0.12	35,35,35,35	0
58	MG	1T	201	1/1	0.97	0.12	46,46,46,46	0
58	MG	1A	3224	1/1	0.97	0.08	48,48,48,48	0
58	MG	1A	3084	1/1	0.97	0.14	32,32,32,32	0
58	MG	2a	1697	1/1	0.97	0.11	40,40,40,40	0
58	MG	1A	3802	1/1	0.97	0.05	40,40,40,40	0
58	MG	2A	3184	1/1	0.97	0.10	43,43,43,43	0
58	MG	1A	3642	1/1	0.97	0.04	15,15,15,15	0
58	MG	1A	3804	1/1	0.97	0.05	23,23,23,23	0
58	MG	1a	1766	1/1	0.97	0.08	66,66,66,66	0
58	MG	2A	3189	1/1	0.97	0.06	63,63,63,63	0
58	MG	1A	3805	1/1	0.97	0.07	22,22,22,22	0
58	MG	1V	201	1/1	0.97	0.17	23,23,23,23	0
58	MG	1A	3226	1/1	0.97	0.11	32,32,32,32	0
58	MG	1A	3125	1/1	0.97	0.15	35,35,35,35	0
58	MG	1A	3438	1/1	0.97	0.14	41,41,41,41	0
58	MG	1A	3229	1/1	0.97	0.08	36,36,36,36	0
58	MG	2A	3749	1/1	0.97	0.05	45,45,45,45	0
58	MG	2a	1712	1/1	0.97	0.14	57,57,57,57	0
58	MG	1A	3171	1/1	0.97	0.05	34,34,34,34	0
58	MG	1A	3175	1/1	0.97	0.09	29,29,29,29	0
58	MG	1W	203	1/1	0.97	0.09	38,38,38,38	0
58	MG	1W	206	1/1	0.97	0.12	26,26,26,26	0
58	MG	2A	3754	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3126	1/1	0.97	0.20	32,32,32,32	0
58	MG	2A	3463	1/1	0.97	0.11	62,62,62,62	0
58	MG	1A	3443	1/1	0.97	0.11	28,28,28,28	0
58	MG	1A	3816	1/1	0.97	0.05	24,24,24,24	0
58	MG	1a	1781	1/1	0.97	0.06	51,51,51,51	0
58	MG	1A	3652	1/1	0.97	0.08	34,34,34,34	0
58	MG	1A	4003	1/1	0.97	0.04	25,25,25,25	0
58	MG	1A	3818	1/1	0.97	0.30	29,29,29,29	0
58	MG	1a	1786	1/1	0.97	0.10	52,52,52,52	0
58	MG	1A	3444	1/1	0.97	0.08	32,32,32,32	0
58	MG	2A	3766	1/1	0.97	0.07	40,40,40,40	0
58	MG	1A	4008	1/1	0.97	0.05	37,37,37,37	0
58	MG	2A	3210	1/1	0.97	0.05	48,48,48,48	0
58	MG	2A	3474	1/1	0.97	0.04	45,45,45,45	0
58	MG	2A	3211	1/1	0.97	0.06	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	4009	1/1	0.97	0.06	29,29,29,29	0
58	MG	1A	4010	1/1	0.97	0.04	37,37,37,37	0
58	MG	1A	3822	1/1	0.97	0.04	25,25,25,25	0
58	MG	1A	3364	1/1	0.97	0.18	32,32,32,32	0
58	MG	1A	4013	1/1	0.97	0.07	66,66,66,66	0
58	MG	1A	3533	1/1	0.97	0.26	39,39,39,39	0
58	MG	1A	3233	1/1	0.97	0.07	62,62,62,62	0
58	MG	1A	3658	1/1	0.97	0.12	55,55,55,55	0
58	MG	1a	1800	1/1	0.97	0.06	60,60,60,60	0
58	MG	1a	1801	1/1	0.97	0.21	48,48,48,48	0
58	MG	1A	3535	1/1	0.97	0.20	41,41,41,41	0
58	MG	1A	3366	1/1	0.97	0.24	37,37,37,37	0
58	MG	1A	3830	1/1	0.97	0.09	29,29,29,29	0
58	MG	1A	3831	1/1	0.97	0.08	48,48,48,48	0
58	MG	2A	3226	1/1	0.97	0.08	42,42,42,42	0
58	MG	2a	1748	1/1	0.97	0.04	58,58,58,58	0
58	MG	12	101	1/1	0.97	0.08	42,42,42,42	0
58	MG	2A	3788	1/1	0.97	0.06	62,62,62,62	0
58	MG	1A	3832	1/1	0.97	0.06	45,45,45,45	0
58	MG	2A	3497	1/1	0.97	0.09	52,52,52,52	0
58	MG	1A	4023	1/1	0.97	0.07	62,62,62,62	0
58	MG	1A	4024	1/1	0.97	0.09	30,30,30,30	0
58	MG	1A	3234	1/1	0.97	0.26	37,37,37,37	0
58	MG	1A	4028	1/1	0.97	0.05	40,40,40,40	0
58	MG	2A	3233	1/1	0.97	0.07	36,36,36,36	0
58	MG	1A	3662	1/1	0.97	0.04	22,22,22,22	0
58	MG	1A	3043	1/1	0.97	0.07	33,33,33,33	0
58	MG	1A	3237	1/1	0.97	0.19	28,28,28,28	0
58	MG	1A	3058	1/1	0.97	0.10	47,47,47,47	0
58	MG	15	104	1/1	0.97	0.27	26,26,26,26	0
58	MG	1A	3014	1/1	0.97	0.11	37,37,37,37	0
58	MG	1A	3668	1/1	0.97	0.05	19,19,19,19	0
58	MG	1A	3455	1/1	0.97	0.19	38,38,38,38	0
58	MG	1A	3130	1/1	0.97	0.13	43,43,43,43	0
58	MG	2A	3805	1/1	0.97	0.10	42,42,42,42	0
58	MG	1A	4038	1/1	0.97	0.08	26,26,26,26	0
58	MG	1A	3842	1/1	0.97	0.11	40,40,40,40	0
58	MG	1A	3008	1/1	0.97	0.04	30,30,30,30	0
58	MG	1A	3675	1/1	0.97	0.05	17,17,17,17	0
58	MG	2A	3517	1/1	0.97	0.06	53,53,53,53	0
58	MG	2a	1774	1/1	0.97	0.07	64,64,64,64	0
58	MG	1A	3845	1/1	0.97	0.09	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	4044	1/1	0.97	0.05	28,28,28,28	0
58	MG	1A	3132	1/1	0.97	0.21	31,31,31,31	0
58	MG	2A	3816	1/1	0.97	0.05	46,46,46,46	0
58	MG	2a	1779	1/1	0.97	0.05	46,46,46,46	0
58	MG	18	104	1/1	0.97	0.14	33,33,33,33	0
58	MG	2A	3252	1/1	0.97	0.12	61,61,61,61	0
58	MG	1A	3547	1/1	0.97	0.07	35,35,35,35	0
58	MG	1A	3548	1/1	0.97	0.05	44,44,44,44	0
58	MG	1A	3849	1/1	0.97	0.13	41,41,41,41	0
58	MG	1A	3851	1/1	0.97	0.17	31,31,31,31	0
58	MG	1A	3852	1/1	0.97	0.06	16,16,16,16	0
58	MG	1A	3681	1/1	0.97	0.10	44,44,44,44	0
58	MG	1A	3550	1/1	0.97	0.18	33,33,33,33	0
58	MG	1A	3134	1/1	0.97	0.08	27,27,27,27	0
58	MG	1A	3046	1/1	0.97	0.13	28,28,28,28	0
58	MG	2A	3003	1/1	0.97	0.28	55,55,55,55	0
58	MG	2A	3004	1/1	0.97	0.26	44,44,44,44	0
58	MG	2A	3265	1/1	0.97	0.14	47,47,47,47	0
58	MG	2A	3535	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	4059	1/1	0.97	0.09	15,15,15,15	0
58	MG	2A	3836	1/1	0.97	0.09	44,44,44,44	0
58	MG	2A	3267	1/1	0.97	0.07	50,50,50,50	0
58	MG	1A	3686	1/1	0.97	0.05	29,29,29,29	0
58	MG	2A	3839	1/1	0.97	0.07	42,42,42,42	0
58	MG	1A	3553	1/1	0.97	0.14	34,34,34,34	0
58	MG	1A	3689	1/1	0.97	0.04	22,22,22,22	0
58	MG	1a	1609	1/1	0.97	0.07	54,54,54,54	0
58	MG	1a	1610	1/1	0.97	0.19	48,48,48,48	0
58	MG	2A	3011	1/1	0.97	0.11	53,53,53,53	0
58	MG	2A	3274	1/1	0.97	0.08	62,62,62,62	0
58	MG	2A	3545	1/1	0.97	0.04	44,44,44,44	0
58	MG	2a	1807	1/1	0.97	0.20	51,51,51,51	0
58	MG	2A	3012	1/1	0.97	0.04	37,37,37,37	0
58	MG	1A	4066	1/1	0.97	0.12	47,47,47,47	0
58	MG	1A	3188	1/1	0.97	0.11	39,39,39,39	0
58	MG	1A	3463	1/1	0.97	0.12	40,40,40,40	0
58	MG	2A	3279	1/1	0.97	0.09	48,48,48,48	0
58	MG	1A	3247	1/1	0.97	0.19	36,36,36,36	0
58	MG	1A	3693	1/1	0.97	0.04	26,26,26,26	0
58	MG	2A	3555	1/1	0.97	0.06	54,54,54,54	0
58	MG	1A	3559	1/1	0.97	0.14	26,26,26,26	0
58	MG	2A	3019	1/1	0.97	0.08	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4072	1/1	0.97	0.08	38,38,38,38	0
58	MG	2A	3559	1/1	0.97	0.06	39,39,39,39	0
58	MG	1A	3560	1/1	0.97	0.06	22,22,22,22	0
58	MG	1a	1619	1/1	0.97	0.05	57,57,57,57	0
58	MG	1A	3063	1/1	0.97	0.09	35,35,35,35	0
58	MG	1A	3384	1/1	0.97	0.26	43,43,43,43	0
58	MG	2A	3027	1/1	0.97	0.05	47,47,47,47	0
58	MG	1A	4077	1/1	0.97	0.13	44,44,44,44	0
58	MG	1A	3318	1/1	0.97	0.09	31,31,31,31	0
58	MG	1A	3566	1/1	0.97	0.26	36,36,36,36	0
58	MG	1a	1625	1/1	0.97	0.12	58,58,58,58	0
58	MG	2A	3569	1/1	0.97	0.10	43,43,43,43	0
58	MG	2A	3032	1/1	0.97	0.05	51,51,51,51	0
58	MG	1A	3028	1/1	0.97	0.12	34,34,34,34	0
58	MG	1A	3193	1/1	0.97	0.11	25,25,25,25	0
58	MG	1A	3706	1/1	0.97	0.04	25,25,25,25	0
58	MG	2f	201	1/1	0.97	0.09	49,49,49,49	0
58	MG	1a	1629	1/1	0.97	0.18	43,43,43,43	0
58	MG	2A	3575	1/1	0.97	0.04	27,27,27,27	0
58	MG	1A	3065	1/1	0.97	0.08	29,29,29,29	0
58	MG	2A	3040	1/1	0.97	0.17	51,51,51,51	0
58	MG	1A	3099	1/1	0.97	0.04	38,38,38,38	0
58	MG	1A	3145	1/1	0.97	0.10	27,27,27,27	0
58	MG	1A	3031	1/1	0.97	0.11	23,23,23,23	0
58	MG	1A	3474	1/1	0.97	0.10	41,41,41,41	0
58	MG	1A	3880	1/1	0.97	0.05	55,55,55,55	0
58	MG	2D	301	1/1	0.97	0.06	39,39,39,39	0
58	MG	2D	302	1/1	0.97	0.22	43,43,43,43	0
58	MG	1A	3576	1/1	0.97	0.09	36,36,36,36	0
58	MG	2r	101	1/1	0.97	0.12	50,50,50,50	0
58	MG	2D	304	1/1	0.97	0.07	34,34,34,34	0
58	MG	1a	1638	1/1	0.97	0.15	57,57,57,57	0
58	MG	1A	3325	1/1	0.97	0.14	30,30,30,30	0
58	MG	1A	4091	1/1	0.97	0.06	47,47,47,47	0
58	MG	1a	1641	1/1	0.97	0.10	70,70,70,70	0
58	MG	2A	3590	1/1	0.97	0.06	47,47,47,47	0
58	MG	1A	3578	1/1	0.97	0.12	49,49,49,49	0
58	MG	1A	3069	1/1	0.97	0.07	16,16,16,16	0
58	MG	1A	3886	1/1	0.97	0.07	48,48,48,48	0
58	MG	1a	1645	1/1	0.97	0.12	44,44,44,44	0
58	MG	1A	3718	1/1	0.97	0.06	36,36,36,36	0
58	MG	1A	3102	1/1	0.97	0.13	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1649	1/1	0.97	0.09	43,43,43,43	0
58	MG	1A	3478	1/1	0.97	0.05	60,60,60,60	0
58	MG	1A	3722	1/1	0.97	0.06	32,32,32,32	0
58	MG	1A	3723	1/1	0.97	0.05	22,22,22,22	0
60	ZN	24	501	1/1	0.97	0.12	124,124,124,124	0
61	SF4	2d	303	8/8	0.97	0.05	77,84,90,103	0
58	MG	1A	3695	1/1	0.98	0.07	23,23,23,23	0
58	MG	1A	3587	1/1	0.98	0.21	29,29,29,29	0
58	MG	2A	3112	1/1	0.98	0.10	45,45,45,45	0
58	MG	1B	202	1/1	0.98	0.13	43,43,43,43	0
58	MG	1a	1764	1/1	0.98	0.05	57,57,57,57	0
58	MG	1A	3174	1/1	0.98	0.10	24,24,24,24	0
58	MG	17	103	1/1	0.98	0.13	25,25,25,25	0
58	MG	2A	3117	1/1	0.98	0.26	62,62,62,62	0
58	MG	1A	3819	1/1	0.98	0.03	21,21,21,21	0
58	MG	1A	3589	1/1	0.98	0.09	40,40,40,40	0
58	MG	1A	3821	1/1	0.98	0.03	21,21,21,21	0
58	MG	1A	3105	1/1	0.98	0.07	28,28,28,28	0
58	MG	1A	3106	1/1	0.98	0.04	26,26,26,26	0
58	MG	1A	3702	1/1	0.98	0.06	28,28,28,28	0
58	MG	1A	3825	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	3020	1/1	0.98	0.04	21,21,21,21	0
58	MG	1A	3704	1/1	0.98	0.04	15,15,15,15	0
58	MG	2A	3761	1/1	0.98	0.06	48,48,48,48	0
58	MG	1A	3108	1/1	0.98	0.15	34,34,34,34	0
58	MG	1A	3504	1/1	0.98	0.07	32,32,32,32	0
58	MG	1A	3110	1/1	0.98	0.04	35,35,35,35	0
58	MG	1B	217	1/1	0.98	0.09	45,45,45,45	0
58	MG	1A	3961	1/1	0.98	0.06	38,38,38,38	0
58	MG	1A	3708	1/1	0.98	0.04	30,30,30,30	0
58	MG	1A	3293	1/1	0.98	0.07	54,54,54,54	0
58	MG	1a	1784	1/1	0.98	0.06	41,41,41,41	0
58	MG	2A	3546	1/1	0.98	0.05	37,37,37,37	0
58	MG	1A	3139	1/1	0.98	0.10	32,32,32,32	0
58	MG	2A	3772	1/1	0.98	0.06	56,56,56,56	0
58	MG	2A	3548	1/1	0.98	0.11	36,36,36,36	0
58	MG	1A	3359	1/1	0.98	0.07	49,49,49,49	0
58	MG	1A	3966	1/1	0.98	0.06	41,41,41,41	0
58	MG	1a	1789	1/1	0.98	0.04	52,52,52,52	0
58	MG	2A	3139	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3140	1/1	0.98	0.06	29,29,29,29	0
58	MG	2A	3141	1/1	0.98	0.12	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	3235	1/1	0.98	0.15	23,23,23,23	0
58	MG	1A	3362	1/1	0.98	0.11	46,46,46,46	0
58	MG	1A	3512	1/1	0.98	0.23	25,25,25,25	0
58	MG	1A	3716	1/1	0.98	0.03	12,12,12,12	0
58	MG	1A	3141	1/1	0.98	0.09	17,17,17,17	0
58	MG	1A	3604	1/1	0.98	0.09	43,43,43,43	0
58	MG	1A	3007	1/1	0.98	0.10	35,35,35,35	0
58	MG	1B	232	1/1	0.98	0.04	46,46,46,46	0
58	MG	1a	1799	1/1	0.98	0.09	51,51,51,51	0
58	MG	1A	3436	1/1	0.98	0.08	42,42,42,42	0
58	MG	2A	3154	1/1	0.98	0.11	41,41,41,41	0
58	MG	1A	3437	1/1	0.98	0.20	33,33,33,33	0
58	MG	1A	3143	1/1	0.98	0.09	54,54,54,54	0
58	MG	1A	3303	1/1	0.98	0.04	29,29,29,29	0
58	MG	1B	237	1/1	0.98	0.03	27,27,27,27	0
58	MG	1D	301	1/1	0.98	0.19	42,42,42,42	0
58	MG	1a	1806	1/1	0.98	0.10	56,56,56,56	0
58	MG	1A	3239	1/1	0.98	0.20	33,33,33,33	0
58	MG	2A	3162	1/1	0.98	0.15	39,39,39,39	0
58	MG	1A	3726	1/1	0.98	0.13	56,56,56,56	0
58	MG	1D	305	1/1	0.98	0.08	33,33,33,33	0
58	MG	1D	306	1/1	0.98	0.14	35,35,35,35	0
58	MG	1A	3611	1/1	0.98	0.09	47,47,47,47	0
58	MG	1A	3983	1/1	0.98	0.04	18,18,18,18	0
58	MG	1e	201	1/1	0.98	0.03	49,49,49,49	0
58	MG	2A	3169	1/1	0.98	0.08	54,54,54,54	0
58	MG	2A	3581	1/1	0.98	0.06	38,38,38,38	0
58	MG	1A	3984	1/1	0.98	0.06	28,28,28,28	0
58	MG	2A	3369	1/1	0.98	0.15	40,40,40,40	0
58	MG	1A	3850	1/1	0.98	0.07	49,49,49,49	0
58	MG	1k	201	1/1	0.98	0.13	45,45,45,45	0
58	MG	1A	3612	1/1	0.98	0.06	29,29,29,29	0
58	MG	1A	3613	1/1	0.98	0.08	36,36,36,36	0
58	MG	1A	3615	1/1	0.98	0.06	19,19,19,19	0
58	MG	2a	1705	1/1	0.98	0.10	60,60,60,60	0
58	MG	1A	3989	1/1	0.98	0.04	40,40,40,40	0
58	MG	2A	3177	1/1	0.98	0.08	31,31,31,31	0
58	MG	2A	3818	1/1	0.98	0.10	69,69,69,69	0
58	MG	1E	303	1/1	0.98	0.15	44,44,44,44	0
58	MG	1A	3991	1/1	0.98	0.05	33,33,33,33	0
58	MG	1E	305	1/1	0.98	0.07	28,28,28,28	0
58	MG	1A	3731	1/1	0.98	0.04	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3732	1/1	0.98	0.03	27,27,27,27	0
58	MG	1A	3733	1/1	0.98	0.05	20,20,20,20	0
58	MG	1E	309	1/1	0.98	0.09	49,49,49,49	0
58	MG	1A	3144	1/1	0.98	0.10	35,35,35,35	0
58	MG	1A	3054	1/1	0.98	0.09	29,29,29,29	0
58	MG	2A	3829	1/1	0.98	0.04	66,66,66,66	0
58	MG	1A	3522	1/1	0.98	0.04	35,35,35,35	0
58	MG	2A	3188	1/1	0.98	0.07	46,46,46,46	0
58	MG	1A	3190	1/1	0.98	0.21	31,31,31,31	0
58	MG	1A	3146	1/1	0.98	0.12	26,26,26,26	0
58	MG	1A	3622	1/1	0.98	0.08	24,24,24,24	0
58	MG	1A	3740	1/1	0.98	0.06	48,48,48,48	0
58	MG	1A	3192	1/1	0.98	0.21	29,29,29,29	0
58	MG	1A	3086	1/1	0.98	0.18	25,25,25,25	0
58	MG	1A	3374	1/1	0.98	0.09	36,36,36,36	0
58	MG	1F	305	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	4006	1/1	0.98	0.03	38,38,38,38	0
58	MG	2A	3397	1/1	0.98	0.15	42,42,42,42	0
58	MG	2A	3398	1/1	0.98	0.11	48,48,48,48	0
58	MG	1A	4007	1/1	0.98	0.04	44,44,44,44	0
58	MG	1A	3068	1/1	0.98	0.10	31,31,31,31	0
58	MG	1A	3035	1/1	0.98	0.05	32,32,32,32	0
58	MG	1A	3377	1/1	0.98	0.07	41,41,41,41	0
58	MG	1A	3631	1/1	0.98	0.04	16,16,16,16	0
58	MG	1A	3378	1/1	0.98	0.13	24,24,24,24	0
58	MG	1A	3452	1/1	0.98	0.05	45,45,45,45	0
58	MG	2A	3850	1/1	0.98	0.09	53,53,53,53	0
58	MG	2A	3406	1/1	0.98	0.19	38,38,38,38	0
58	MG	1A	4014	1/1	0.98	0.06	37,37,37,37	0
58	MG	1A	3089	1/1	0.98	0.07	32,32,32,32	0
58	MG	2A	3855	1/1	0.98	0.04	64,64,64,64	0
58	MG	1A	3874	1/1	0.98	0.23	29,29,29,29	0
58	MG	1A	3454	1/1	0.98	0.17	50,50,50,50	0
58	MG	1A	3876	1/1	0.98	0.12	29,29,29,29	0
58	MG	1A	3249	1/1	0.98	0.05	43,43,43,43	0
58	MG	1A	3250	1/1	0.98	0.06	48,48,48,48	0
58	MG	1A	3382	1/1	0.98	0.04	33,33,33,33	0
58	MG	2A	3630	1/1	0.98	0.07	46,46,46,46	0
58	MG	1N	203	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3538	1/1	0.98	0.14	37,37,37,37	0
58	MG	1N	205	1/1	0.98	0.04	36,36,36,36	0
58	MG	1A	3117	1/1	0.98	0.11	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1755	1/1	0.98	0.04	64,64,64,64	0
58	MG	2A	3021	1/1	0.98	0.06	30,30,30,30	0
58	MG	2A	3022	1/1	0.98	0.09	42,42,42,42	0
58	MG	2A	3637	1/1	0.98	0.06	36,36,36,36	0
58	MG	1A	3317	1/1	0.98	0.05	43,43,43,43	0
58	MG	1A	3385	1/1	0.98	0.30	25,25,25,25	0
58	MG	1A	3118	1/1	0.98	0.05	35,35,35,35	0
58	MG	1A	3885	1/1	0.98	0.05	43,43,43,43	0
58	MG	1A	3387	1/1	0.98	0.16	21,21,21,21	0
58	MG	1P	203	1/1	0.98	0.17	32,32,32,32	0
58	MG	1A	3199	1/1	0.98	0.10	23,23,23,23	0
58	MG	1A	3647	1/1	0.98	0.06	27,27,27,27	0
58	MG	1A	3201	1/1	0.98	0.12	31,31,31,31	0
58	MG	2A	3647	1/1	0.98	0.15	55,55,55,55	0
58	MG	2A	3648	1/1	0.98	0.12	63,63,63,63	0
58	MG	1A	3037	1/1	0.98	0.09	34,34,34,34	0
58	MG	1A	3257	1/1	0.98	0.11	38,38,38,38	0
58	MG	2A	3034	1/1	0.98	0.06	49,49,49,49	0
58	MG	1A	3038	1/1	0.98	0.21	31,31,31,31	0
58	MG	1A	4037	1/1	0.98	0.10	26,26,26,26	0
58	MG	2A	3037	1/1	0.98	0.15	44,44,44,44	0
58	MG	2A	3234	1/1	0.98	0.27	37,37,37,37	0
58	MG	1Q	205	1/1	0.98	0.04	45,45,45,45	0
58	MG	2D	305	1/1	0.98	0.24	39,39,39,39	0
58	MG	2A	3438	1/1	0.98	0.16	46,46,46,46	0
58	MG	2A	3439	1/1	0.98	0.23	53,53,53,53	0
58	MG	1A	3155	1/1	0.98	0.13	27,27,27,27	0
58	MG	1A	3156	1/1	0.98	0.04	30,30,30,30	0
58	MG	2A	3661	1/1	0.98	0.08	38,38,38,38	0
58	MG	1R	201	1/1	0.98	0.08	30,30,30,30	0
58	MG	2E	305	1/1	0.98	0.08	35,35,35,35	0
58	MG	1A	3121	1/1	0.98	0.16	29,29,29,29	0
58	MG	1A	4041	1/1	0.98	0.09	36,36,36,36	0
58	MG	2A	3665	1/1	0.98	0.17	41,41,41,41	0
58	MG	1A	3896	1/1	0.98	0.06	41,41,41,41	0
58	MG	1A	3396	1/1	0.98	0.05	32,32,32,32	0
58	MG	1A	3775	1/1	0.98	0.06	20,20,20,20	0
58	MG	1A	3899	1/1	0.98	0.08	49,49,49,49	0
58	MG	1A	4046	1/1	0.98	0.06	42,42,42,42	0
58	MG	1U	201	1/1	0.98	0.10	30,30,30,30	0
58	MG	1A	3048	1/1	0.98	0.08	25,25,25,25	0
58	MG	1A	3159	1/1	0.98	0.09	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	1A	3778	1/1	0.98	0.04	33,33,33,33	0
58	MG	1A	3074	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	3558	1/1	0.98	0.06	28,28,28,28	0
58	MG	1U	209	1/1	0.98	0.07	44,44,44,44	0
58	MG	1A	4052	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	3060	1/1	0.98	0.10	49,49,49,49	0
58	MG	2A	3461	1/1	0.98	0.08	51,51,51,51	0
58	MG	1V	204	1/1	0.98	0.19	30,30,30,30	0
58	MG	1V	205	1/1	0.98	0.18	29,29,29,29	0
58	MG	1A	3906	1/1	0.98	0.07	36,36,36,36	0
58	MG	1V	207	1/1	0.98	0.03	36,36,36,36	0
58	MG	1A	3211	1/1	0.98	0.15	33,33,33,33	0
58	MG	1A	4057	1/1	0.98	0.03	43,43,43,43	0
58	MG	2A	3261	1/1	0.98	0.05	53,53,53,53	0
58	MG	1A	3402	1/1	0.98	0.07	39,39,39,39	0
58	MG	1A	3096	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3097	1/1	0.98	0.07	33,33,33,33	0
58	MG	1W	204	1/1	0.98	0.09	30,30,30,30	0
58	MG	1W	205	1/1	0.98	0.10	32,32,32,32	0
58	MG	1A	3565	1/1	0.98	0.27	38,38,38,38	0
58	MG	1A	3214	1/1	0.98	0.12	34,34,34,34	0
58	MG	1A	3669	1/1	0.98	0.04	18,18,18,18	0
58	MG	1A	3789	1/1	0.98	0.04	45,45,45,45	0
58	MG	2A	3478	1/1	0.98	0.06	48,48,48,48	0
58	MG	1X	103	1/1	0.98	0.23	43,43,43,43	0
58	MG	1X	104	1/1	0.98	0.10	33,33,33,33	0
58	MG	23	104	1/1	0.98	0.07	49,49,49,49	0
58	MG	1X	105	1/1	0.98	0.04	47,47,47,47	0
58	MG	1Y	201	1/1	0.98	0.05	41,41,41,41	0
58	MG	1A	3568	1/1	0.98	0.18	35,35,35,35	0
58	MG	1a	1728	1/1	0.98	0.05	38,38,38,38	0
58	MG	1A	3077	1/1	0.98	0.06	29,29,29,29	0
58	MG	1A	3078	1/1	0.98	0.10	26,26,26,26	0
58	MG	1A	3674	1/1	0.98	0.08	24,24,24,24	0
58	MG	1A	3029	1/1	0.98	0.14	22,22,22,22	0
58	MG	1A	3485	1/1	0.98	0.07	36,36,36,36	0
58	MG	2A	3490	1/1	0.98	0.14	33,33,33,33	0
58	MG	10	103	1/1	0.98	0.05	35,35,35,35	0
58	MG	2A	3283	1/1	0.98	0.25	52,52,52,52	0
58	MG	1A	3218	1/1	0.98	0.06	37,37,37,37	0
58	MG	1A	4075	1/1	0.98	0.13	46,46,46,46	0
58	MG	1A	3410	1/1	0.98	0.06	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	2A	3717	1/1	0.98	0.04	33,33,33,33	0
58	MG	1A	3080	1/1	0.98	0.17	29,29,29,29	0
58	MG	1A	3275	1/1	0.98	0.13	21,21,21,21	0
58	MG	1A	3012	1/1	0.98	0.14	30,30,30,30	0
58	MG	1A	3684	1/1	0.98	0.05	22,22,22,22	0
58	MG	2A	3722	1/1	0.98	0.06	38,38,38,38	0
58	MG	1A	3221	1/1	0.98	0.10	32,32,32,32	0
58	MG	2A	3724	1/1	0.98	0.10	50,50,50,50	0
58	MG	1a	1744	1/1	0.98	0.14	38,38,38,38	0
58	MG	1A	3929	1/1	0.98	0.04	48,48,48,48	0
58	MG	1A	3930	1/1	0.98	0.04	58,58,58,58	0
58	MG	1A	3931	1/1	0.98	0.05	29,29,29,29	0
58	MG	1a	1748	1/1	0.98	0.10	61,61,61,61	0
58	MG	2A	3730	1/1	0.98	0.04	61,61,61,61	0
58	MG	1A	3032	1/1	0.98	0.25	29,29,29,29	0
58	MG	1A	3133	1/1	0.98	0.04	33,33,33,33	0
58	MG	1A	3688	1/1	0.98	0.05	26,26,26,26	0
58	MG	1A	3937	1/1	0.98	0.11	46,46,46,46	0
58	MG	1A	3938	1/1	0.98	0.03	36,36,36,36	0
58	MG	1A	3581	1/1	0.98	0.03	37,37,37,37	0
58	MG	1A	3172	1/1	0.98	0.13	40,40,40,40	0
58	MG	1A	3282	1/1	0.98	0.12	39,39,39,39	0
58	MG	1A	3173	1/1	0.98	0.22	31,31,31,31	0
58	MG	1A	3284	1/1	0.98	0.05	50,50,50,50	0
58	MG	1A	3944	1/1	0.98	0.07	40,40,40,40	0
60	ZN	2Y	202	1/1	0.98	0.04	96,96,96,96	0
58	MG	2A	3742	1/1	0.98	0.04	49,49,49,49	0
60	ZN	25	106	1/1	0.98	0.03	67,67,67,67	0
60	ZN	29	501	1/1	0.98	0.04	62,62,62,62	0
60	ZN	2n	102	1/1	0.98	0.05	92,92,92,92	0
61	SF4	1d	302	8/8	0.98	0.06	62,67,71,80	0
58	MG	1A	3285	1/1	0.98	0.23	46,46,46,46	0
58	MG	2A	3365	1/1	0.99	0.08	37,37,37,37	0
58	MG	1A	3066	1/1	0.99	0.02	27,27,27,27	0
58	MG	1A	3696	1/1	0.99	0.03	37,37,37,37	0
58	MG	1A	3036	1/1	0.99	0.10	24,24,24,24	0
58	MG	1A	3623	1/1	0.99	0.05	22,22,22,22	0
58	MG	1A	3561	1/1	0.99	0.23	30,30,30,30	0
58	MG	1A	3625	1/1	0.99	0.07	51,51,51,51	0
58	MG	2A	3450	1/1	0.99	0.15	26,26,26,26	0
58	MG	1F	306	1/1	0.99	0.06	42,42,42,42	0
58	MG	1A	3935	1/1	0.99	0.06	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	3936	1/1	0.99	0.03	40,40,40,40	0
58	MG	1A	3990	1/1	0.99	0.05	44,44,44,44	0
58	MG	1A	3022	1/1	0.99	0.04	16,16,16,16	0
58	MG	1A	3252	1/1	0.99	0.04	26,26,26,26	0
58	MG	2A	3149	1/1	0.99	0.06	36,36,36,36	0
58	MG	1A	3744	1/1	0.99	0.07	20,20,20,20	0
58	MG	2A	3151	1/1	0.99	0.04	37,37,37,37	0
58	MG	1A	3298	1/1	0.99	0.09	23,23,23,23	0
58	MG	1B	216	1/1	0.99	0.04	43,43,43,43	0
58	MG	2A	3708	1/1	0.99	0.03	49,49,49,49	0
58	MG	1A	3746	1/1	0.99	0.03	11,11,11,11	0
58	MG	1A	3160	1/1	0.99	0.05	24,24,24,24	0
58	MG	1A	4054	1/1	0.99	0.06	22,22,22,22	0
58	MG	1a	1770	1/1	0.99	0.03	39,39,39,39	0
58	MG	1A	3013	1/1	0.99	0.03	26,26,26,26	0
58	MG	1A	3666	1/1	0.99	0.03	36,36,36,36	0
58	MG	1A	3750	1/1	0.99	0.03	26,26,26,26	0
58	MG	1A	3796	1/1	0.99	0.09	21,21,21,21	0
58	MG	1A	4001	1/1	0.99	0.03	30,30,30,30	0
58	MG	1A	3567	1/1	0.99	0.19	39,39,39,39	0
58	MG	1A	3070	1/1	0.99	0.05	28,28,28,28	0
58	MG	1A	3302	1/1	0.99	0.04	32,32,32,32	0
58	MG	1a	1633	1/1	0.99	0.11	28,28,28,28	0
58	MG	1A	4064	1/1	0.99	0.04	31,31,31,31	0
58	MG	1A	3800	1/1	0.99	0.04	34,34,34,34	0
58	MG	1A	3178	1/1	0.99	0.09	33,33,33,33	0
58	MG	1A	3635	1/1	0.99	0.05	27,27,27,27	0
58	MG	1A	3672	1/1	0.99	0.06	30,30,30,30	0
58	MG	1A	3093	1/1	0.99	0.06	17,17,17,17	0
58	MG	1A	3279	1/1	0.99	0.12	28,28,28,28	0
58	MG	1A	3806	1/1	0.99	0.03	32,32,32,32	0
58	MG	2A	3813	1/1	0.99	0.06	32,32,32,32	0
58	MG	12	102	1/1	0.99	0.06	39,39,39,39	0
58	MG	2A	3815	1/1	0.99	0.04	43,43,43,43	0
58	MG	1A	3807	1/1	0.99	0.04	26,26,26,26	0
58	MG	1A	3011	1/1	0.99	0.04	26,26,26,26	0
58	MG	1A	3462	1/1	0.99	0.10	35,35,35,35	0
58	MG	1A	3677	1/1	0.99	0.04	27,27,27,27	0
58	MG	1A	3762	1/1	0.99	0.07	35,35,35,35	0
58	MG	1a	1648	1/1	0.99	0.03	49,49,49,49	0
58	MG	1D	304	1/1	0.99	0.04	19,19,19,19	0
58	MG	1A	3003	1/1	0.99	0.06	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3492	1/1	0.99	0.11	25,25,25,25	0
58	MG	2A	3825	1/1	0.99	0.07	20,20,20,20	0
58	MG	1A	3911	1/1	0.99	0.03	23,23,23,23	0
58	MG	1D	307	1/1	0.99	0.12	28,28,28,28	0
58	MG	1A	3679	1/1	0.99	0.02	27,27,27,27	0
58	MG	2A	3496	1/1	0.99	0.03	61,61,61,61	0
58	MG	1A	3200	1/1	0.99	0.03	30,30,30,30	0
58	MG	1R	203	1/1	0.99	0.12	34,34,34,34	0
58	MG	1A	3721	1/1	0.99	0.04	40,40,40,40	0
58	MG	1A	3109	1/1	0.99	0.13	28,28,28,28	0
58	MG	17	101	1/1	0.99	0.05	29,29,29,29	0
58	MG	1A	3030	1/1	0.99	0.14	23,23,23,23	0
58	MG	1A	3184	1/1	0.99	0.04	35,35,35,35	0
58	MG	2W	202	1/1	0.99	0.15	37,37,37,37	0
58	MG	1A	4025	1/1	0.99	0.03	26,26,26,26	0
58	MG	1A	4026	1/1	0.99	0.03	41,41,41,41	0
58	MG	2A	3587	1/1	0.99	0.04	35,35,35,35	0
58	MG	1A	3549	1/1	0.99	0.17	36,36,36,36	0
58	MG	1a	1736	1/1	0.99	0.08	41,41,41,41	0
58	MG	1U	202	1/1	0.99	0.15	36,36,36,36	0
58	MG	1A	3056	1/1	0.99	0.05	29,29,29,29	0
58	MG	1A	3186	1/1	0.99	0.11	34,34,34,34	0
58	MG	2A	3511	1/1	0.99	0.07	38,38,38,38	0
58	MG	1A	3098	1/1	0.99	0.11	16,16,16,16	0
58	MG	1A	3614	1/1	0.99	0.05	34,34,34,34	0
58	MG	1U	207	1/1	0.99	0.13	26,26,26,26	0
58	MG	1A	3975	1/1	0.99	0.03	49,49,49,49	0
58	MG	1A	3289	1/1	0.99	0.09	24,24,24,24	0
58	MG	25	104	1/1	0.99	0.05	52,52,52,52	0
60	ZN	1Y	204	1/1	0.99	0.03	70,70,70,70	0
58	MG	1A	3075	1/1	0.99	0.02	33,33,33,33	0
60	ZN	19	501	1/1	0.99	0.11	60,60,60,60	0
60	ZN	1n	103	1/1	0.99	0.02	65,65,65,65	0
58	MG	1A	3042	1/1	0.99	0.20	33,33,33,33	0
58	MG	1V	203	1/1	0.99	0.04	34,34,34,34	0
58	MG	2A	3854	1/1	0.99	0.13	39,39,39,39	0
60	ZN	26	501	1/1	0.99	0.05	61,61,61,61	0
58	MG	1E	312	1/1	0.99	0.11	21,21,21,21	0
58	MG	1A	3343	1/1	0.99	0.11	34,34,34,34	0
58	MG	1A	3228	1/1	0.99	0.15	33,33,33,33	0
58	MG	1A	3655	1/1	0.99	0.06	30,30,30,30	0
58	MG	1a	1787	1/1	1.00	0.02	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	4065	1/1	1.00	0.04	22,22,22,22	0
58	MG	1A	3295	1/1	1.00	0.02	28,28,28,28	0
58	MG	1A	4060	1/1	1.00	0.04	21,21,21,21	0
60	ZN	15	107	1/1	1.00	0.01	38,38,38,38	0
60	ZN	16	103	1/1	1.00	0.02	39,39,39,39	0
58	MG	1A	3618	1/1	1.00	0.05	31,31,31,31	0
58	MG	2A	3700	1/1	1.00	0.06	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.