



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2020 – 01:32 PM BST

PDB ID : 6CAE
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with NOSO-95179 antibiotic and bound to mRNA and A-, P- and E-site tRNAs at 2.6Å resolution
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Deposited on : 2018-01-30
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.1

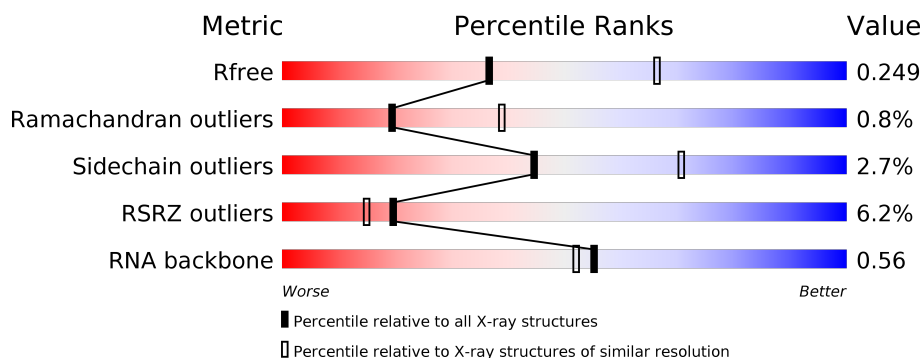
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	2A	2915	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>.</div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>93%</div> <div>6%</div> <div>..</div> </div> </div>
2	2B	121	<div> <div></div> <div> <div></div> <div>78%</div> <div>21%</div> <div>.</div> </div> </div>
3	1D	276	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>.</div> </div> </div>

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

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Mol	Chain	Length	Quality of chain
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	
28	16	54	

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

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Mol	Chain	Length	Quality of chain
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	
53	1v	27	

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Mol	Chain	Length	Quality of chain
53	2v	27	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	
56	A	9	
56	B	9	
56	C	9	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	PSU	1w	55	-	-	-	X
54	CM0	2y	34	-	-	-	X
54	5MU	2y	54	-	-	-	X
56	IAR	A	9	-	-	-	X
56	IAR	B	7	-	-	-	X
56	IAR	C	9	-	-	-	X
57	MG	1A	3084	-	-	-	X
57	MG	1A	3086	-	-	-	X
57	MG	1A	3232	-	-	-	X
57	MG	1A	3297	-	-	-	X
57	MG	1A	3363	-	-	-	X
57	MG	1A	3446	-	-	-	X
57	MG	1A	3473	-	-	-	X
57	MG	1A	3931	-	-	-	X
57	MG	1A	3945	-	-	-	X
57	MG	1E	301	-	-	-	X
57	MG	1P	203	-	-	-	X
57	MG	1a	1645	-	-	-	X
57	MG	1a	1648	-	-	-	X
57	MG	1a	1659	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1a	1671	-	-	-	X
57	MG	1a	1870	-	-	-	X
57	MG	1w	104	-	-	-	X
57	MG	1w	106	-	-	-	X
57	MG	1x	3014	-	-	-	X
57	MG	23	101	-	-	-	X
57	MG	28	101	-	-	-	X
57	MG	29	101	-	-	-	X
57	MG	2A	3082	-	-	-	X
57	MG	2A	3122	-	-	-	X
57	MG	2A	3179	-	-	-	X
57	MG	2A	3209	-	-	-	X
57	MG	2A	3213	-	-	-	X
57	MG	2A	3219	-	-	-	X
57	MG	2A	3222	-	-	-	X
57	MG	2A	3224	-	-	-	X
57	MG	2A	3227	-	-	-	X
57	MG	2A	3237	-	-	-	X
57	MG	2A	3240	-	-	-	X
57	MG	2A	3281	-	-	-	X
57	MG	2A	3292	-	-	-	X
57	MG	2A	3312	-	-	-	X
57	MG	2A	3317	-	-	-	X
57	MG	2A	3327	-	-	-	X
57	MG	2A	3342	-	-	-	X
57	MG	2A	3557	-	-	-	X
57	MG	2A	3675	-	-	-	X
57	MG	2A	3832	-	-	-	X
57	MG	2A	3834	-	-	-	X
57	MG	2A	3843	-	-	-	X
57	MG	2A	3845	-	-	-	X
57	MG	2A	3850	-	-	-	X
57	MG	2X	3001	-	-	-	X
57	MG	2a	1693	-	-	-	X
57	MG	2a	1802	-	-	-	X
57	MG	2v	101	-	-	-	X
57	MG	2y	3003	-	-	-	X
57	MG	C	8002	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 301143 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 mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			276	124	48	91	13			
53	2v	13	Total	C	N	O	P	0	0	0
			276	124	48	91	13			

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	73	Total	C	N	O	P	S	0	0
			1568	700	282	512	73	1		
54	1y	74	Total	C	N	O	P	S	0	0
			1591	710	287	519	74	1		
54	2w	73	Total	C	N	O	P	S	0	0
			1568	700	282	512	73	1		
54	2y	73	Total	C	N	O	P	S	0	0
			1568	700	282	512	73	1		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
55	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 56 is a protein called NOSO-95179 antibiotic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	A	9	Total	C	N	O	0	0	0
			72	43	18	11			
56	B	7	Total	C	N	O	0	0	0
			55	33	14	8			
56	C	9	Total	C	N	O	0	0	0
			72	43	18	11			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2E	10	Total	Mg	0	0
			10	10		
57	17	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2d	1	Total Mg 1 1	0	0
57	1T	2	Total Mg 2 2	0	0
57	1N	7	Total Mg 7 7	0	0
57	20	2	Total Mg 2 2	0	0
57	18	4	Total Mg 4 4	0	0
57	2W	2	Total Mg 2 2	0	0
57	1Y	3	Total Mg 3 3	0	0
57	13	2	Total Mg 2 2	0	0
57	1f	1	Total Mg 1 1	0	0
57	C	2	Total Mg 2 2	0	0
57	1P	4	Total Mg 4 4	0	0
57	2B	21	Total Mg 21 21	0	0
57	2a	202	Total Mg 202 202	0	0
57	1E	10	Total Mg 10 10	0	0
57	1b	2	Total Mg 2 2	0	0
57	2l	3	Total Mg 3 3	0	0
57	2F	3	Total Mg 3 3	0	0
57	16	1	Total Mg 1 1	0	0
57	28	3	Total Mg 3 3	0	0
57	2e	2	Total Mg 2 2	0	0
57	1W	5	Total Mg 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1149	Total 1149	Mg 1149	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1n	1	Total 1	Mg 1	0	0
57	1X	6	Total 6	Mg 6	0	0
57	12	2	Total 2	Mg 2	0	0
57	1y	6	Total 6	Mg 6	0	0
57	2i	1	Total 1	Mg 1	0	0
57	1S	3	Total 3	Mg 3	0	0
57	25	3	Total 3	Mg 3	0	0
57	2T	4	Total 4	Mg 4	0	0
57	1D	9	Total 9	Mg 9	0	0
57	2N	1	Total 1	Mg 1	0	0
57	1e	2	Total 2	Mg 2	0	0
57	2G	1	Total 1	Mg 1	0	0
57	1I	1	Total 1	Mg 1	0	0
57	29	1	Total 1	Mg 1	0	0
57	2f	2	Total 2	Mg 2	0	0
57	1V	2	Total 2	Mg 2	0	0
57	2X	3	Total 3	Mg 3	0	0
57	1w	8	Total 8	Mg 8	0	0
57	26	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1a	314	Total Mg 314 314	0	0
57	2Q	3	Total Mg 3 3	0	0
57	15	2	Total Mg 2 2	0	0
57	1x	14	Total Mg 14 14	0	0
57	2j	2	Total Mg 2 2	0	0
57	1R	3	Total Mg 3 3	0	0
57	1s	1	Total Mg 1 1	0	0
57	1m	1	Total Mg 1 1	0	0
57	2U	4	Total Mg 4 4	0	0
57	1G	5	Total Mg 5 5	0	0
57	2O	2	Total Mg 2 2	0	0
57	11	2	Total Mg 2 2	0	0
57	1d	2	Total Mg 2 2	0	0
57	2n	1	Total Mg 1 1	0	0
57	21	2	Total Mg 2 2	0	0
57	2g	1	Total Mg 1 1	0	0
57	1v	1	Total Mg 1 1	0	0
57	2x	6	Total Mg 6 6	0	0
57	2R	2	Total Mg 2 2	0	0
57	1Z	4	Total Mg 4 4	0	0
57	2D	4	Total Mg 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2q	3	Total Mg 3 3	0	0
57	1U	6	Total Mg 6 6	0	0
57	2r	1	Total Mg 1 1	0	0
57	1O	4	Total Mg 4 4	0	0
57	1r	1	Total Mg 1 1	0	0
57	19	1	Total Mg 1 1	0	0
57	1l	2	Total Mg 2 2	0	0
57	2V	2	Total Mg 2 2	0	0
57	1F	8	Total Mg 8 8	0	0
57	10	6	Total Mg 6 6	0	0
57	2t	1	Total Mg 1 1	0	0
57	1Q	5	Total Mg 5 5	0	0
57	2A	861	Total Mg 861 861	0	0
57	23	2	Total Mg 2 2	0	0
57	2Z	1	Total Mg 1 1	0	0
57	1B	36	Total Mg 36 36	0	0
57	2y	7	Total Mg 7 7	0	0
57	2v	2	Total Mg 2 2	0	0

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total K 1 1	0	0

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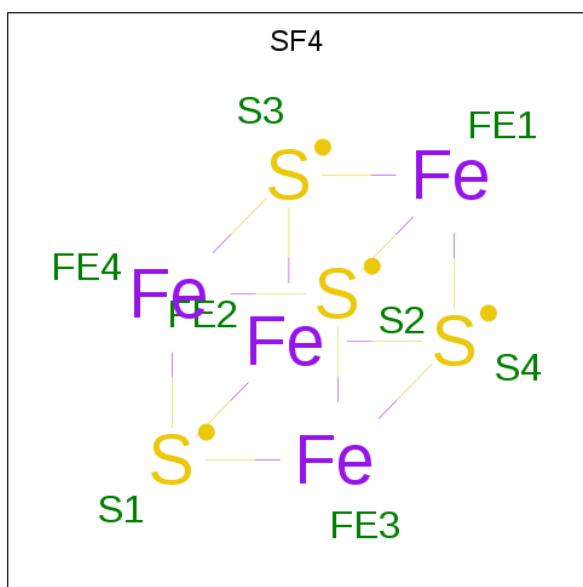
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	2A	1	Total K 1 1	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0
59	14	1	Total Zn 1 1	0	0
59	1n	1	Total Zn 1 1	0	0
59	15	1	Total Zn 1 1	0	0
59	29	1	Total Zn 1 1	0	0
59	19	1	Total Zn 1 1	0	0
59	26	1	Total Zn 1 1	0	0
59	25	1	Total Zn 1 1	0	0
59	24	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0
59	2Y	1	Total Zn 1 1	0	0
59	16	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total	Fe	S	0	0
			8	4	4		
60	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2172	Total	O	0	0
			2172	2172		
61	1B	71	Total	O	0	0
			71	71		
61	1D	28	Total	O	0	0
			28	28		
61	1E	29	Total	O	0	0
			29	29		
61	1F	18	Total	O	0	0
			18	18		
61	1G	7	Total	O	0	0
			7	7		
61	1H	2	Total	O	0	0
			2	2		
61	1I	2	Total	O	0	0
			2	2		
61	1N	5	Total	O	0	0
			5	5		
61	1O	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1P	23	Total 23	O 23	0	0
61	1Q	11	Total 11	O 11	0	0
61	1R	18	Total 18	O 18	0	0
61	1S	3	Total 3	O 3	0	0
61	1T	10	Total 10	O 10	0	0
61	1U	11	Total 11	O 11	0	0
61	1V	8	Total 8	O 8	0	0
61	1W	7	Total 7	O 7	0	0
61	1X	7	Total 7	O 7	0	0
61	1Y	4	Total 4	O 4	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	11	Total 11	O 11	0	0
61	11	9	Total 9	O 9	0	0
61	12	5	Total 5	O 5	0	0
61	13	6	Total 6	O 6	0	0
61	15	5	Total 5	O 5	0	0
61	16	4	Total 4	O 4	0	0
61	17	7	Total 7	O 7	0	0
61	18	12	Total 12	O 12	0	0
61	19	1	Total 1	O 1	0	0
61	1a	686	Total 686	O 686	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1b	1	Total 1	O 1	0	0
61	1d	3	Total 3	O 3	0	0
61	1f	1	Total 1	O 1	0	0
61	1g	1	Total 1	O 1	0	0
61	1i	1	Total 1	O 1	0	0
61	1l	10	Total 10	O 10	0	0
61	1m	1	Total 1	O 1	0	0
61	1o	2	Total 2	O 2	0	0
61	1p	3	Total 3	O 3	0	0
61	1q	5	Total 5	O 5	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	6	Total 6	O 6	0	0
61	1w	7	Total 7	O 7	0	0
61	1x	17	Total 17	O 17	0	0
61	1y	4	Total 4	O 4	0	0
61	2A	1348	Total 1348	O 1348	0	0
61	2B	27	Total 27	O 27	0	0
61	2D	26	Total 26	O 26	0	0
61	2E	12	Total 12	O 12	0	0
61	2F	17	Total 17	O 17	0	0
61	2I	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2N	2	Total 2	O 2	0	0
61	2O	2	Total 2	O 2	0	0
61	2P	14	Total 14	O 14	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	3	Total 3	O 3	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	4	Total 4	O 4	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	5	Total 5	O 5	0	0
61	2X	6	Total 6	O 6	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	5	Total 5	O 5	0	0
61	21	12	Total 12	O 12	0	0
61	22	1	Total 1	O 1	0	0
61	23	1	Total 1	O 1	0	0
61	25	4	Total 4	O 4	0	0
61	26	1	Total 1	O 1	0	0
61	27	3	Total 3	O 3	0	0
61	28	5	Total 5	O 5	0	0
61	29	1	Total 1	O 1	0	0

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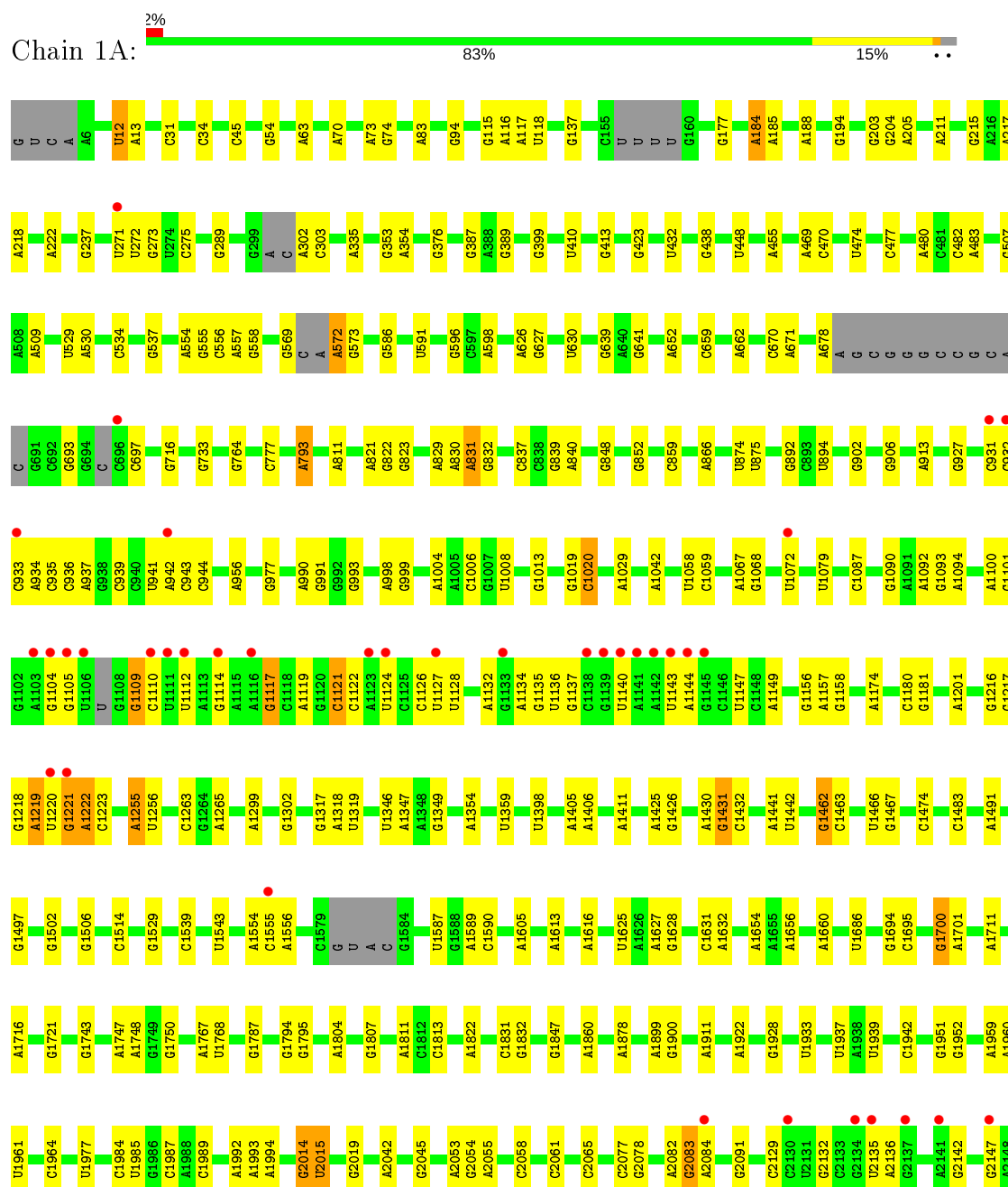
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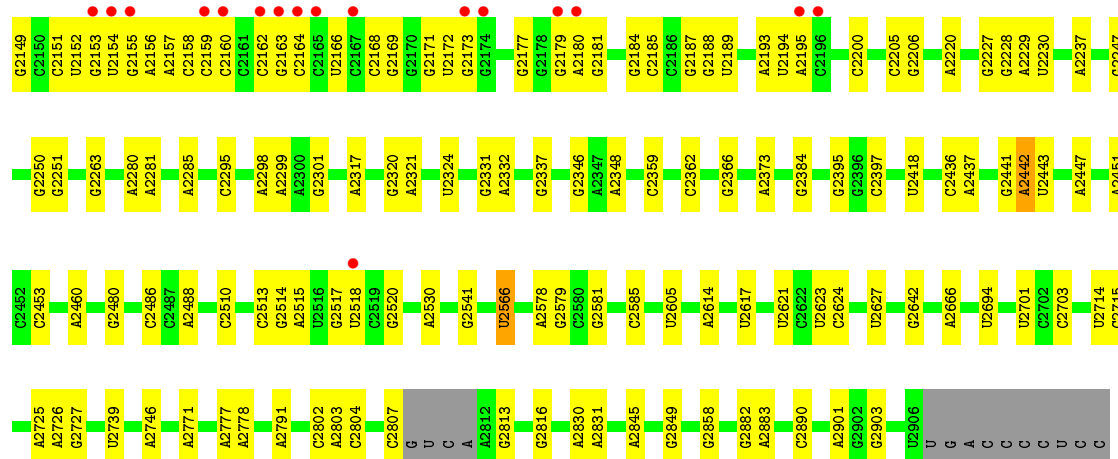
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	270	Total 270	O 270	0	0
61	2d	1	Total 1	O 1	0	0
61	2g	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	5	Total 5	O 5	0	0
61	2m	1	Total 1	O 1	0	0
61	2o	1	Total 1	O 1	0	0
61	2p	2	Total 2	O 2	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	2	Total 2	O 2	0	0
61	2v	4	Total 4	O 4	0	0
61	2w	4	Total 4	O 4	0	0
61	2x	7	Total 7	O 7	0	0
61	2y	19	Total 19	O 19	0	0
61	C	4	Total 4	O 4	0	0

3 Residue-property plots [i](#)

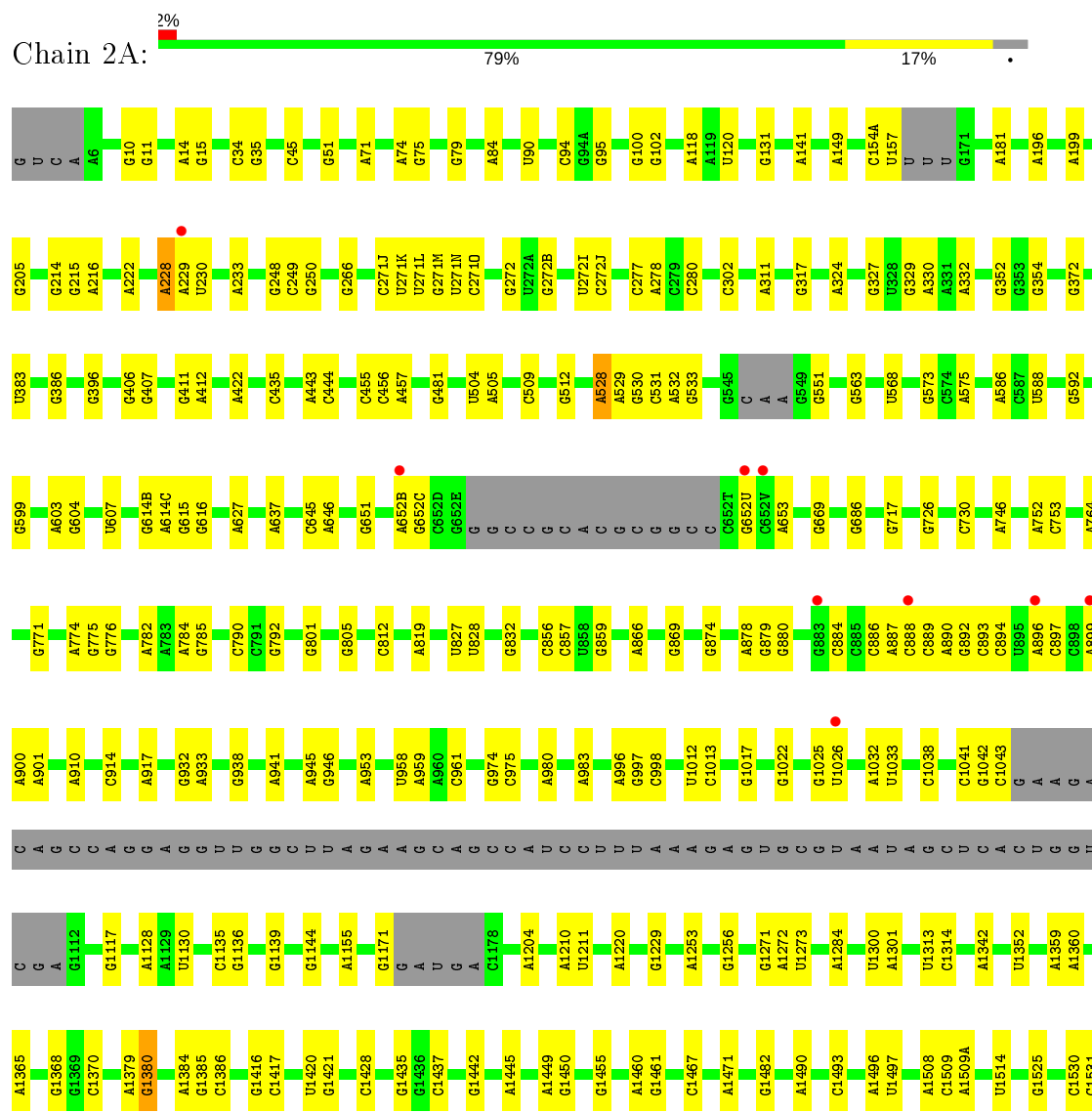
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S Ribosomal RNA

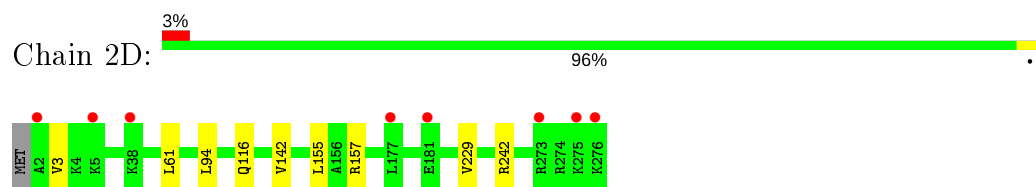




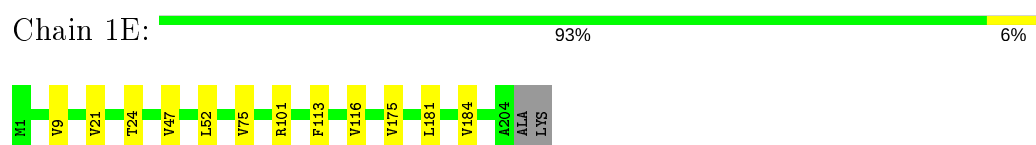
• Molecule 1: 23S Ribosomal RNA



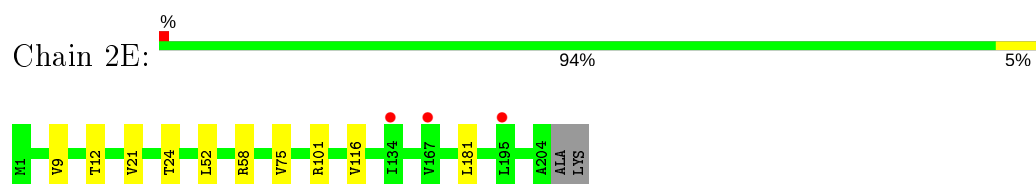
- Molecule 3: 50S ribosomal protein L2



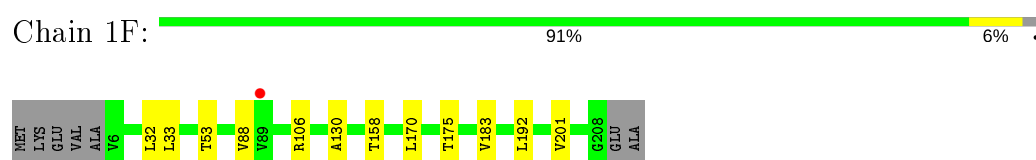
- Molecule 4: 50S ribosomal protein L3



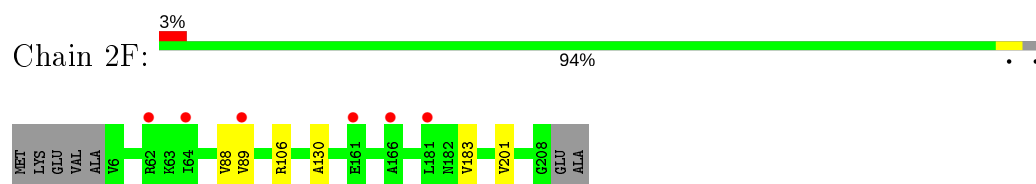
- Molecule 4: 50S ribosomal protein L3



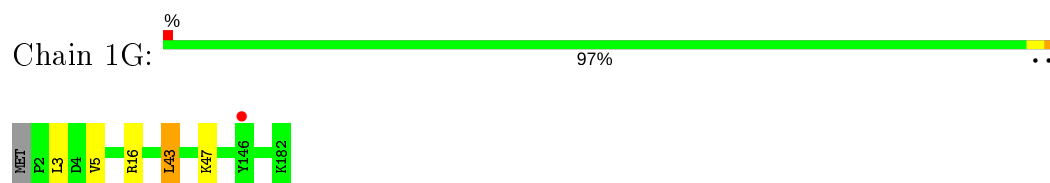
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4

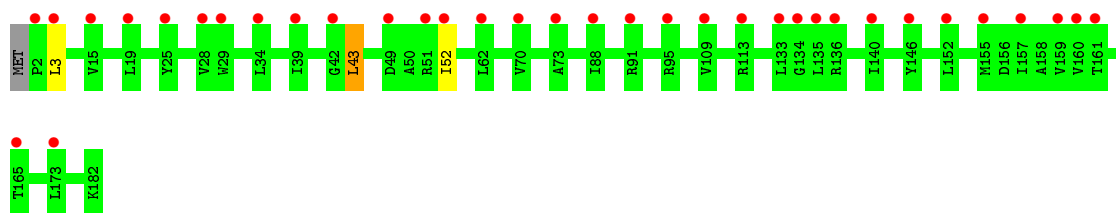


- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5

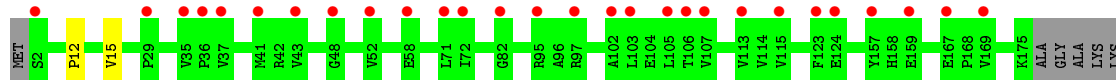




- Molecule 7: 50S ribosomal protein L6



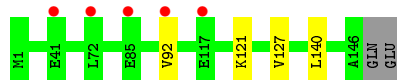
- Molecule 7: 50S ribosomal protein L6



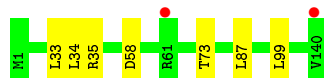
- Molecule 8: 50S ribosomal protein L9



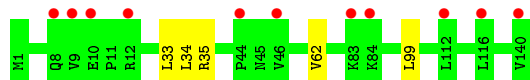
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13



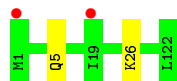
- Molecule 10: 50S ribosomal protein L14

Chain 1O:  98%



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  98%



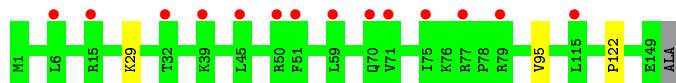
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  96%



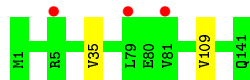
- Molecule 11: 50S ribosomal protein L15

Chain 2P:  97%



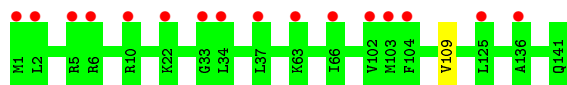
- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  99%



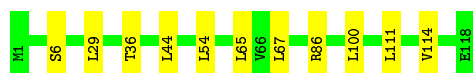
- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  99%

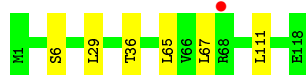


- Molecule 13: 50S ribosomal protein L17

Chain 1R:  91% 9%



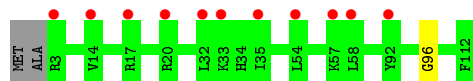
- Molecule 13: 50S ribosomal protein L17



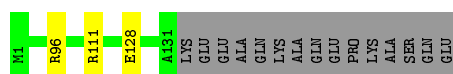
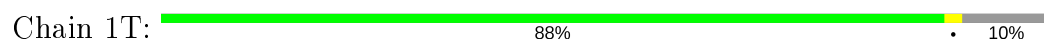
- Molecule 14: 50S ribosomal protein L18



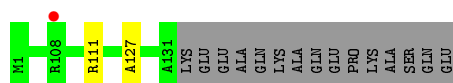
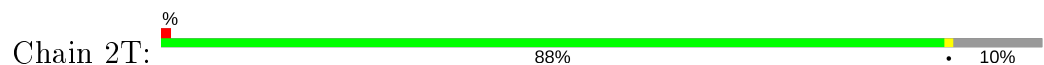
- Molecule 14: 50S ribosomal protein L18



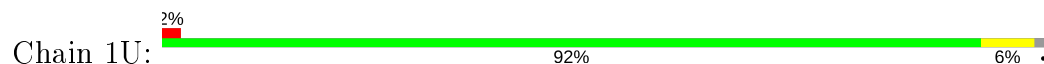
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19

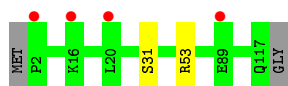


- Molecule 16: 50S ribosomal protein L20

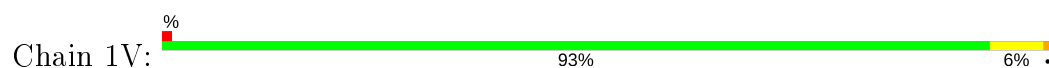


- Molecule 16: 50S ribosomal protein L20

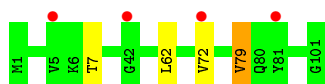




- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



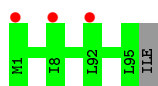
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  93% 5% .




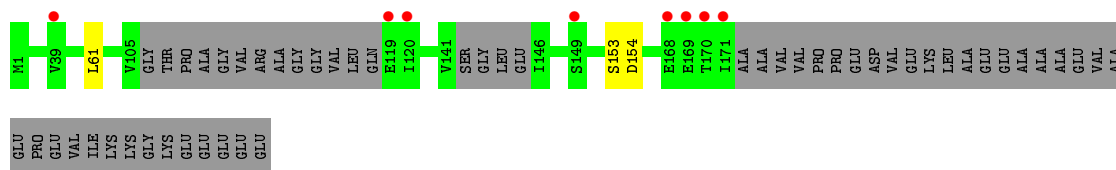
- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  15% 95% . .




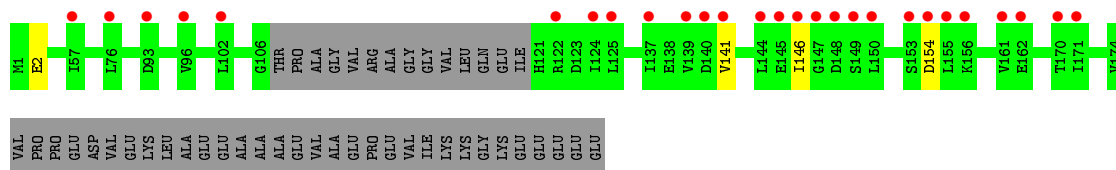
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  4% 73% 25%



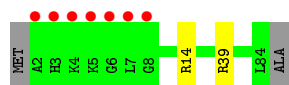
- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  13% 76% 22%



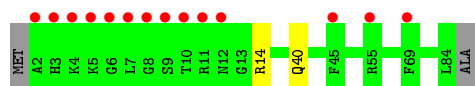
- Molecule 22: 50S ribosomal protein L27

Chain 10:  8% 95% . .



- Molecule 22: 50S ribosomal protein L27

Chain 20:  16% 95% . .

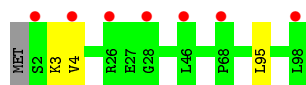


- Molecule 23: 50S ribosomal protein L28

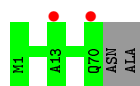
Chain 11:  4% 96% . .



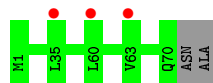
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



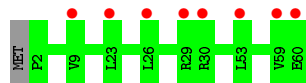
- Molecule 24: 50S ribosomal protein L29



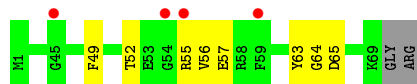
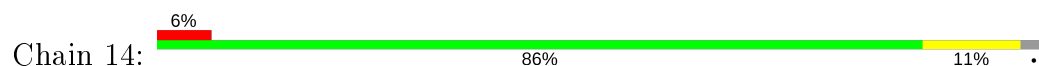
- Molecule 25: 50S ribosomal protein L30



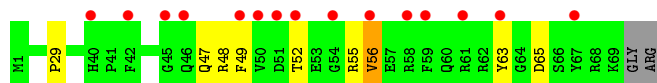
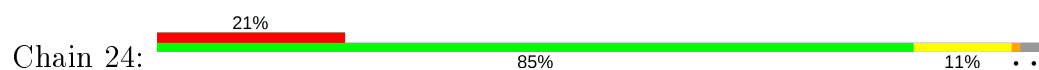
- Molecule 25: 50S ribosomal protein L30



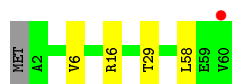
- Molecule 26: 50S ribosomal protein L31



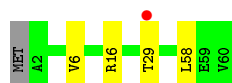
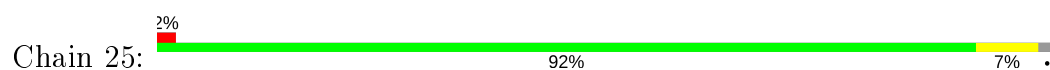
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



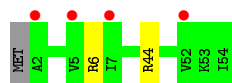
- Molecule 27: 50S ribosomal protein L32



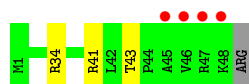
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35

Chain 18:  94% 5% .



- Molecule 30: 50S ribosomal protein L35

Chain 28:  8% 97% ..



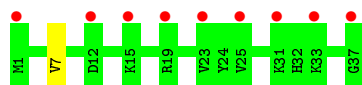
- Molecule 31: 50S ribosomal protein L36

Chain 19:  97% .




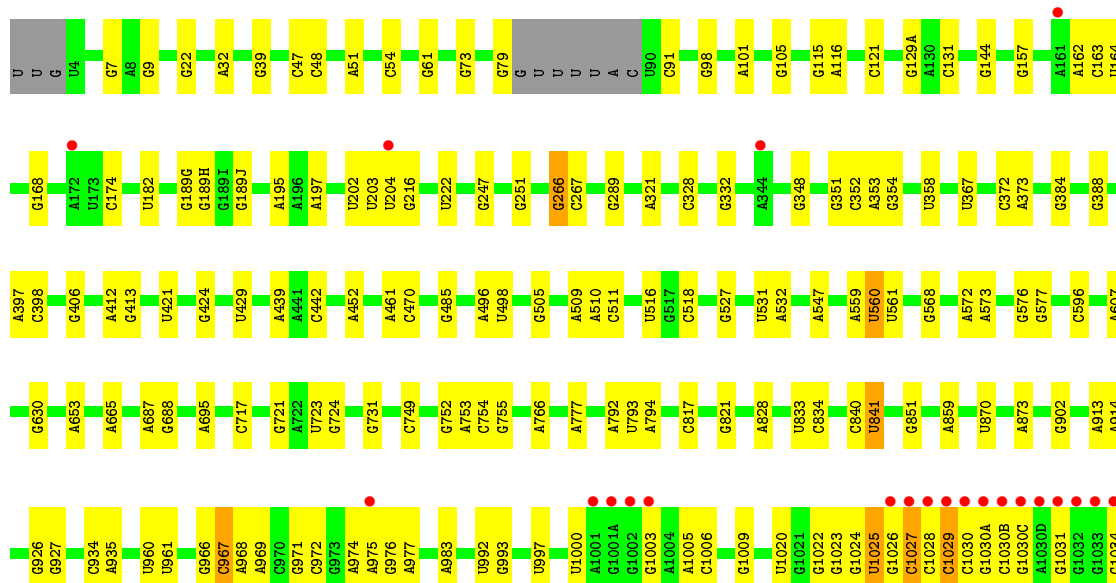
- Molecule 31: 50S ribosomal protein L36

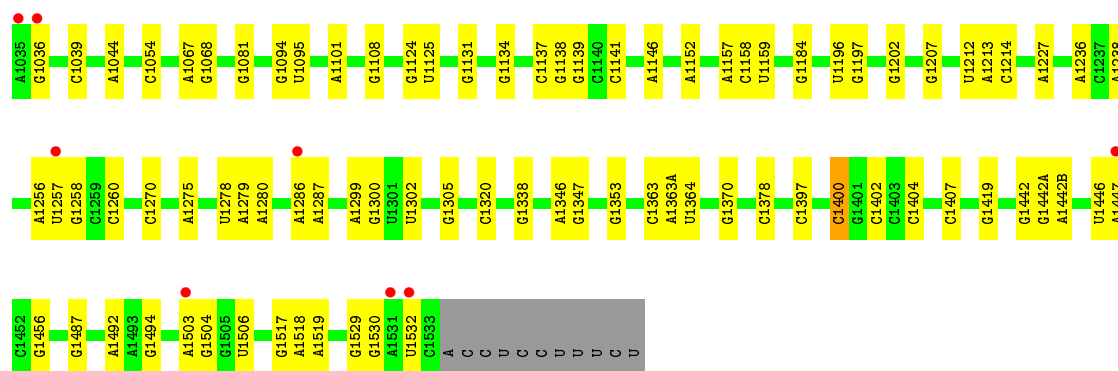
Chain 29:  24% 97% .



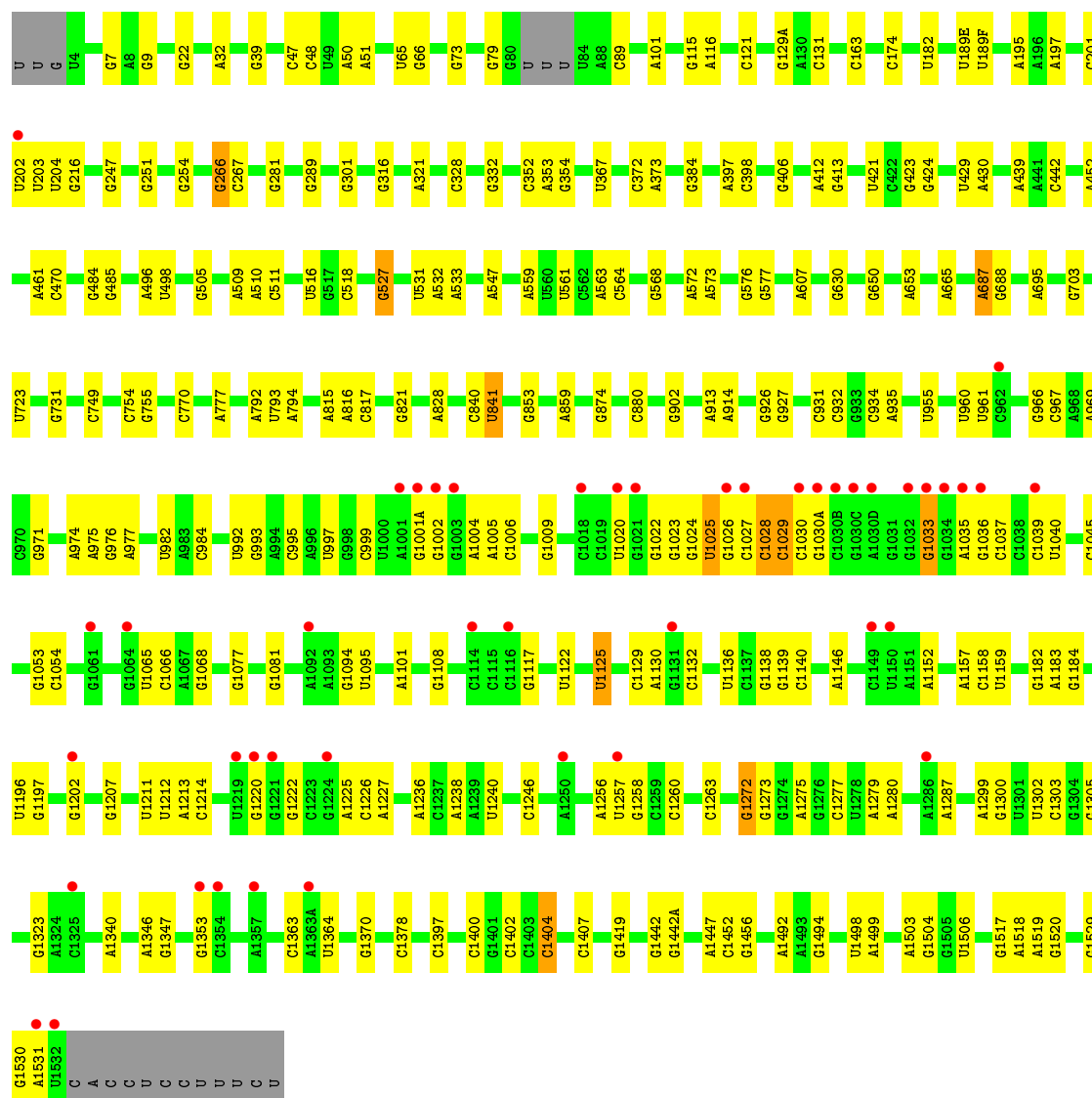
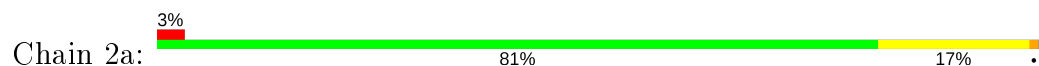
- Molecule 32: 16S Ribosomal RNA

Chain 1a:  2% 82% 16% ..

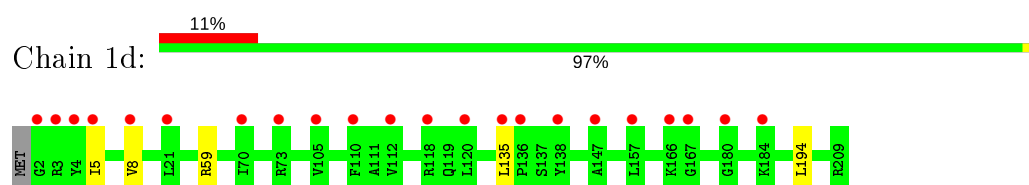
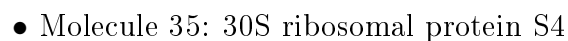
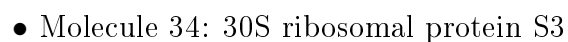
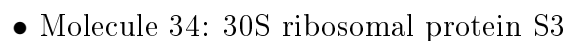
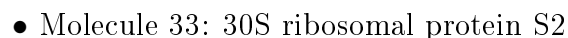




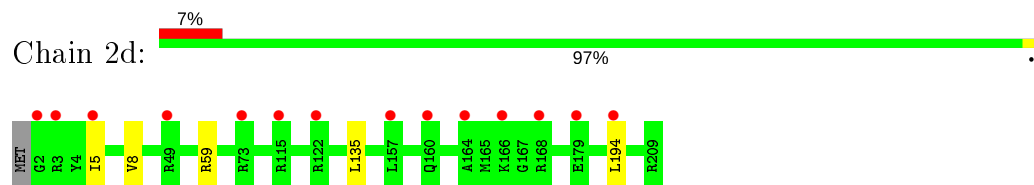
• Molecule 32: 16S Ribosomal RNA



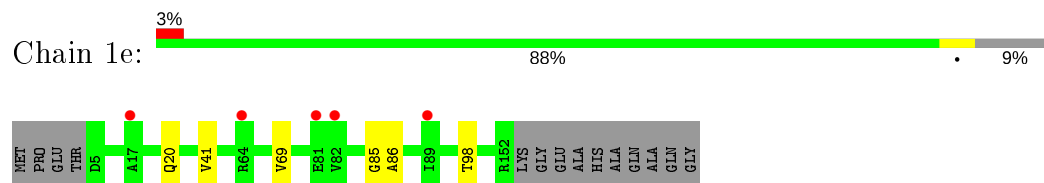
• Molecule 33: 30S ribosomal protein S2



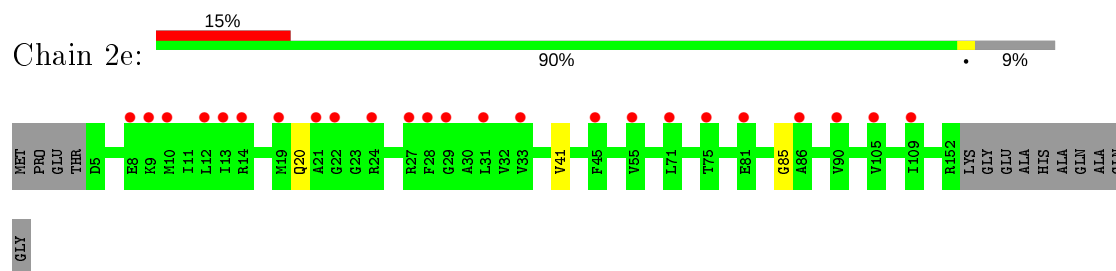
• Molecule 35: 30S ribosomal protein S4



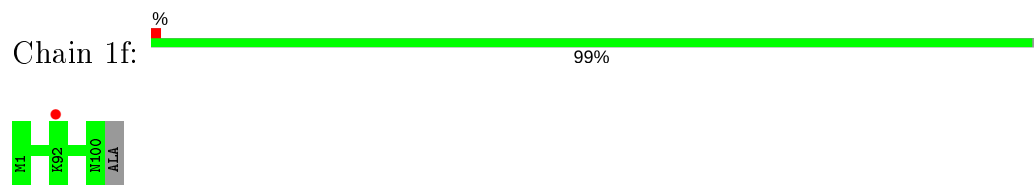
• Molecule 36: 30S ribosomal protein S5



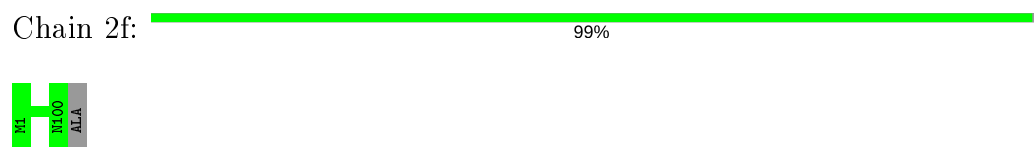
• Molecule 36: 30S ribosomal protein S5



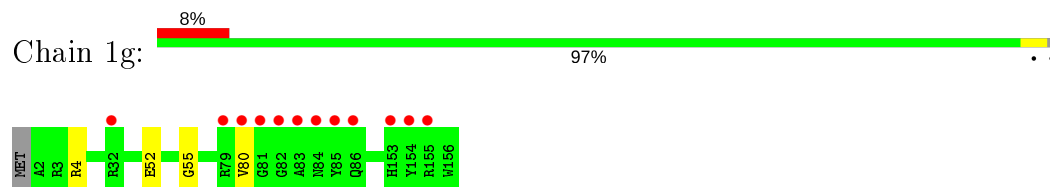
• Molecule 37: 30S ribosomal protein S6



• Molecule 37: 30S ribosomal protein S6

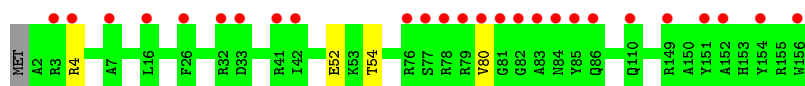


• Molecule 38: 30S ribosomal protein S7



• Molecule 38: 30S ribosomal protein S7

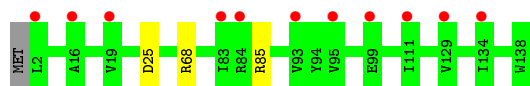




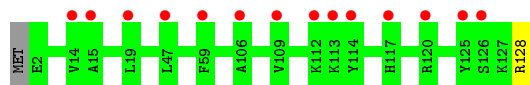
- Molecule 39: 30S ribosomal protein S8



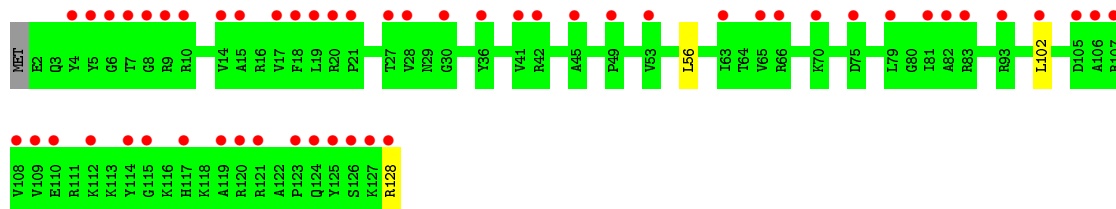
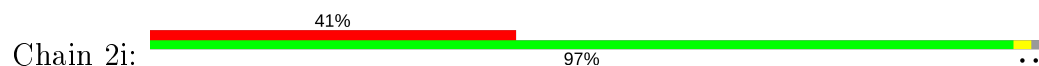
- Molecule 39: 30S ribosomal protein S8



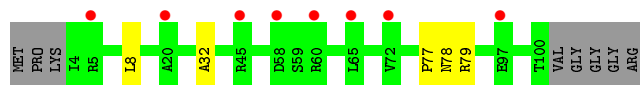
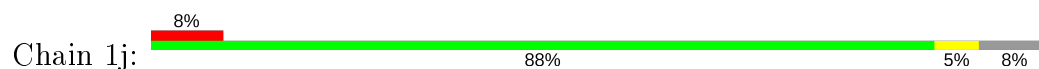
- Molecule 40: 30S ribosomal protein S9



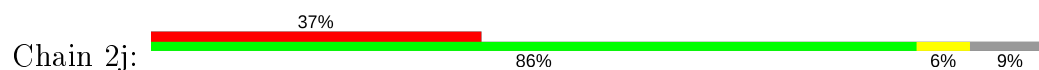
- Molecule 40: 30S ribosomal protein S9

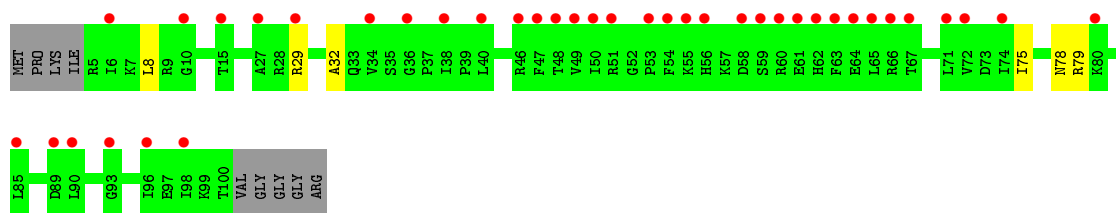


- Molecule 41: 30S ribosomal protein S10

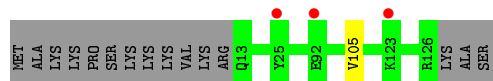
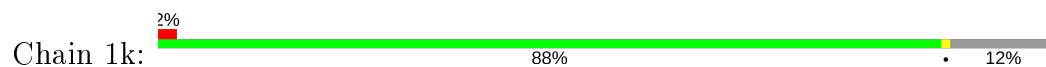


- Molecule 41: 30S ribosomal protein S10

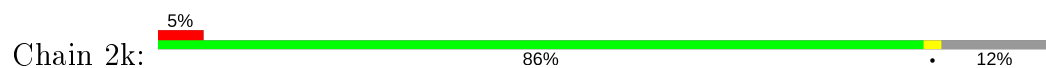




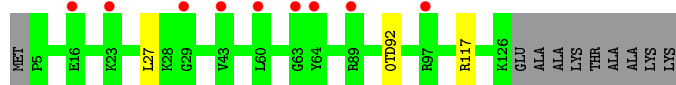
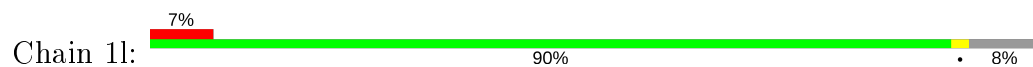
- Molecule 42: 30S ribosomal protein S11



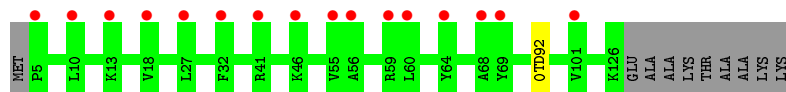
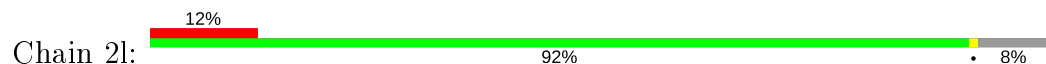
- Molecule 42: 30S ribosomal protein S11



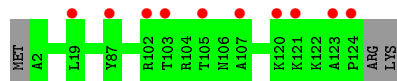
- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12

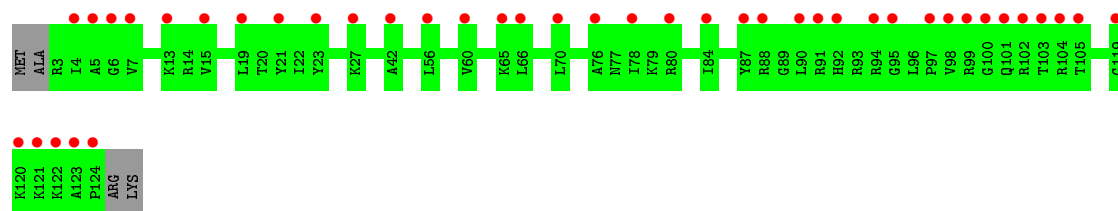


- Molecule 44: 30S ribosomal protein S13

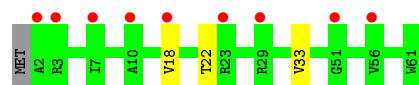


- Molecule 44: 30S ribosomal protein S13

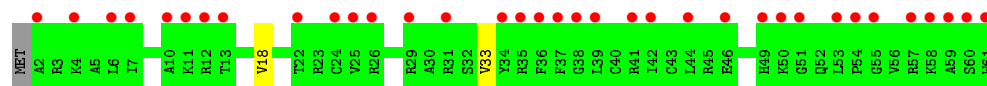




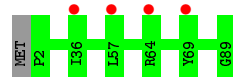
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



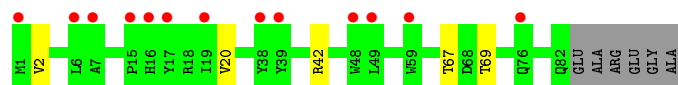
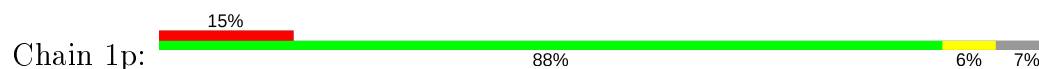
- Molecule 46: 30S ribosomal protein S15



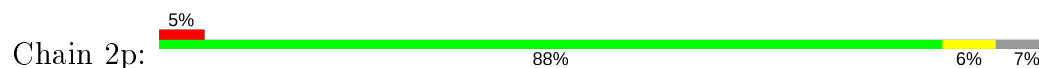
- Molecule 46: 30S ribosomal protein S15

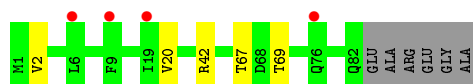


- Molecule 47: 30S ribosomal protein S16

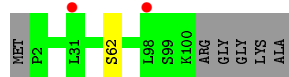


- Molecule 47: 30S ribosomal protein S16

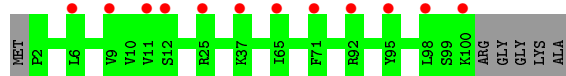




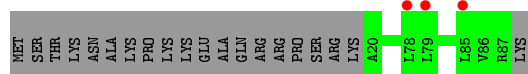
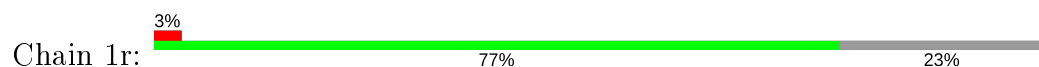
- Molecule 48: 30S ribosomal protein S17



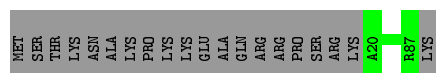
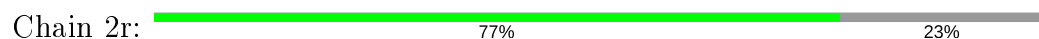
- Molecule 48: 30S ribosomal protein S17



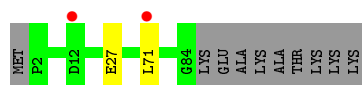
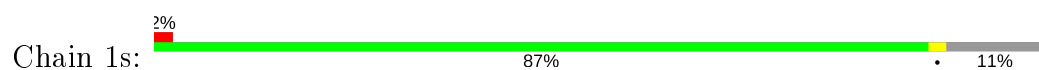
- Molecule 49: 30S ribosomal protein S18



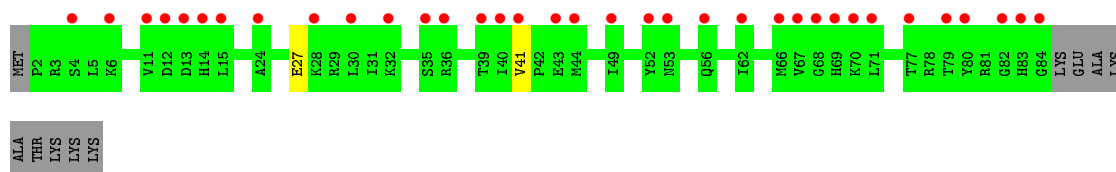
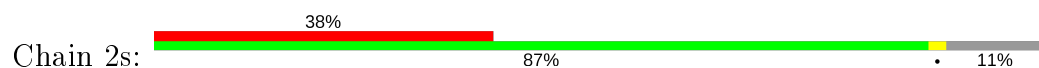
- Molecule 49: 30S ribosomal protein S18



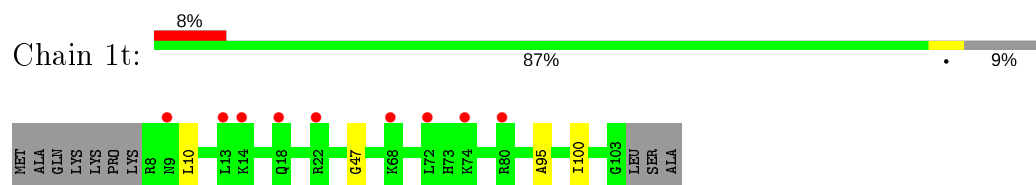
- Molecule 50: 30S ribosomal protein S19



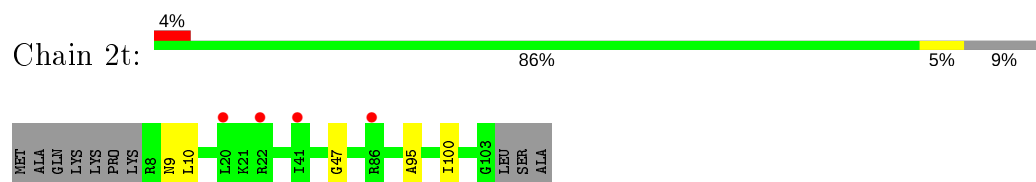
- Molecule 50: 30S ribosomal protein S19



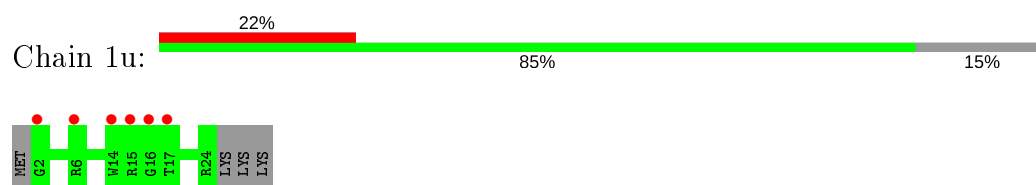
- Molecule 51: 30S ribosomal protein S20



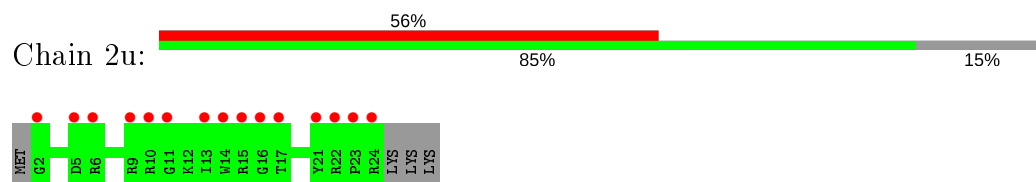
- Molecule 51: 30S ribosomal protein S20



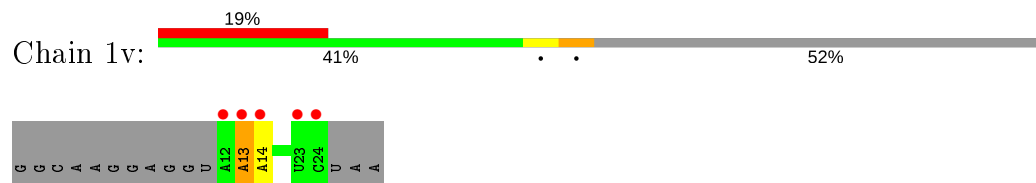
- Molecule 52: 30S ribosomal protein Thx



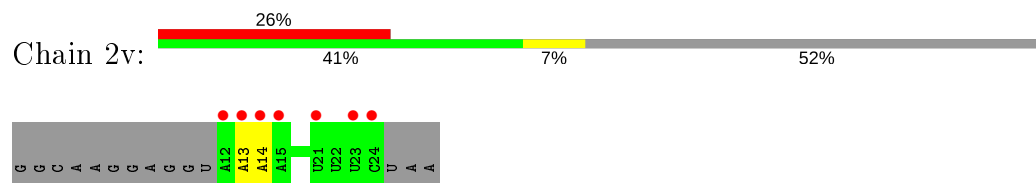
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



- Molecule 53: mRNA

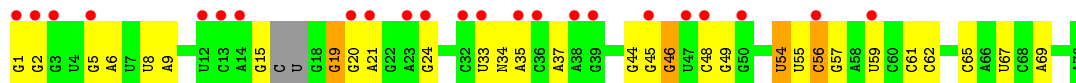


- Molecule 54: A-site and E-site tRNAs

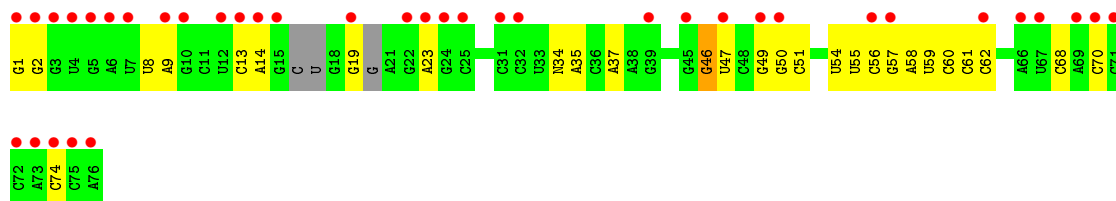




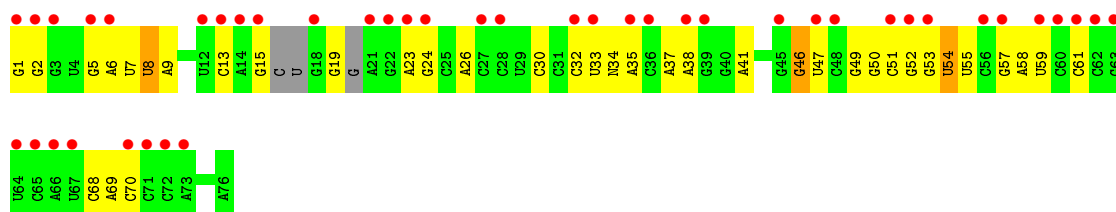
• Molecule 54: A-site and E-site tRNAs



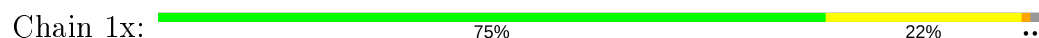
• Molecule 54: A-site and E-site tRNAs



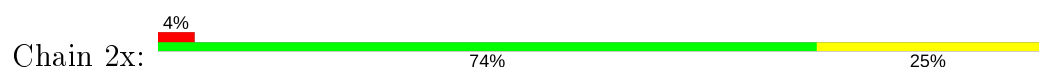
• Molecule 54: A-site and E-site tRNAs



• Molecule 55: P-site tRNA



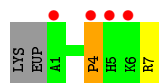
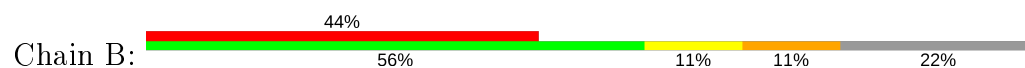
• Molecule 55: P-site tRNA



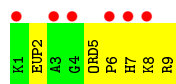
- Molecule 56: NOSO-95179 antibiotic



- Molecule 56: NOSO-95179 antibiotic



- Molecule 56: NOSO-95179 antibiotic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.17Å 448.69Å 618.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.63 – 2.60 363.19 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (154.63-2.60) 98.9 (363.19-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.212 , 0.249 0.212 , 0.249	Depositor DCC
R_{free} test set	87360 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	301143	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

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

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: MA6, SF4, 0TD, PSU, 2MA, 2MG, 2MU, UR3, M2G, 7MG, ZN, K, 6MZ, EUP, IAR, 5MU, MG, OMG, 5MC, 4OC, ORD, 4SU, CM0

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	0.52	0/69009	0.94	67/107712 (0.1%)
1	2A	0.38	0/67293	0.84	26/105034 (0.0%)
2	1B	0.44	1/2882 (0.0%)	0.84	0/4494
2	2B	0.38	1/2879 (0.0%)	0.82	1/4487 (0.0%)
3	1D	0.38	0/2186	0.59	0/2944
3	2D	0.33	0/2186	0.54	0/2944
4	1E	0.36	0/1592	0.56	0/2149
4	2E	0.31	0/1592	0.52	0/2149
5	1F	0.34	0/1619	0.52	0/2193
5	2F	0.29	0/1615	0.47	0/2188
6	1G	0.30	0/1448	0.48	0/1957
6	2G	0.29	0/1453	0.47	0/1963
7	1H	0.31	0/1356	0.48	0/1834
7	2H	0.28	0/1356	0.45	0/1834
8	1I	0.27	0/1112	0.47	0/1514
8	2I	0.27	0/1079	0.47	0/1475
9	1N	0.34	0/1144	0.52	0/1543
9	2N	0.28	0/1144	0.46	0/1543
10	1O	0.35	0/943	0.53	0/1269
10	2O	0.33	0/943	0.52	0/1269
11	1P	0.33	0/1152	0.55	0/1533
11	2P	0.29	0/1152	0.51	0/1533
12	1Q	0.35	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.32	0/982	0.53	0/1312
13	2R	0.27	0/982	0.50	0/1312
14	1S	0.30	0/883	0.49	0/1176
14	2S	0.29	0/880	0.46	0/1172
15	1T	0.34	0/1105	0.51	0/1477
15	2T	0.29	0/1097	0.47	0/1468
16	1U	0.37	0/977	0.52	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.29	0/977	0.44	0/1301
17	1V	0.43	1/782 (0.1%)	0.55	0/1049
17	2V	0.30	0/782	0.50	0/1049
18	1W	0.36	0/897	0.53	0/1205
18	2W	0.31	0/897	0.48	0/1205
19	1X	0.38	0/764	0.56	0/1025
19	2X	0.30	0/764	0.48	0/1025
20	1Y	0.36	0/819	0.53	0/1095
20	2Y	0.31	0/819	0.53	0/1095
21	1Z	0.33	0/1267	0.51	0/1717
21	2Z	0.29	0/1299	0.50	0/1763
22	10	0.35	0/662	0.55	0/881
22	20	0.29	0/662	0.50	0/881
23	11	0.34	0/762	0.51	0/1014
23	21	0.30	0/762	0.50	0/1014
24	12	0.31	0/590	0.46	0/781
24	22	0.28	0/590	0.40	0/781
25	13	0.33	0/474	0.51	0/635
25	23	0.29	0/469	0.45	0/630
26	14	0.37	0/565	0.55	0/761
26	24	0.32	0/545	0.60	0/737
27	15	0.36	0/469	0.56	0/635
27	25	0.33	0/469	0.51	0/635
28	16	0.35	0/460	0.52	0/613
28	26	0.29	0/456	0.48	0/608
29	17	0.34	0/426	0.52	0/561
29	27	0.28	0/426	0.51	0/561
30	18	0.34	0/525	0.57	0/691
30	28	0.30	0/525	0.48	0/691
31	19	0.31	0/310	0.50	0/407
31	29	0.29	0/310	0.50	0/407
32	1a	0.36	0/35795	0.85	27/55864 (0.0%)
32	2a	0.35	2/35886 (0.0%)	0.86	40/56005 (0.1%)
33	1b	0.35	1/1881 (0.1%)	0.47	0/2542
33	2b	0.29	0/1860	0.48	0/2518
34	1c	0.28	0/1572	0.44	0/2126
34	2c	0.28	0/1566	0.45	0/2119
35	1d	0.29	0/1685	0.46	0/2262
35	2d	0.28	0/1704	0.46	0/2284
36	1e	0.29	0/1145	0.50	0/1543
36	2e	0.29	0/1149	0.48	0/1548
37	1f	0.28	0/823	0.46	0/1115
37	2f	0.29	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.27	0/1250	0.42	0/1679
38	2g	0.27	0/1254	0.41	0/1683
39	1h	0.28	0/1108	0.47	0/1494
39	2h	0.27	0/1108	0.45	0/1494
40	1i	0.29	0/1002	0.49	0/1346
40	2i	0.29	0/997	0.48	0/1343
41	1j	0.28	0/722	0.49	0/982
41	2j	0.28	0/727	0.46	0/988
42	1k	0.28	0/844	0.47	0/1145
42	2k	0.27	0/848	0.47	0/1149
43	1l	0.30	0/937	0.51	0/1260
43	2l	0.28	0/937	0.49	0/1260
44	1m	0.27	0/969	0.47	0/1302
44	2m	0.30	0/961	0.47	0/1291
45	1n	0.31	0/501	0.47	0/664
45	2n	0.29	0/501	0.46	0/664
46	1o	0.27	0/739	0.43	0/985
46	2o	0.26	0/739	0.44	0/985
47	1p	0.28	0/697	0.47	0/939
47	2p	0.28	0/693	0.49	0/935
48	1q	0.29	0/836	0.47	0/1117
48	2q	0.28	0/836	0.47	0/1117
49	1r	0.27	0/560	0.46	0/746
49	2r	0.27	0/560	0.43	0/746
50	1s	0.27	0/667	0.51	0/900
50	2s	0.30	0/661	0.53	0/893
51	1t	0.26	0/730	0.39	0/965
51	2t	0.26	0/729	0.42	0/965
52	1u	0.27	0/203	0.44	0/266
52	2u	0.29	0/203	0.48	0/266
53	1v	0.44	0/308	0.95	2/477 (0.4%)
53	2v	0.40	0/308	0.86	0/477
54	1w	0.50	1/1600 (0.1%)	0.96	2/2482 (0.1%)
54	1y	0.51	1/1627 (0.1%)	1.01	4/2527 (0.2%)
54	2w	0.49	1/1600 (0.1%)	0.91	0/2482
54	2y	0.55	1/1600 (0.1%)	1.06	3/2482 (0.1%)
55	1x	0.50	1/1725 (0.1%)	1.05	14/2689 (0.5%)
55	2x	0.43	0/1725	1.06	8/2689 (0.3%)
56	A	1.35	1/43 (2.3%)	1.38	0/51
56	B	1.82	2/35 (5.7%)	1.45	1/43 (2.3%)
56	C	1.36	1/43 (2.3%)	1.81	1/51 (2.0%)
All	All	0.40	15/316879 (0.0%)	0.80	196/474354 (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
26	14	0	1
26	24	0	1
33	1b	0	1
33	2b	0	1
All	All	0	4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	1	G	OP3-P	-10.30	1.48	1.61
54	2y	1	G	OP3-P	-10.27	1.48	1.61
54	2w	1	G	OP3-P	-10.27	1.48	1.61
54	1w	1	G	OP3-P	-10.08	1.49	1.61
2	2B	1	U	OP3-P	-10.02	1.49	1.61
2	1B	1	U	OP3-P	-9.92	1.49	1.61
33	1b	233	SER	C-N	9.03	1.51	1.34
32	2a	1272	G	N1-C2	-8.30	1.31	1.37
32	2a	1272	G	C6-N1	-7.87	1.34	1.39
56	A	6	PRO	CA-C	-6.86	1.39	1.52
56	C	6	PRO	CA-C	-5.75	1.41	1.52
17	1V	34	GLU	C-N	-5.52	1.21	1.34
55	1x	14	A	C8-N7	-5.43	1.27	1.31
56	B	4	PRO	N-CA	5.28	1.56	1.47
56	B	4	PRO	CA-C	-5.27	1.42	1.52

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	19.70	130.72	118.90
32	2a	1272	G	C5-C6-O6	19.34	140.20	128.60
32	2a	1272	G	N3-C2-N2	17.23	131.96	119.90
32	2a	1272	G	N1-C2-N2	-15.44	102.30	116.20
32	2a	1263	C	C2-N3-C4	13.51	126.65	119.90
32	2a	1272	G	C6-N1-C2	11.84	132.20	125.10
32	2a	1272	G	C5-C6-N1	-11.23	105.88	111.50
1	1A	848	G	O5'-P-OP2	-11.16	95.66	105.70
32	2a	1263	C	N3-C2-O2	-10.40	114.62	121.90
55	2x	17	C	N1-C2-O2	10.18	125.01	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	N1-C6-O6	-10.02	113.89	119.90
32	2a	1263	C	C5-C6-N1	9.65	125.83	121.00
2	2B	80	U	O4'-C1'-N1	8.93	115.34	108.20
55	1x	14	A	C5-N7-C8	8.91	108.36	103.90
1	1A	537	G	O4'-C1'-N9	8.89	115.31	108.20
1	1A	1807	G	O5'-P-OP2	-8.78	97.80	105.70
1	1A	1020	C	N1-C2-O2	-8.72	113.67	118.90
1	2A	2136	C	N1-C2-O2	8.69	124.11	118.90
1	1A	1132	A	N1-C6-N6	-8.44	113.54	118.60
55	1x	14	A	C4-C5-C6	8.29	121.14	117.00
32	2a	1272	G	C2-N3-C4	-8.29	107.76	111.90
55	2x	17	C	N3-C2-O2	-8.23	116.14	121.90
1	1A	1686	U	O5'-P-OP2	-8.19	98.33	105.70
55	1x	46	G	C6-N1-C2	-7.91	120.36	125.10
55	2x	17	C	C2-N1-C1'	7.89	127.48	118.80
1	1A	2015	U	O5'-P-OP1	-7.71	98.77	105.70
32	2a	1029	C	N1-C2-O2	7.64	123.48	118.90
1	1A	591	U	C5-C4-O4	-7.63	121.32	125.90
32	1a	841	U	C5-C6-N1	7.62	126.51	122.70
1	1A	1121	C	N1-C2-O2	7.61	123.46	118.90
32	1a	1025	U	N1-C2-O2	7.58	128.10	122.80
1	2A	2473	U	C2-N1-C1'	7.57	126.79	117.70
1	1A	2694	U	O5'-P-OP2	-7.57	98.89	105.70
54	1y	56	C	N1-C2-O2	7.47	123.38	118.90
1	1A	2189	U	C2-N1-C1'	7.37	126.54	117.70
32	2a	841	U	C2-N1-C1'	7.35	126.52	117.70
32	1a	1030(B)	C	C2-N1-C1'	7.32	126.85	118.80
1	1A	2189	U	N1-C2-O2	7.31	127.92	122.80
55	2x	14	A	C5-N7-C8	7.29	107.55	103.90
32	2a	1263	C	C2-N1-C1'	7.29	126.82	118.80
1	2A	2167	U	N1-C2-O2	7.22	127.86	122.80
1	1A	1660	A	O5'-P-OP1	-7.22	99.20	105.70
32	1a	1027	C	N3-C4-C5	-7.20	119.02	121.90
32	2a	841	U	C5-C6-N1	7.15	126.27	122.70
32	1a	1030(B)	C	C6-N1-C2	-7.06	117.47	120.30
1	1A	2858	G	O4'-C1'-N9	6.98	113.78	108.20
54	1y	56	C	C2-N3-C4	6.97	123.39	119.90
1	1A	12	U	C2-N1-C1'	6.91	125.99	117.70
1	1A	2802	C	O4'-C1'-N1	6.81	113.65	108.20
32	2a	1263	C	C6-N1-C2	-6.79	117.58	120.30
1	1A	2083	G	O5'-P-OP2	-6.75	99.62	105.70
1	1A	1121	C	C2-N3-C4	6.75	123.28	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1027	C	C5-C4-N4	6.72	124.90	120.20
1	1A	2189	U	N3-C2-O2	-6.71	117.50	122.20
1	1A	1117	G	N3-C4-N9	-6.69	121.99	126.00
56	B	4	PRO	CA-N-CD	-6.65	102.19	111.50
1	2A	2248	C	O5'-P-OP2	-6.61	99.75	105.70
1	2A	2167	U	C2-N1-C1'	6.60	125.62	117.70
32	1a	1030(B)	C	N1-C2-O2	6.58	122.85	118.90
32	1a	1027	C	C6-N1-C1'	6.56	128.67	120.80
32	2a	1263	C	N1-C2-N3	-6.54	114.62	119.20
1	1A	2566	U	O5'-P-OP1	-6.50	99.85	105.70
1	2A	2167	U	N3-C2-O2	-6.49	117.66	122.20
56	C	6	PRO	C-N-CA	6.49	137.92	121.70
32	1a	841	U	C2-N1-C1'	6.48	125.47	117.70
32	2a	1263	C	C4-C5-C6	-6.45	114.18	117.40
55	1x	14	A	C8-N9-C1'	-6.42	116.15	127.70
32	1a	1025	U	C2-N1-C1'	6.40	125.38	117.70
1	2A	2473	U	N1-C2-O2	6.37	127.26	122.80
32	2a	1263	C	C5-C4-N4	6.37	124.66	120.20
1	1A	1221	G	OP1-P-O3'	6.34	119.16	105.20
32	2a	754	C	C2-N1-C1'	6.27	125.70	118.80
32	2a	254	G	O5'-P-OP1	-6.25	100.08	105.70
55	1x	22	G	N1-C6-O6	-6.24	116.16	119.90
55	1x	22	G	C4-C5-C6	-6.22	115.07	118.80
1	1A	892	G	O4'-C1'-N9	6.22	113.17	108.20
1	1A	215	G	O4'-C1'-N9	6.19	113.15	108.20
1	2A	2473	U	N3-C2-O2	-6.13	117.91	122.20
1	2A	2061	G	O5'-P-OP2	-6.12	100.19	105.70
54	2y	50	G	C5-C6-O6	6.09	132.25	128.60
32	1a	1030(B)	C	N3-C2-O2	-6.08	117.64	121.90
32	1a	266	G	P-O3'-C3'	6.06	126.98	119.70
1	1A	2014	G	P-O3'-C3'	6.04	126.95	119.70
1	2A	1992	G	P-O3'-C3'	6.00	126.89	119.70
55	1x	14	A	C4-N9-C1'	5.99	137.08	126.30
1	2A	801	G	O5'-P-OP2	-5.99	100.31	105.70
1	1A	2442	A	O5'-P-OP2	-5.97	100.33	105.70
55	1x	22	G	N3-C4-N9	-5.95	122.43	126.00
54	1y	19	G	C5-C6-O6	5.94	132.16	128.60
32	2a	1028	C	C2-N3-C4	5.90	122.85	119.90
32	2a	1272	G	C4-N9-C1'	5.88	134.14	126.50
32	2a	1225	A	C5-C6-N6	5.87	128.39	123.70
1	1A	1020	C	C2-N1-C1'	-5.83	112.39	118.80
32	1a	1027	C	C2-N1-C1'	-5.82	112.40	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2802	C	C2-N1-C1'	-5.82	112.40	118.80
1	2A	512	G	O4'-C1'-N9	5.77	112.82	108.20
1	2A	2140	C	N1-C2-O2	5.76	122.36	118.90
1	1A	1109	G	C5-C6-O6	5.76	132.05	128.60
1	2A	2140	C	C2-N1-C1'	5.71	125.08	118.80
1	2A	383	U	O4'-C1'-N1	5.69	112.75	108.20
1	1A	840	A	O5'-P-OP2	-5.69	100.58	105.70
55	1x	22	G	C5-N7-C8	-5.69	101.46	104.30
1	1A	1132	A	C5-C6-N1	5.68	120.54	117.70
55	1x	14	A	C5-C6-N1	-5.68	114.86	117.70
55	1x	22	G	C8-N9-C1'	5.67	134.38	127.00
1	1A	821	A	C8-N9-C4	-5.67	103.53	105.80
54	1w	44	G	P-O3'-C3'	5.67	126.50	119.70
1	1A	1128	U	N3-C4-O4	-5.64	115.45	119.40
1	1A	572	A	P-O3'-C3'	5.63	126.46	119.70
1	1A	1109	G	C6-N1-C2	5.61	128.46	125.10
32	2a	563	A	O4'-C1'-N9	5.60	112.68	108.20
1	1A	31	C	O5'-P-OP1	-5.60	100.66	105.70
54	1y	19	G	C6-N1-C2	5.59	128.45	125.10
32	2a	79	G	C5-C6-O6	5.59	131.95	128.60
32	2a	266	G	P-O3'-C3'	5.58	126.40	119.70
32	2a	1272	G	C8-N9-C1'	-5.58	119.75	127.00
1	2A	1313	U	C2-N1-C1'	5.57	124.38	117.70
55	2x	17	C	C6-N1-C2	-5.52	118.09	120.30
55	2x	14	A	C4-C5-C6	5.52	119.76	117.00
32	1a	1036	G	N3-C2-N2	-5.50	116.05	119.90
32	2a	687	A	P-O3'-C3'	5.50	126.30	119.70
1	2A	2689	U	P-O3'-C3'	5.49	126.28	119.70
1	1A	831	A	OP1-P-O3'	5.46	117.21	105.20
1	1A	1462	G	O4'-C1'-N9	5.46	112.57	108.20
54	1w	44	G	OP1-P-O3'	5.46	117.20	105.20
1	1A	410	U	C2-N1-C1'	-5.45	111.16	117.70
32	1a	754	C	N1-C2-O2	5.44	122.16	118.90
1	1A	2627	U	O5'-P-OP1	-5.43	100.81	105.70
53	1v	13	A	P-O3'-C3'	5.43	126.22	119.70
55	1x	46	G	C5-C6-N1	5.42	114.21	111.50
32	1a	1034	G	N3-C2-N2	5.41	123.69	119.90
32	2a	1025	U	C2-N1-C1'	5.41	124.19	117.70
1	1A	1700	G	P-O3'-C3'	5.40	126.19	119.70
32	1a	841	U	C6-N1-C2	-5.40	117.76	121.00
1	2A	1204	A	O4'-C1'-N9	5.39	112.52	108.20
1	1A	1255	A	P-O3'-C3'	5.38	126.15	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2520	G	N1-C6-O6	-5.36	116.68	119.90
1	1A	1431	G	O4'-C1'-N9	5.36	112.49	108.20
32	2a	1033	G	C5-C6-O6	5.34	131.80	128.60
55	2x	17	C	C6-N1-C1'	-5.33	114.40	120.80
1	1A	184	A	P-O3'-C3'	5.32	126.08	119.70
55	2x	46	G	C6-N1-C2	-5.32	121.91	125.10
32	1a	1025	U	C6-N1-C1'	-5.31	113.77	121.20
32	1a	1030	C	N1-C2-O2	5.30	122.08	118.90
1	1A	2331	G	N3-C4-C5	5.30	131.25	128.60
32	1a	1158	C	C2-N1-C1'	5.26	124.59	118.80
32	1a	1029	C	C2-N3-C4	5.26	122.53	119.90
1	1A	1359	U	N3-C2-O2	-5.24	118.53	122.20
1	1A	1117	G	N3-C4-C5	5.24	131.22	128.60
55	1x	14	A	C4-C5-N7	-5.24	108.08	110.70
1	1A	1013	G	N1-C6-O6	-5.24	116.76	119.90
1	1A	1222	A	O5'-P-OP1	-5.23	100.99	105.70
1	1A	2331	G	N3-C4-N9	-5.22	122.86	126.00
1	2A	528	A	P-O3'-C3'	5.22	125.97	119.70
32	1a	1034	G	C6-N1-C2	5.22	128.23	125.10
1	1A	2513	C	C2-N1-C1'	-5.21	113.07	118.80
54	2y	47	U	C2-N1-C1'	5.21	123.95	117.70
1	1A	894	U	C2-N1-C1'	5.20	123.94	117.70
1	2A	528	A	OP1-P-O3'	5.20	116.63	105.20
1	1A	1219	A	OP1-P-O3'	5.19	116.62	105.20
32	2a	1125	U	C2-N1-C1'	5.18	123.92	117.70
1	1A	793	A	O4'-C1'-N9	5.18	112.34	108.20
32	2a	1263	C	N3-C4-N4	-5.18	114.38	118.00
53	1v	13	A	OP1-P-O3'	5.17	116.58	105.20
1	2A	2136	C	N3-C2-O2	-5.17	118.28	121.90
32	1a	1067	A	P-O3'-C3'	5.16	125.89	119.70
1	2A	2155	G	N3-C4-N9	5.16	129.09	126.00
32	2a	65	U	P-O3'-C3'	5.15	125.88	119.70
1	1A	2605	U	N3-C4-C5	5.15	117.69	114.60
32	2a	1225	A	N1-C6-N6	-5.14	115.51	118.60
32	2a	754	C	N1-C2-O2	5.14	121.98	118.90
32	2a	913	A	P-O3'-C3'	5.14	125.86	119.70
55	1x	22	G	C6-C5-N7	5.13	133.48	130.40
1	1A	591	U	N3-C4-C5	5.12	117.67	114.60
1	1A	1716	A	O4'-C1'-N9	5.12	112.30	108.20
32	1a	560	U	C3'-C2'-C1'	5.12	105.59	101.50
1	2A	746	A	O4'-C1'-N9	5.11	112.28	108.20
32	2a	115	G	P-O3'-C3'	5.11	125.83	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	754	C	C2-N1-C1'	5.09	124.41	118.80
1	1A	399	G	O4'-C1'-N9	5.09	112.27	108.20
1	1A	993	G	O5'-P-OP1	-5.08	101.12	105.70
1	1A	2054	G	C5-N7-C8	5.07	106.84	104.30
32	2a	1158	C	C2-N1-C1'	5.07	124.38	118.80
1	1A	1117	G	C4-N9-C1'	-5.07	119.92	126.50
1	1A	1126	C	N1-C2-O2	5.06	121.94	118.90
1	1A	1221	G	P-O3'-C3'	5.06	125.78	119.70
1	1A	999	G	O5'-P-OP1	-5.06	101.15	105.70
1	2A	2629	A	O4'-C1'-N9	5.05	112.24	108.20
1	2A	228	A	P-O3'-C3'	5.04	125.75	119.70
1	2A	1380	G	O5'-P-OP2	-5.04	101.17	105.70
32	1a	913	A	P-O3'-C3'	5.03	125.73	119.70
54	2y	68	C	N1-C2-O2	5.02	121.92	118.90
1	1A	2802	C	C6-N1-C1'	5.02	126.83	120.80
32	2a	955	U	C2-N3-C4	5.02	130.01	127.00
32	1a	560	U	C2-N1-C1'	5.01	123.71	117.70
1	1A	2058	C	O5'-P-OP1	-5.00	101.20	105.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	63	TYR	Peptide
33	1b	124	SER	Peptide
26	24	63	TYR	Peptide
33	2b	124	SER	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	34	57
3	2D	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	34	57
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29	52
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	52
5	1F	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	29	52
5	2F	201/210 (96%)	193 (96%)	6 (3%)	2 (1%)	15	32
6	1G	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	14	30
6	2G	179/182 (98%)	162 (90%)	15 (8%)	2 (1%)	14	30
7	1H	172/180 (96%)	163 (95%)	9 (5%)	0	100	100
7	2H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	25	47
8	1I	144/148 (97%)	126 (88%)	15 (10%)	3 (2%)	7	13
8	2I	144/148 (97%)	131 (91%)	13 (9%)	0	100	100
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	113 (94%)	5 (4%)	2 (2%)	9	18
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	140 (95%)	5 (3%)	2 (1%)	11	22
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	17	35
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19	39
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	32
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	30
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	99 (94%)	4 (4%)	2 (2%)	8	15
20	2Y	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	15	32
21	1Z	148/206 (72%)	127 (86%)	21 (14%)	0	100	100
21	2Z	156/206 (76%)	143 (92%)	10 (6%)	3 (2%)	8	15
22	10	81/85 (95%)	81 (100%)	0	0	100	100
22	20	81/85 (95%)	81 (100%)	0	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	30
23	21	95/98 (97%)	94 (99%)	0	1 (1%)	14	30
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1
26	24	67/71 (94%)	56 (84%)	6 (9%)	5 (8%)	1	1
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	202 (88%)	22 (10%)	5 (2%)	6	12
33	2b	229/256 (90%)	204 (89%)	20 (9%)	5 (2%)	6	12
34	1c	204/239 (85%)	183 (90%)	19 (9%)	2 (1%)	15	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	2c	204/239 (85%)	187 (92%)	16 (8%)	1 (0%)	29	52
35	1d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	29	52
35	2d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	52
36	1e	146/162 (90%)	138 (94%)	4 (3%)	4 (3%)	5	8
36	2e	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	22	43
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	144 (94%)	5 (3%)	4 (3%)	5	9
38	2g	153/156 (98%)	141 (92%)	8 (5%)	4 (3%)	5	9
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	22	43
40	1i	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
40	2i	125/128 (98%)	116 (93%)	8 (6%)	1 (1%)	19	39
41	1j	95/105 (90%)	85 (90%)	6 (6%)	4 (4%)	3	3
41	2j	94/105 (90%)	82 (87%)	7 (7%)	5 (5%)	2	2
42	1k	112/129 (87%)	108 (96%)	3 (3%)	1 (1%)	17	35
42	2k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8	16
43	1l	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100	100
44	2m	120/126 (95%)	113 (94%)	7 (6%)	0	100	100
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
47	1p	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
47	2p	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
48	1q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	1s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	13	27
50	2s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	13	27
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	4	6
51	2t	94/106 (89%)	86 (92%)	3 (3%)	5 (5%)	2	2
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
56	A	4/9 (44%)	2 (50%)	1 (25%)	1 (25%)	0	0
56	B	4/9 (44%)	2 (50%)	2 (50%)	0	100	100
56	C	4/9 (44%)	1 (25%)	2 (50%)	1 (25%)	0	0
All	All	11382/12155 (94%)	10712 (94%)	575 (5%)	95 (1%)	19	39

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
26	14	65	ASP
5	2F	130	ALA
6	2G	52	ILE
17	2V	79	VAL
21	2Z	146	ILE
26	24	55	ARG
26	24	56	VAL
33	2b	125	PRO
51	2t	10	LEU
56	C	7	HIS
6	1G	47	LYS
17	1V	79	VAL
19	1X	93	GLU
23	11	3	LYS
36	1e	85	GLY
38	1g	4	ARG
51	1t	47	GLY
10	2O	5	GLN
23	21	3	LYS
33	2b	17	PHE
33	2b	36	ARG
36	2e	85	GLY
41	2j	75	ILE
41	2j	79	ARG

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Mol	Chain	Res	Type
42	2k	49	GLY
6	1G	43	LEU
20	1Y	103	GLY
26	14	55	ARG
33	1b	17	PHE
33	1b	125	PRO
34	1c	107	GLN
41	1j	79	ARG
50	1s	27	GLU
21	2Z	2	GLU
26	24	47	GLN
26	24	65	ASP
33	2b	20	GLU
38	2g	52	GLU
39	2h	68	ARG
41	2j	29	ARG
3	1D	3	VAL
4	1E	52	LEU
33	1b	78	GLN
35	1d	5	ILE
36	1e	86	ALA
36	1e	98	THR
38	1g	80	VAL
41	1j	32	ALA
41	1j	78	ASN
4	2E	52	LEU
10	2O	26	LYS
38	2g	54	THR
50	2s	27	GLU
51	2t	9	ASN
51	2t	47	GLY
8	1I	11	ASN
8	1I	39	ALA
26	14	57	GLU
38	1g	52	GLU
51	1t	95	ALA
3	2D	3	VAL
11	2P	29	LYS
15	2T	127	ALA
26	24	29	PRO
33	2b	78	GLN
38	2g	4	ARG

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Mol	Chain	Res	Type
40	2i	56	LEU
41	2j	32	ALA
41	2j	78	ASN
8	1I	104	GLN
20	1Y	55	TYR
26	14	64	GLY
33	1b	36	ARG
6	2G	43	LEU
11	2P	122	PRO
20	2Y	55	TYR
51	2t	95	ALA
41	1j	77	PRO
51	1t	100	ILE
7	2H	12	PRO
35	2d	5	ILE
14	2S	96	GLY
34	2c	66	VAL
36	1e	69	VAL
38	1g	55	GLY
42	1k	105	VAL
38	2g	80	VAL
56	A	4	GLY
33	1b	231	GLU
5	2F	89	VAL
42	2k	105	VAL
34	1c	66	VAL
21	2Z	141	VAL
51	2t	100	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	204 (95%)	11 (5%)	24	46
3	2D	215/218 (99%)	207 (96%)	8 (4%)	34	60
4	1E	164/166 (99%)	153 (93%)	11 (7%)	16	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	155 (94%)	9 (6%)	21	43
5	1F	160/166 (96%)	149 (93%)	11 (7%)	15	31
5	2F	159/166 (96%)	155 (98%)	4 (2%)	47	73
6	1G	143/156 (92%)	139 (97%)	4 (3%)	43	69
6	2G	143/156 (92%)	141 (99%)	2 (1%)	67	85
7	1H	144/148 (97%)	141 (98%)	3 (2%)	53	77
7	2H	144/148 (97%)	143 (99%)	1 (1%)	84	94
8	1I	113/124 (91%)	111 (98%)	2 (2%)	59	80
8	2I	105/124 (85%)	102 (97%)	3 (3%)	42	68
9	1N	118/119 (99%)	111 (94%)	7 (6%)	19	39
9	2N	118/119 (99%)	113 (96%)	5 (4%)	30	55
10	1O	100/100 (100%)	98 (98%)	2 (2%)	55	78
10	2O	100/100 (100%)	100 (100%)	0	100	100
11	1P	115/116 (99%)	110 (96%)	5 (4%)	29	54
11	2P	115/116 (99%)	114 (99%)	1 (1%)	78	91
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	59	80
12	2Q	111/111 (100%)	110 (99%)	1 (1%)	78	91
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	11
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19	39
14	1S	86/88 (98%)	82 (95%)	4 (5%)	26	50
14	2S	85/88 (97%)	85 (100%)	0	100	100
15	1T	115/127 (91%)	112 (97%)	3 (3%)	46	72
15	2T	113/127 (89%)	112 (99%)	1 (1%)	78	91
16	1U	93/94 (99%)	86 (92%)	7 (8%)	13	27
16	2U	93/94 (99%)	91 (98%)	2 (2%)	52	76
17	1V	80/82 (98%)	74 (92%)	6 (8%)	13	27
17	2V	80/82 (98%)	76 (95%)	4 (5%)	24	47
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21	42
18	2W	90/92 (98%)	88 (98%)	2 (2%)	52	76
19	1X	77/78 (99%)	76 (99%)	1 (1%)	69	86
19	2X	77/78 (99%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	85/91 (93%)	82 (96%)	3 (4%)	36	62
20	2Y	85/91 (93%)	83 (98%)	2 (2%)	49	74
21	1Z	135/179 (75%)	132 (98%)	3 (2%)	52	76
21	2Z	137/179 (76%)	136 (99%)	1 (1%)	84	94
22	10	65/67 (97%)	63 (97%)	2 (3%)	40	66
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	66
23	11	80/83 (96%)	78 (98%)	2 (2%)	47	73
23	21	80/83 (96%)	78 (98%)	2 (2%)	47	73
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	50 (98%)	1 (2%)	55	78
25	23	50/52 (96%)	50 (100%)	0	100	100
26	14	59/63 (94%)	56 (95%)	3 (5%)	24	46
26	24	53/63 (84%)	49 (92%)	4 (8%)	13	27
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	24
27	25	50/52 (96%)	46 (92%)	4 (8%)	12	24
28	16	51/52 (98%)	46 (90%)	5 (10%)	8	15
28	26	50/52 (96%)	48 (96%)	2 (4%)	31	57
29	17	41/42 (98%)	38 (93%)	3 (7%)	14	28
29	27	41/42 (98%)	40 (98%)	1 (2%)	49	74
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	42
30	28	54/55 (98%)	53 (98%)	1 (2%)	57	79
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	68
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	68
33	1b	192/220 (87%)	188 (98%)	4 (2%)	53	77
33	2b	187/220 (85%)	184 (98%)	3 (2%)	62	82
34	1c	142/188 (76%)	138 (97%)	4 (3%)	43	69
34	2c	140/188 (74%)	140 (100%)	0	100	100
35	1d	169/181 (93%)	165 (98%)	4 (2%)	49	74
35	2d	173/181 (96%)	169 (98%)	4 (2%)	50	75
36	1e	113/123 (92%)	111 (98%)	2 (2%)	59	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	114/123 (93%)	112 (98%)	2 (2%)	59	80
37	1f	84/90 (93%)	84 (100%)	0	100	100
37	2f	85/90 (94%)	85 (100%)	0	100	100
38	1g	119/127 (94%)	119 (100%)	0	100	100
38	2g	120/127 (94%)	120 (100%)	0	100	100
39	1h	114/119 (96%)	112 (98%)	2 (2%)	59	80
39	2h	114/119 (96%)	112 (98%)	2 (2%)	59	80
40	1i	90/99 (91%)	89 (99%)	1 (1%)	73	88
40	2i	89/99 (90%)	87 (98%)	2 (2%)	52	76
41	1j	66/92 (72%)	65 (98%)	1 (2%)	65	83
41	2j	69/92 (75%)	68 (99%)	1 (1%)	67	85
42	1k	82/99 (83%)	82 (100%)	0	100	100
42	2k	83/99 (84%)	82 (99%)	1 (1%)	71	87
43	1l	96/108 (89%)	94 (98%)	2 (2%)	53	77
43	2l	96/108 (89%)	96 (100%)	0	100	100
44	1m	93/101 (92%)	93 (100%)	0	100	100
44	2m	92/101 (91%)	92 (100%)	0	100	100
45	1n	49/50 (98%)	46 (94%)	3 (6%)	18	38
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	56
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69	86
47	1p	69/74 (93%)	64 (93%)	5 (7%)	14	29
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13	28
48	1q	94/97 (97%)	93 (99%)	1 (1%)	73	88
48	2q	94/97 (97%)	94 (100%)	0	100	100
49	1r	59/77 (77%)	59 (100%)	0	100	100
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	68 (99%)	1 (1%)	67	85
50	2s	67/80 (84%)	66 (98%)	1 (2%)	65	83
51	1t	70/82 (85%)	69 (99%)	1 (1%)	67	85
51	2t	70/82 (85%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
56	A	4/4 (100%)	2 (50%)	2 (50%)	0	0
56	B	3/4 (75%)	2 (67%)	1 (33%)	0	0
56	C	4/4 (100%)	3 (75%)	1 (25%)	0	1
All	All	9314/10076 (92%)	9061 (97%)	253 (3%)	44	71

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	14	ARG
3	1D	32	SER
3	1D	94	LEU
3	1D	113	VAL
3	1D	116	GLN
3	1D	142	VAL
3	1D	155	LEU
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
4	1E	9	VAL
4	1E	21	VAL
4	1E	24	THR
4	1E	47	VAL
4	1E	75	VAL
4	1E	101	ARG
4	1E	113	PHE
4	1E	116	VAL
4	1E	175	VAL
4	1E	181	LEU
4	1E	184	VAL
5	1F	32	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	88	VAL
5	1F	106	ARG
5	1F	158	THR
5	1F	170	LEU
5	1F	175	THR

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Mol	Chain	Res	Type
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	16	ARG
6	1G	43	LEU
7	1H	15	VAL
7	1H	69	ARG
7	1H	71	LEU
8	1I	92	VAL
8	1I	140	LEU
9	1N	33	LEU
9	1N	34	LEU
9	1N	35	ARG
9	1N	58	ASP
9	1N	73	THR
9	1N	87	LEU
9	1N	99	LEU
10	1O	28	SER
10	1O	69	ILE
11	1P	3	LEU
11	1P	56	SER
11	1P	83	VAL
11	1P	95	VAL
11	1P	125	VAL
12	1Q	35	VAL
12	1Q	109	VAL
13	1R	6	SER
13	1R	29	LEU
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	86	ARG
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	23	ARG
14	1S	50	SER
14	1S	52	SER

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Mol	Chain	Res	Type
14	1S	69	VAL
15	1T	96	ARG
15	1T	111	ARG
15	1T	128	GLU
16	1U	8	VAL
16	1U	31	SER
16	1U	50	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	85	LYS
16	1U	95	LEU
17	1V	18	LEU
17	1V	51	VAL
17	1V	61	VAL
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
18	1W	11	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	107	LEU
19	1X	35	THR
20	1Y	43	ASN
20	1Y	97	ARG
20	1Y	99	CYS
21	1Z	61	LEU
21	1Z	153	SER
21	1Z	154	ASP
22	10	14	ARG
22	10	39	ARG
23	11	30	VAL
23	11	95	LEU
25	13	23	LEU
26	14	49	PHE
26	14	52	THR
26	14	56	VAL
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	58	LEU
28	16	6	ARG

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Mol	Chain	Res	Type
28	16	14	THR
28	16	44	ARG
28	16	48	VAL
28	16	52	VAL
29	17	34	ARG
29	17	41	ARG
29	17	43	THR
30	18	14	VAL
30	18	31	HIS
30	18	32	LEU
31	19	4	ARG
33	1b	111	ARG
33	1b	122	PHE
33	1b	154	LEU
33	1b	175	ARG
34	1c	3	ASN
34	1c	15	THR
34	1c	70	VAL
34	1c	115	LEU
35	1d	8	VAL
35	1d	59	ARG
35	1d	135	LEU
35	1d	194	LEU
36	1e	20	GLN
36	1e	41	VAL
39	1h	104	ARG
39	1h	133	LEU
40	1i	128	ARG
41	1j	8	LEU
43	1l	27	LEU
43	1l	117	ARG
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
47	1p	2	VAL
47	1p	20	VAL
47	1p	42	ARG
47	1p	67	THR
47	1p	69	THR
48	1q	62	SER
50	1s	71	LEU
51	1t	10	LEU

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Mol	Chain	Res	Type
3	2D	61	LEU
3	2D	94	LEU
3	2D	116	GLN
3	2D	142	VAL
3	2D	155	LEU
3	2D	157	ARG
3	2D	229	VAL
3	2D	242	ARG
4	2E	9	VAL
4	2E	12	THR
4	2E	21	VAL
4	2E	24	THR
4	2E	58	ARG
4	2E	75	VAL
4	2E	101	ARG
4	2E	116	VAL
4	2E	181	LEU
5	2F	88	VAL
5	2F	106	ARG
5	2F	183	VAL
5	2F	201	VAL
6	2G	3	LEU
6	2G	43	LEU
7	2H	15	VAL
8	2I	92	VAL
8	2I	127	VAL
8	2I	140	LEU
9	2N	33	LEU
9	2N	34	LEU
9	2N	35	ARG
9	2N	62	VAL
9	2N	99	LEU
11	2P	95	VAL
12	2Q	109	VAL
13	2R	6	SER
13	2R	29	LEU
13	2R	36	THR
13	2R	65	LEU
13	2R	67	LEU
13	2R	111	LEU
15	2T	111	ARG
16	2U	31	SER

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Mol	Chain	Res	Type
16	2U	53	ARG
17	2V	7	THR
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
18	2W	19	LEU
18	2W	107	LEU
20	2Y	43	ASN
20	2Y	85	VAL
21	2Z	154	ASP
22	20	14	ARG
22	20	40	GLN
23	21	4	VAL
23	21	95	LEU
26	24	48	ARG
26	24	49	PHE
26	24	52	THR
26	24	56	VAL
27	25	6	VAL
27	25	16	ARG
27	25	29	THR
27	25	58	LEU
28	26	6	ARG
28	26	44	ARG
29	27	43	THR
30	28	32	LEU
31	29	7	VAL
33	2b	124	SER
33	2b	128	GLU
33	2b	175	ARG
35	2d	8	VAL
35	2d	59	ARG
35	2d	135	LEU
35	2d	194	LEU
36	2e	20	GLN
36	2e	41	VAL
39	2h	25	ASP
39	2h	85	ARG
40	2i	102	LEU
40	2i	128	ARG
41	2j	8	LEU
42	2k	14	VAL

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Mol	Chain	Res	Type
45	2n	18	VAL
45	2n	33	VAL
46	2o	39	LEU
47	2p	2	VAL
47	2p	20	VAL
47	2p	42	ARG
47	2p	67	THR
47	2p	69	THR
50	2s	41	VAL
56	A	1	LYS
56	A	8	LYS
56	B	4	PRO
56	C	8	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	116	GLN
3	1D	126	GLN
5	1F	69	HIS
5	1F	203	GLN
10	1O	3	GLN
13	1R	24	GLN
14	1S	95	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	65	GLN
21	1Z	73	GLN
22	10	50	ASN
23	11	56	GLN
24	12	65	ASN
25	13	32	GLN
26	14	47	GLN
33	1b	78	GLN
34	1c	6	HIS
34	1c	162	GLN
34	1c	176	HIS
35	1d	77	ASN
35	1d	119	GLN

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Mol	Chain	Res	Type
35	1d	123	HIS
35	1d	125	HIS
35	1d	161	ASN
36	1e	78	HIS
37	1f	13	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	86	GLN
40	1i	3	GLN
40	1i	31	GLN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
44	1m	77	ASN
44	1m	92	HIS
49	1r	63	GLN
50	1s	57	HIS
50	1s	69	HIS
50	1s	83	HIS
3	2D	116	GLN
4	2E	48	GLN
5	2F	69	HIS
5	2F	75	HIS
8	2I	133	HIS
8	2I	139	GLN
13	2R	24	GLN
15	2T	58	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	43	ASN
21	2Z	55	HIS
21	2Z	65	GLN
23	21	56	GLN
24	22	65	ASN
33	2b	40	HIS
33	2b	78	GLN
34	2c	6	HIS
35	2d	77	ASN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS

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Mol	Chain	Res	Type
35	2d	161	ASN
36	2e	78	HIS
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	148	ASN
40	2i	3	GLN
40	2i	58	HIS
41	2j	56	HIS
44	2m	12	ASN
47	2p	16	HIS
49	2r	63	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	42	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	405 (14%)	29 (1%)
1	2A	2788/2915 (95%)	467 (16%)	22 (0%)
2	1B	120/121 (99%)	7 (5%)	1 (0%)
2	2B	118/121 (97%)	24 (20%)	0
32	1a	1494/1521 (98%)	235 (15%)	0
32	2a	1498/1521 (98%)	247 (16%)	0
53	1v	12/27 (44%)	2 (16%)	0
53	2v	12/27 (44%)	2 (16%)	0
54	1w	68/76 (89%)	22 (32%)	0
54	1y	70/76 (92%)	25 (35%)	0
54	2w	68/76 (89%)	22 (32%)	0
54	2y	68/76 (89%)	30 (44%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	12 (16%)	0
All	All	9327/9626 (96%)	1512 (16%)	52 (0%)

All (1512) RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
1	1A	45	C
1	1A	54	G
1	1A	63	A
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	83	A
1	1A	94	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	137	G
1	1A	177	G
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	203	G
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	275	C
1	1A	289	G
1	1A	303	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	376	G
1	1A	387	G
1	1A	389	G
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	448	U
1	1A	455	A

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Mol	Chain	Res	Type
1	1A	469	A
1	1A	470	C
1	1A	474	U
1	1A	477	C
1	1A	480	A
1	1A	482	C
1	1A	483	A
1	1A	507	G
1	1A	529	U
1	1A	530	A
1	1A	534	C
1	1A	554	A
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	652	A
1	1A	659	C
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	678	A
1	1A	693	G
1	1A	697	C
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	811	A
1	1A	822	G
1	1A	823	G
1	1A	829	A

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Mol	Chain	Res	Type
1	1A	830	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	859	C
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	902	G
1	1A	906	G
1	1A	913	A
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	939	C
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	956	A
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	998	A
1	1A	1004	A
1	1A	1006	C
1	1A	1008	U
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U

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Mol	Chain	Res	Type
1	1A	1079	U
1	1A	1087	C
1	1A	1090	G
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1101	G
1	1A	1104	G
1	1A	1105	G
1	1A	1109	G
1	1A	1110	C
1	1A	1112	U
1	1A	1114	G
1	1A	1117	G
1	1A	1119	A
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1127	U
1	1A	1134	A
1	1A	1135	G
1	1A	1136	U
1	1A	1137	G
1	1A	1140	U
1	1A	1143	U
1	1A	1144	A
1	1A	1147	U
1	1A	1149	A
1	1A	1156	G
1	1A	1157	A
1	1A	1158	G
1	1A	1174	A
1	1A	1180	C
1	1A	1181	G
1	1A	1201	A
1	1A	1216	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G

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Mol	Chain	Res	Type
1	1A	1222	A
1	1A	1223	C
1	1A	1256	U
1	1A	1263	C
1	1A	1265	A
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1354	A
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1432	C
1	1A	1441	A
1	1A	1442	U
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1483	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1506	G
1	1A	1514	C
1	1A	1529	G
1	1A	1539	C
1	1A	1543	U
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1587	U

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Mol	Chain	Res	Type
1	1A	1589	A
1	1A	1590	C
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1656	A
1	1A	1694	G
1	1A	1695	C
1	1A	1701	A
1	1A	1711	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1750	G
1	1A	1767	A
1	1A	1768	U
1	1A	1787	G
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1878	A
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1951	G
1	1A	1952	G

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Mol	Chain	Res	Type
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1987	C
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2129	C
1	1A	2132	G
1	1A	2135	U
1	1A	2136	A
1	1A	2142	G
1	1A	2147	G
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2159	C
1	1A	2160	C
1	1A	2162	C
1	1A	2163	G

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Mol	Chain	Res	Type
1	1A	2164	C
1	1A	2166	U
1	1A	2168	C
1	1A	2169	G
1	1A	2171	G
1	1A	2172	U
1	1A	2173	G
1	1A	2177	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2184	G
1	1A	2185	C
1	1A	2187	G
1	1A	2188	G
1	1A	2193	A
1	1A	2194	U
1	1A	2195	A
1	1A	2200	C
1	1A	2206	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2230	U
1	1A	2237	A
1	1A	2247	G
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2285	A
1	1A	2295	C
1	1A	2298	A
1	1A	2299	A
1	1A	2301	G
1	1A	2317	A
1	1A	2320	G
1	1A	2321	A
1	1A	2324	U
1	1A	2332	A
1	1A	2337	G

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Mol	Chain	Res	Type
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2366	G
1	1A	2373	A
1	1A	2384	G
1	1A	2395	G
1	1A	2397	C
1	1A	2418	U
1	1A	2436	C
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2480	G
1	1A	2486	C
1	1A	2488	A
1	1A	2510	C
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2541	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2581	G
1	1A	2585	C
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2642	G
1	1A	2666	A
1	1A	2701	U
1	1A	2703	C
1	1A	2714	U

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Mol	Chain	Res	Type
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2771	A
1	1A	2777	A
1	1A	2778	A
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2807	C
1	1A	2813	G
1	1A	2816	G
1	1A	2830	A
1	1A	2831	A
1	1A	2845	A
1	1A	2849	G
1	1A	2882	G
1	1A	2883	A
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
2	1B	2	C
2	1B	13	A
2	1B	15	A
2	1B	56	G
2	1B	73	A
2	1B	85	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	73	G

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Mol	Chain	Res	Type
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	129(A)	G
32	1a	131	C
32	1a	144	G
32	1a	157	G
32	1a	162	A
32	1a	163	C
32	1a	164	U
32	1a	168	G
32	1a	174	C
32	1a	182	U
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U

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Mol	Chain	Res	Type
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	388	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	687	A

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Mol	Chain	Res	Type
32	1a	688	G
32	1a	695	A
32	1a	717	C
32	1a	721	G
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	749	C
32	1a	752	G
32	1a	753	A
32	1a	755	G
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	833	U
32	1a	834	C
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	870	U
32	1a	873	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	967	5MC
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A

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Mol	Chain	Res	Type
32	1a	976	G
32	1a	977	A
32	1a	983	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1044	A
32	1a	1054	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1124	G
32	1a	1125	U
32	1a	1131	G
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A

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Mol	Chain	Res	Type
32	1a	1157	A
32	1a	1159	U
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1364	U
32	1a	1370	G
32	1a	1378	C
32	1a	1397	C
32	1a	1400	5MC
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G

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Mol	Chain	Res	Type
32	1a	1442(B)	A
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	14	A
54	1w	2	G
54	1w	6	A
54	1w	8	4SU
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	23	A
54	1w	45	G
54	1w	46	7MG
54	1w	47	U
54	1w	49	G
54	1w	50	G
54	1w	51	C
54	1w	56	C
54	1w	57	G
54	1w	58	A
54	1w	59	U
54	1w	61	C
54	1w	62	C
54	1w	68	C
54	1w	70	C
54	1w	74	C
55	1x	6	G
55	1x	9	G
55	1x	18	G
55	1x	19	G

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Mol	Chain	Res	Type
55	1x	21	A
55	1x	22	G
55	1x	31	G
55	1x	47	U
55	1x	61	C
55	1x	63	G
55	1x	69	C
55	1x	76	A
54	1y	2	G
54	1y	5	G
54	1y	6	A
54	1y	9	A
54	1y	15	G
54	1y	19	G
54	1y	20	G
54	1y	21	A
54	1y	24	G
54	1y	33	U
54	1y	35	A
54	1y	44	G
54	1y	45	G
54	1y	46	7MG
54	1y	48	C
54	1y	49	G
54	1y	54	5MU
54	1y	56	C
54	1y	57	G
54	1y	59	U
54	1y	61	C
54	1y	62	C
54	1y	65	C
54	1y	67	U
54	1y	69	A
1	2A	10	G
1	2A	11	G
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	51	G
1	2A	71	A

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Mol	Chain	Res	Type
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	149	A
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	266	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272	G
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C

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Mol	Chain	Res	Type
1	2A	277	C
1	2A	278	A
1	2A	280	C
1	2A	302	C
1	2A	311	A
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	332	A
1	2A	352	G
1	2A	354	G
1	2A	372	G
1	2A	386	G
1	2A	396	G
1	2A	406	G
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	435	C
1	2A	443	A
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A

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Mol	Chain	Res	Type
1	2A	586	A
1	2A	588	U
1	2A	592	G
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G

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Mol	Chain	Res	Type
1	2A	856	C
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	874	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	899	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	997	G

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Mol	Chain	Res	Type
1	2A	998	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1032	A
1	2A	1033	U
1	2A	1038	C
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1117	G
1	2A	1128	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1144	G
1	2A	1155	A
1	2A	1171	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1229	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1342	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C

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Mol	Chain	Res	Type
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1435	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1514	U
1	2A	1525	G
1	2A	1530	C
1	2A	1531	C
1	2A	1532	C
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A

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Mol	Chain	Res	Type
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A

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Mol	Chain	Res	Type
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2096	U
1	2A	2097	C
1	2A	2099	U
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A

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Mol	Chain	Res	Type
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2140	C
1	2A	2141	G
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2177	C
1	2A	2178	C
1	2A	2182	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A

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Mol	Chain	Res	Type
1	2A	2294	C
1	2A	2302	G
1	2A	2305	A
1	2A	2308	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2469	A
1	2A	2476	A
1	2A	2490	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2572	A
1	2A	2573	C
1	2A	2602	A
1	2A	2609	U

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Mol	Chain	Res	Type
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2662	A
1	2A	2663	G
1	2A	2689	U
1	2A	2690	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2751	G
1	2A	2757	A
1	2A	2759	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2793	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2836	U
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2883	A
1	2A	2886	G
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	4	C
2	2B	5	C

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Mol	Chain	Res	Type
2	2B	8	U
2	2B	13	A
2	2B	19	G
2	2B	20	C
2	2B	34	U
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	67	G
2	2B	69	G
2	2B	73	A
2	2B	75	G
2	2B	85	G
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	114	C
2	2B	119	G
2	2B	120	A
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	73	G
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	189(F)	U

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Mol	Chain	Res	Type
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	281	G
32	2a	289	G
32	2a	301	G
32	2a	316	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	484	G
32	2a	485	G

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Mol	Chain	Res	Type
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	7MG
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	607	A
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	703	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	770	C
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	816	A
32	2a	817	C
32	2a	821	G

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Mol	Chain	Res	Type
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	859	A
32	2a	874	G
32	2a	880	C
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	932	C
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	984	C
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1024	G
32	2a	1025	U
32	2a	1026	G

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Mol	Chain	Res	Type
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1033	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1136	U
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G

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Mol	Chain	Res	Type
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1220	G
32	2a	1222	G
32	2a	1226	C
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1246	C
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1272	G
32	2a	1273	G
32	2a	1275	A
32	2a	1277	C
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1323	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1364	U
32	2a	1370	G
32	2a	1378	C
32	2a	1397	C
32	2a	1404	5MC
32	2a	1419	G
32	2a	1442	G

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Mol	Chain	Res	Type
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
53	2v	13	A
53	2v	14	A
54	2w	2	G
54	2w	9	A
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	23	A
54	2w	35	A
54	2w	46	7MG
54	2w	47	U
54	2w	49	G
54	2w	50	G
54	2w	51	C
54	2w	56	C
54	2w	57	G
54	2w	58	A
54	2w	59	U
54	2w	60	C
54	2w	61	C
54	2w	62	C
54	2w	68	C
54	2w	70	C
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	20	U

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Mol	Chain	Res	Type
55	2x	21	A
55	2x	22	G
55	2x	47	U
55	2x	48	C
55	2x	52	G
55	2x	56	C
55	2x	68	C
55	2x	73	A
55	2x	76	A
54	2y	2	G
54	2y	5	G
54	2y	6	A
54	2y	7	U
54	2y	8	4SU
54	2y	9	A
54	2y	13	C
54	2y	15	G
54	2y	19	G
54	2y	23	A
54	2y	24	G
54	2y	26	A
54	2y	30	C
54	2y	32	C
54	2y	33	U
54	2y	35	A
54	2y	38	A
54	2y	41	A
54	2y	46	7MG
54	2y	49	G
54	2y	51	C
54	2y	52	G
54	2y	53	G
54	2y	54	5MU
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	61	C
54	2y	69	A
54	2y	70	C

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	184	A
1	1A	185	A
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	572	A
1	1A	793	A
1	1A	811	A
1	1A	913	A
1	1A	941	U
1	1A	1019	G
1	1A	1067	A
1	1A	1093	G
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1425	A
1	1A	1554	A
1	1A	1654	A
1	1A	1700	G
1	1A	2014	G
1	1A	2156	A
1	1A	2205	C
1	1A	2418	U
1	1A	2442	A
1	1A	2451	A
2	1B	1	U
1	2A	34	C
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A

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Mol	Chain	Res	Type
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	CM0	2w	34	54	16,26,27	1.07	1 (6%)	18,37,40	2.00	4 (22%)
32	7MG	1a	527	32,57	22,26,27	1.82	4 (18%)	28,39,42	2.68	8 (28%)
32	5MC	1a	1407	32	15,22,23	1.37	1 (6%)	19,32,35	1.27	3 (15%)
54	5MU	1y	54	54	15,22,23	1.09	1 (6%)	16,32,35	1.77	2 (12%)
43	0TD	1l	92	43	4,9,10	3.20	1 (25%)	3,11,13	6.08	1 (33%)
55	5MU	2x	54	55	15,22,23	1.11	1 (6%)	16,32,35	1.79	1 (6%)
32	M2G	1a	966	32	20,27,28	1.39	3 (15%)	22,40,43	2.11	6 (27%)
32	5MC	2a	1400	32	15,22,23	1.38	1 (6%)	19,32,35	1.25	3 (15%)
54	7MG	2w	46	54	22,26,27	1.82	4 (18%)	28,39,42	2.72	8 (28%)
32	5MC	2a	1404	32	15,22,23	1.42	1 (6%)	19,32,35	1.28	2 (10%)
32	5MC	1a	1404	32	15,22,23	1.21	1 (6%)	19,32,35	1.22	2 (10%)
43	0TD	2l	92	43	4,9,10	3.18	1 (25%)	3,11,13	8.96	1 (33%)
55	5MU	1x	54	55,57	15,22,23	1.09	2 (13%)	16,32,35	2.12	2 (12%)
32	UR3	2a	1498	32	14,22,23	0.79	1 (7%)	15,32,35	0.70	0
54	CM0	1y	34	54	16,26,27	1.11	1 (6%)	18,37,40	2.08	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	1407	32,57	15,22,23	1.33	1 (6%)	19,32,35	1.41	3 (15%)
1	5MC	2A	1962	1,57	15,22,23	1.32	1 (6%)	19,32,35	1.35	3 (15%)
56	IAR	C	9	54,56	9,11,11	1.80	3 (33%)	6,13,13	1.77	1 (16%)
54	PSU	2y	55	54	17,21,22	1.46	2 (11%)	20,30,33	3.20	6 (30%)
32	4OC	1a	1402	32	16,23,24	0.64	0	17,32,35	1.33	1 (5%)
55	5MC	2x	32	55	15,22,23	1.29	1 (6%)	19,32,35	1.45	4 (21%)
54	PSU	1w	55	54	17,21,22	1.33	2 (11%)	20,30,33	3.34	6 (30%)
32	MA6	1a	1518	32	19,26,27	0.98	1 (5%)	18,38,41	1.58	3 (16%)
1	OMG	1A	2263	1,55,57	18,26,27	1.20	2 (11%)	20,38,41	2.30	6 (30%)
32	M2G	2a	966	32	20,27,28	1.41	3 (15%)	22,40,43	2.08	6 (27%)
32	5MC	1a	1400	32	15,22,23	1.36	1 (6%)	19,32,35	1.33	3 (15%)
1	PSU	2A	1911	1	17,21,22	1.56	3 (17%)	20,30,33	3.13	6 (30%)
55	4SU	1x	8	55	14,21,22	1.50	2 (14%)	15,30,33	2.65	2 (13%)
54	4SU	2y	8	54	14,21,22	1.18	1 (7%)	15,30,33	1.68	2 (13%)
32	MA6	2a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.62	5 (27%)
32	2MG	1a	1207	32	19,26,27	1.21	2 (10%)	21,38,41	2.28	8 (38%)
1	4OC	1A	1942	1	15,22,24	0.74	0	17,31,35	1.47	2 (11%)
1	5MC	1A	1964	1	15,22,23	1.25	1 (6%)	19,32,35	1.36	3 (15%)
55	4SU	2x	8	55	14,21,22	1.32	2 (14%)	15,30,33	2.41	2 (13%)
1	5MC	2A	1942	1	15,22,23	1.30	1 (6%)	19,32,35	1.34	3 (15%)
56	EUP	A	2	56	4,7,8	0.55	0	5,8,10	1.46	1 (20%)
54	4SU	1y	8	54	14,21,22	1.28	1 (7%)	15,30,33	1.57	2 (13%)
54	4SU	1w	8	54	14,21,22	1.29	1 (7%)	15,30,33	1.48	2 (13%)
54	PSU	2w	55	54	17,21,22	1.31	2 (11%)	20,30,33	3.30	6 (30%)
32	2MG	2a	1207	32	19,26,27	1.35	2 (10%)	21,38,41	2.32	7 (33%)
32	UR3	1a	1498	32	14,22,23	0.75	0	15,32,35	0.70	0
54	5MU	1w	54	54	15,22,23	1.07	1 (6%)	16,32,35	1.83	2 (12%)
54	7MG	1y	46	54	22,26,27	1.91	4 (18%)	28,39,42	3.11	12 (42%)
1	5MU	2A	1915	1	15,22,23	1.07	1 (6%)	16,32,35	1.84	2 (12%)
1	4OC	2A	1920	1	15,22,24	0.68	0	17,31,35	1.37	1 (5%)
56	ORD	A	5	56	6,7,8	0.49	0	2,7,9	0.61	0
1	OMG	2A	2251	1,55,57	18,26,27	1.15	2 (11%)	20,38,41	2.16	6 (30%)
54	5MU	2y	54	54	15,22,23	1.09	1 (6%)	16,32,35	1.74	2 (12%)
55	PSU	2x	55	55	17,21,22	1.63	2 (11%)	20,30,33	3.06	6 (30%)
54	5MU	2w	54	54	15,22,23	1.01	1 (6%)	16,32,35	2.02	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PSU	1x	55	55	17,21,22	1.61	2 (11%)	20,30,33	3.12	6 (30%)
32	5MC	2a	967	32	15,22,23	1.40	1 (6%)	19,32,35	1.26	3 (15%)
56	IAR	B	7	56	9,11,11	2.12	3 (33%)	6,13,13	2.26	1 (16%)
54	6MZ	2w	37	54	18,25,26	0.97	1 (5%)	16,36,39	2.03	4 (25%)
54	6MZ	2y	37	54,32	18,25,26	1.01	1 (5%)	16,36,39	2.00	4 (25%)
1	PSU	1A	1933	1	17,21,22	1.59	4 (23%)	20,30,33	3.08	6 (30%)
1	2MA	1A	2515	1,57	17,25,26	1.14	2 (11%)	19,37,40	2.08	3 (15%)
32	PSU	1a	516	32	17,21,22	1.55	3 (17%)	20,30,33	3.03	6 (30%)
1	5MU	1A	1961	1	15,22,23	1.06	2 (13%)	16,32,35	1.79	2 (12%)
32	MA6	2a	1518	32	19,26,27	1.01	1 (5%)	18,38,41	1.67	4 (22%)
1	5MC	1A	1984	1,57	15,22,23	1.34	1 (6%)	19,32,35	1.25	3 (15%)
32	MA6	1a	1519	32	19,26,27	1.07	1 (5%)	18,38,41	1.55	4 (22%)
56	IAR	A	9	56	9,11,11	1.65	2 (22%)	6,13,13	3.45	1 (16%)
56	ORD	B	3	56	6,7,8	0.51	0	2,7,9	0.49	0
54	CM0	1w	34	54	16,26,27	1.10	1 (6%)	18,37,40	2.10	5 (27%)
54	PSU	1y	55	54	17,21,22	1.56	3 (17%)	20,30,33	3.09	7 (35%)
1	5MU	1A	1937	1	15,22,23	1.08	1 (6%)	16,32,35	1.79	1 (6%)
54	CM0	2y	34	54	16,26,27	1.16	1 (6%)	18,37,40	2.06	4 (22%)
54	7MG	1w	46	54	22,26,27	1.83	4 (18%)	28,39,42	2.75	9 (32%)
1	PSU	2A	2605	1	17,21,22	1.53	3 (17%)	20,30,33	3.22	6 (30%)
54	6MZ	1w	37	54	18,25,26	0.94	1 (5%)	16,36,39	2.10	4 (25%)
54	6MZ	1y	37	54	18,25,26	1.02	1 (5%)	16,36,39	2.18	4 (25%)
56	EUP	C	2	56	4,7,8	0.51	0	5,8,10	1.36	1 (20%)
1	PSU	2A	1917	1	17,21,22	1.56	3 (17%)	20,30,33	3.07	6 (30%)
1	PSU	1A	1939	1	17,21,22	1.59	2 (11%)	20,30,33	3.34	6 (30%)
32	7MG	2a	527	32,57	22,26,27	1.79	4 (18%)	28,39,42	2.67	8 (28%)
54	7MG	2y	46	54	22,26,27	1.84	3 (13%)	28,39,42	2.99	10 (35%)
1	2MU	1A	2564	1	14,22,24	0.89	0	14,31,36	0.72	0
1	2MU	2A	2552	1,57	14,22,24	0.95	1 (7%)	14,31,36	0.89	1 (7%)
1	2MA	2A	2503	1	17,25,26	1.26	2 (11%)	19,37,40	1.91	3 (15%)
55	5MC	1x	32	55	15,22,23	1.32	1 (6%)	19,32,35	1.59	4 (21%)
1	5MU	2A	1939	1	15,22,23	1.09	2 (13%)	16,32,35	1.65	2 (12%)
56	ORD	C	5	32,56	6,7,8	1.35	1 (16%)	2,7,9	0.78	0
54	4SU	2w	8	54	14,21,22	1.31	1 (7%)	15,30,33	1.20	2 (13%)
32	4OC	2a	1402	32,57	16,23,24	0.65	0	17,32,35	1.67	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	1a	967	32	15,22,23	1.23	1 (6%)	19,32,35	1.36	2 (10%)
32	PSU	2a	516	32,57	17,21,22	1.56	3 (17%)	20,30,33	3.05	7 (35%)
1	PSU	1A	2617	1	17,21,22	1.82	3 (17%)	20,30,33	3.02	6 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	CM0	2w	34	54	-	5/8/30/31	0/2/2/2
32	7MG	1a	527	32,57	-	3/7/37/38	0/3/3/3
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/5/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
55	5MU	1x	54	55,57	-	0/5/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
54	CM0	1y	34	54	-	0/8/30/31	0/2/2/2
32	5MC	2a	1407	32,57	-	0/5/25/26	0/2/2/2
1	5MC	2A	1962	1,57	-	2/5/25/26	0/2/2/2
56	IAR	C	9	54,56	-	2/6/11/11	-
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
55	5MC	2x	32	55	-	1/5/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
1	OMG	1A	2263	1,55,57	-	1/5/27/28	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
54	4SU	2y	8	54	-	1/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	4OC	1A	1942	1	-	1/7/27/30	0/2/2/2
1	5MC	1A	1964	1	-	0/5/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
56	EUP	A	2	56	-	1/7/8/10	-
54	4SU	1y	8	54	-	1/5/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	2/5/27/28	0/3/3/3
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/7/27/30	0/2/2/2
56	ORD	A	5	56	-	2/5/6/8	-
1	OMG	2A	2251	1,55,57	-	0/5/27/28	0/3/3/3
54	5MU	2y	54	54	-	2/5/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
56	IAR	B	7	56	-	2/6/11/11	-
54	6MZ	2w	37	54	-	0/5/27/28	0/3/3/3
54	6MZ	2y	37	54,32	-	1/5/27/28	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	1,57	-	2/3/25/26	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1	-	0/5/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
1	5MC	1A	1984	1,57	-	2/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
56	IAR	A	9	56	-	3/6/11/11	-
56	ORD	B	3	56	-	4/5/6/8	-
54	CM0	1w	34	54	-	5/8/30/31	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/5/25/26	0/2/2/2
54	CM0	2y	34	54	-	4/8/30/31	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	6MZ	1w	37	54	-	0/5/27/28	0/3/3/3
54	6MZ	1y	37	54	-	0/5/27/28	0/3/3/3
56	EUP	C	2	56	-	3/7/8/10	-
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,57	-	3/7/37/38	0/3/3/3
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3
1	2MU	1A	2564	1	-	0/7/27/28	0/2/2/2
1	2MU	2A	2552	1,57	-	0/7/27/28	0/2/2/2
1	2MA	2A	2503	1	-	1/3/25/26	0/3/3/3
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
1	5MU	2A	1939	1	-	1/5/25/26	0/2/2/2
56	ORD	C	5	32,56	-	3/5/6/8	-
54	4SU	2w	8	54	-	0/5/25/26	0/2/2/2
32	4OC	2a	1402	32,57	-	3/9/29/30	0/2/2/2
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
32	PSU	2a	516	32,57	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-6.11	1.69	1.84
43	1l	92	0TD	CB-SB	-6.01	1.69	1.84
1	1A	2617	PSU	C5-C1'	-5.35	1.47	1.52
32	2a	527	7MG	C6-C5	5.27	1.48	1.41
32	1a	527	7MG	C6-C5	5.13	1.48	1.41
54	1y	46	7MG	C5-C4	5.08	1.49	1.39
32	2a	967	5MC	C5-C4	5.07	1.49	1.41
32	2a	1404	5MC	C5-C4	5.03	1.49	1.41
54	1y	46	7MG	C6-C5	5.00	1.48	1.41
54	1w	46	7MG	C6-C5	4.98	1.48	1.41
54	2w	46	7MG	C6-C5	4.92	1.48	1.41
54	2y	46	7MG	C6-C5	4.89	1.48	1.41
32	2a	1400	5MC	C5-C4	4.87	1.48	1.41
32	1a	1400	5MC	C5-C4	4.83	1.48	1.41
54	2y	46	7MG	C5-C4	4.81	1.48	1.39
1	1A	1984	5MC	C5-C4	4.79	1.48	1.41
32	1a	1407	5MC	C5-C4	4.79	1.48	1.41
55	2x	55	PSU	C5-C1'	-4.71	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	32	5MC	C5-C4	4.69	1.48	1.41
54	2w	46	7MG	C5-C4	4.68	1.48	1.39
32	2a	1407	5MC	C5-C4	4.66	1.48	1.41
1	2A	1962	5MC	C5-C4	4.64	1.48	1.41
55	2x	32	5MC	C5-C4	4.63	1.48	1.41
1	2A	1942	5MC	C5-C4	4.60	1.48	1.41
55	1x	55	PSU	C5-C1'	-4.58	1.48	1.52
54	1w	46	7MG	C5-C4	4.57	1.48	1.39
32	2a	1207	2MG	C6-C5	4.57	1.49	1.41
54	1y	55	PSU	C5-C1'	-4.47	1.48	1.52
32	2a	527	7MG	C5-C4	4.46	1.47	1.39
1	1A	1964	5MC	C5-C4	4.46	1.48	1.41
32	1a	527	7MG	C5-C4	4.45	1.47	1.39
1	1A	1939	PSU	C5-C1'	-4.39	1.48	1.52
32	1a	967	5MC	C5-C4	4.35	1.48	1.41
56	B	7	IAR	CA-N	4.34	1.38	1.27
32	1a	1207	2MG	C6-C5	4.33	1.48	1.41
1	2A	1911	PSU	C5-C1'	-4.29	1.48	1.52
32	1a	1404	5MC	C5-C4	4.23	1.47	1.41
1	1A	1933	PSU	C5-C1'	-4.21	1.48	1.52
56	C	9	IAR	CA-N	4.20	1.37	1.27
32	1a	966	M2G	C6-C5	4.20	1.48	1.41
32	2a	516	PSU	C5-C1'	-4.16	1.48	1.52
1	2A	2605	PSU	C5-C1'	-4.10	1.48	1.52
54	2w	8	4SU	C4-S4	-4.09	1.60	1.67
54	1w	8	4SU	C4-S4	-4.07	1.60	1.67
1	2A	1917	PSU	C5-C1'	-4.06	1.48	1.52
32	1a	516	PSU	C5-C1'	-4.05	1.48	1.52
32	2a	966	M2G	C6-C5	4.04	1.48	1.41
54	1y	8	4SU	C4-S4	-4.02	1.60	1.67
1	2A	2503	2MA	C6-C5	3.95	1.47	1.41
56	A	9	IAR	CA-N	3.94	1.37	1.27
55	1x	8	4SU	C2-N3	-3.84	1.30	1.38
54	2y	8	4SU	C4-S4	-3.82	1.60	1.67
55	1x	8	4SU	C4-S4	-3.81	1.60	1.67
1	2A	2251	OMG	C6-C5	3.78	1.47	1.41
1	1A	2263	OMG	C6-C5	3.72	1.47	1.41
1	1A	2515	2MA	C6-C5	3.66	1.46	1.41
54	2y	55	PSU	C4-C5	3.65	1.49	1.41
54	2y	34	CM0	C4-C5	3.63	1.49	1.40
56	B	7	IAR	C-CA	3.60	1.57	1.52
54	2y	54	5MU	C4-C5	3.57	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1915	5MU	C4-C5	3.56	1.49	1.41
55	2x	54	5MU	C4-C5	3.56	1.49	1.41
55	2x	8	4SU	C4-S4	-3.55	1.61	1.67
54	1y	34	CM0	C4-C5	3.53	1.48	1.40
54	2y	46	7MG	C5-N7	-3.52	1.33	1.39
32	2a	966	M2G	C2-N2	3.51	1.40	1.34
54	1w	34	CM0	C4-C5	3.49	1.48	1.40
54	1y	54	5MU	C4-C5	3.47	1.48	1.41
55	2x	55	PSU	C4-C5	3.44	1.48	1.41
1	1A	1933	PSU	C4-C5	3.43	1.48	1.41
1	2A	1917	PSU	C4-C5	3.43	1.48	1.41
32	1a	527	7MG	C5-N7	-3.41	1.34	1.39
54	1w	54	5MU	C4-C5	3.40	1.48	1.41
32	2a	516	PSU	C4-C5	3.39	1.48	1.41
54	2y	55	PSU	C5-C1'	-3.38	1.49	1.52
54	2w	34	CM0	C4-C5	3.38	1.48	1.40
54	2w	55	PSU	C4-C5	3.37	1.48	1.41
1	1A	2617	PSU	C4-C5	3.37	1.48	1.41
32	1a	516	PSU	C4-C5	3.36	1.48	1.41
1	1A	1937	5MU	C4-C5	3.35	1.48	1.41
54	1w	55	PSU	C4-C5	3.33	1.48	1.41
1	2A	1939	5MU	C4-C5	3.30	1.48	1.41
54	1y	46	7MG	C5-N7	-3.28	1.34	1.39
54	1w	46	7MG	C5-N7	-3.27	1.34	1.39
1	2A	1911	PSU	C4-C5	3.26	1.48	1.41
55	1x	54	5MU	C4-C5	3.25	1.48	1.41
55	1x	55	PSU	C4-C5	3.24	1.48	1.41
54	1y	55	PSU	C4-C5	3.22	1.48	1.41
54	2w	54	5MU	C4-C5	3.20	1.48	1.41
32	2a	527	7MG	C5-N7	-3.19	1.34	1.39
54	2w	46	7MG	C5-N7	-3.18	1.34	1.39
32	1a	966	M2G	C2-N2	3.16	1.40	1.34
1	1A	1939	PSU	C4-C5	3.09	1.48	1.41
1	1A	1961	5MU	C4-C5	3.07	1.48	1.41
1	2A	2605	PSU	C4-C5	3.04	1.48	1.41
55	2x	8	4SU	C2-N3	-3.02	1.32	1.38
56	C	5	ORD	CB-CA	2.81	1.57	1.53
54	2y	37	6MZ	C5-C4	2.81	1.48	1.40
32	2a	1518	MA6	C5-C4	2.71	1.48	1.40
54	1y	37	6MZ	C5-C4	2.67	1.48	1.40
32	2a	1207	2MG	C5-C4	2.67	1.48	1.40
32	2a	1519	MA6	C5-C4	2.63	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	37	6MZ	C5-C4	2.61	1.47	1.40
54	2w	55	PSU	C5-C1'	-2.60	1.50	1.52
32	1a	1519	MA6	C5-C4	2.60	1.47	1.40
32	1a	527	7MG	C4-N9	-2.57	1.33	1.38
54	1w	37	6MZ	C5-C4	2.53	1.47	1.40
32	2a	966	M2G	C5-C4	2.52	1.47	1.40
32	1a	1518	MA6	C5-C4	2.51	1.47	1.40
32	1a	966	M2G	C5-C4	2.51	1.47	1.40
54	1w	55	PSU	C5-C1'	-2.48	1.50	1.52
54	1w	46	7MG	C4-N9	-2.43	1.33	1.38
1	1A	2617	PSU	C2-N3	-2.39	1.33	1.38
54	1y	46	7MG	C4-N3	2.38	1.37	1.34
1	2A	2251	OMG	C5-C4	2.36	1.47	1.40
1	2A	2503	2MA	C5-C4	2.33	1.47	1.40
54	2w	46	7MG	C4-N9	-2.32	1.34	1.38
56	B	7	IAR	CB-CA	2.28	1.56	1.50
1	1A	2263	OMG	C5-C4	2.24	1.46	1.40
56	C	9	IAR	C-CA	2.23	1.55	1.52
32	2a	1498	UR3	C4-N3	2.19	1.41	1.38
32	1a	1207	2MG	C5-C4	2.19	1.46	1.40
55	1x	54	5MU	C2-N3	-2.18	1.33	1.38
1	1A	1961	5MU	C2-N3	-2.16	1.33	1.38
32	2a	516	PSU	O4'-C1'	-2.15	1.41	1.44
1	2A	2552	2MU	C2-N3	-2.14	1.33	1.38
32	1a	516	PSU	O4'-C1'	-2.10	1.41	1.44
56	C	9	IAR	CB-CA	2.10	1.56	1.50
32	2a	527	7MG	C4-N9	-2.09	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.08	1.34	1.38
1	1A	1933	PSU	O4'-C1'	-2.07	1.41	1.44
56	A	9	IAR	CB-CA	2.07	1.56	1.50
1	2A	1911	PSU	O4'-C1'	-2.05	1.41	1.44
1	1A	1933	PSU	C2-N3	-2.03	1.34	1.38
1	1A	2515	2MA	C5-C4	2.03	1.46	1.40
1	2A	1917	PSU	C2-N3	-2.01	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.00	1.34	1.38
54	1y	55	PSU	O4'-C1'	-2.00	1.41	1.44

All (318) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-15.48	71.40	101.85
43	1l	92	0TD	CSB-SB-CB	-10.45	81.30	101.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	46	7MG	N3-C4-N9	9.91	139.64	126.91
54	2y	46	7MG	N3-C4-N9	9.84	139.54	126.91
54	1w	55	PSU	N1-C2-N3	-9.67	120.74	128.43
54	2w	55	PSU	N1-C2-N3	-9.05	121.24	128.43
1	1A	1939	PSU	N1-C2-N3	-9.03	121.25	128.43
55	1x	8	4SU	C2-N3-C4	8.96	128.15	115.15
1	2A	2605	PSU	N1-C2-N3	-8.91	121.35	128.43
54	1w	46	7MG	N3-C4-N9	8.72	138.11	126.91
54	2w	46	7MG	N3-C4-N9	8.70	138.08	126.91
32	1a	527	7MG	N3-C4-N9	8.69	138.07	126.91
1	2A	1911	PSU	N1-C2-N3	-8.60	121.59	128.43
32	2a	527	7MG	N3-C4-N9	8.56	137.90	126.91
54	2y	55	PSU	N1-C2-N3	-8.48	121.69	128.43
32	2a	516	PSU	N1-C2-N3	-8.39	121.76	128.43
55	1x	55	PSU	N1-C2-N3	-8.20	121.91	128.43
1	1A	1933	PSU	N1-C2-N3	-8.18	121.93	128.43
56	A	9	IAR	CG-CB-CA	8.17	127.65	113.35
32	1a	516	PSU	N1-C2-N3	-8.16	121.94	128.43
54	1y	55	PSU	N1-C2-N3	-8.02	122.05	128.43
55	2x	8	4SU	C2-N3-C4	7.95	126.68	115.15
55	2x	55	PSU	N1-C2-N3	-7.87	122.17	128.43
54	1w	55	PSU	C4-N3-C2	7.81	121.73	115.14
55	1x	54	5MU	C4-N3-C2	7.80	121.73	115.14
1	1A	2617	PSU	N1-C2-N3	-7.65	122.35	128.43
1	2A	1917	PSU	N1-C2-N3	-7.64	122.36	128.43
54	2w	55	PSU	C4-N3-C2	7.42	121.41	115.14
54	2y	55	PSU	C4-N3-C2	7.40	121.39	115.14
54	2w	54	5MU	C4-N3-C2	7.36	121.36	115.14
1	1A	1939	PSU	C4-N3-C2	7.25	121.26	115.14
54	2y	34	CM0	C4-N3-C2	6.93	120.99	115.14
1	2A	2605	PSU	C4-N3-C2	6.84	120.92	115.14
54	1y	55	PSU	C4-N3-C2	6.80	120.88	115.14
54	1w	34	CM0	C4-N3-C2	6.77	120.86	115.14
1	1A	2515	2MA	C2-N3-C4	6.77	121.02	115.52
1	2A	1911	PSU	C4-N3-C2	6.76	120.85	115.14
54	2w	34	CM0	C4-N3-C2	6.75	120.84	115.14
1	2A	1915	5MU	C4-N3-C2	6.71	120.81	115.14
1	1A	1933	PSU	C4-N3-C2	6.70	120.80	115.14
1	1A	1937	5MU	C4-N3-C2	6.63	120.74	115.14
55	2x	54	5MU	C4-N3-C2	6.59	120.71	115.14
32	1a	516	PSU	C4-N3-C2	6.57	120.69	115.14
1	2A	1917	PSU	C4-N3-C2	6.55	120.67	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	516	PSU	C4-N3-C2	6.47	120.61	115.14
54	1y	37	6MZ	C2-N1-C6	6.46	122.13	116.59
54	1y	46	7MG	C6-N1-C2	6.37	126.06	115.93
54	1y	34	CM0	C4-N3-C2	6.35	120.51	115.14
55	1x	55	PSU	C4-N3-C2	6.27	120.44	115.14
54	1y	54	5MU	C4-N3-C2	6.25	120.42	115.14
55	2x	55	PSU	C4-N3-C2	6.18	120.36	115.14
54	1w	37	6MZ	C2-N1-C6	6.14	121.85	116.59
54	1w	54	5MU	C4-N3-C2	6.13	120.31	115.14
54	2y	54	5MU	C4-N3-C2	6.05	120.25	115.14
54	2y	37	6MZ	C2-N1-C6	5.96	121.70	116.59
1	1A	1961	5MU	C4-N3-C2	5.95	120.16	115.14
1	1A	2617	PSU	C4-N3-C2	5.87	120.09	115.14
32	2a	1402	4OC	CM4-N4-C4	-5.85	117.94	122.97
54	2y	55	PSU	C5-C4-N3	-5.84	117.83	125.36
1	2A	2503	2MA	C2-N3-C4	5.82	120.25	115.52
54	1y	55	PSU	C5-C4-N3	-5.79	117.90	125.36
54	2w	37	6MZ	C2-N1-C6	5.59	121.38	116.59
54	2y	46	7MG	C5-C4-N3	-5.54	117.45	126.49
1	2A	1917	PSU	C5-C4-N3	-5.52	118.25	125.36
32	2a	527	7MG	N7-C8-N9	-5.48	95.54	103.38
55	2x	55	PSU	C5-C4-N3	-5.41	118.39	125.36
1	1A	1933	PSU	C5-C4-N3	-5.40	118.40	125.36
1	1A	1939	PSU	C5-C4-N3	-5.40	118.41	125.36
54	1w	46	7MG	N7-C8-N9	-5.39	95.67	103.38
56	B	7	IAR	CG-CB-CA	5.38	122.77	113.35
54	2y	46	7MG	C6-N1-C2	5.35	124.44	115.93
54	2w	46	7MG	N7-C8-N9	-5.33	95.75	103.38
54	2w	55	PSU	C5-C4-N3	-5.31	118.52	125.36
54	1w	55	PSU	C5-C4-N3	-5.28	118.56	125.36
32	1a	516	PSU	C5-C4-N3	-5.26	118.59	125.36
1	2A	1911	PSU	C5-C4-N3	-5.22	118.63	125.36
55	1x	55	PSU	C5-C4-N3	-5.21	118.65	125.36
1	1A	2263	OMG	C2-N3-C4	5.18	121.27	115.36
32	2a	966	M2G	C2-N3-C4	5.16	121.14	115.28
32	2a	516	PSU	C5-C4-N3	-5.16	118.71	125.36
32	1a	527	7MG	N7-C8-N9	-5.15	96.02	103.38
54	1y	46	7MG	C5-C4-N3	-5.13	118.11	126.49
32	1a	527	7MG	C5-C4-N3	-5.08	118.19	126.49
32	1a	966	M2G	C2-N3-C4	5.03	120.98	115.28
1	2A	2605	PSU	C5-C4-N3	-5.02	118.90	125.36
32	2a	527	7MG	C5-C4-N3	-5.00	118.33	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1939	5MU	C4-N3-C2	4.99	119.36	115.14
1	1A	2617	PSU	C5-C4-N3	-4.97	118.96	125.36
32	2a	966	M2G	C6-N1-C2	4.96	122.08	116.18
32	1a	1207	2MG	C2-N3-C4	4.87	120.81	115.28
55	2x	55	PSU	C5-C6-N1	-4.84	118.49	124.44
54	2w	46	7MG	C6-N1-C2	4.82	123.59	115.93
32	1a	966	M2G	C6-N1-C2	4.80	121.89	116.18
54	1y	46	7MG	N7-C8-N9	-4.78	96.54	103.38
54	1w	46	7MG	C5-C4-N3	-4.76	118.72	126.49
32	2a	1207	2MG	C2-N3-C4	4.76	120.68	115.28
1	1A	2617	PSU	C5-C6-N1	-4.74	118.61	124.44
54	2y	46	7MG	N7-C8-N9	-4.73	96.62	103.38
54	1w	46	7MG	C6-N1-C2	4.71	123.41	115.93
54	1y	8	4SU	C2-N3-C4	4.69	121.95	115.15
54	2w	46	7MG	C5-C4-N3	-4.65	118.89	126.49
54	2y	8	4SU	C2-N3-C4	4.61	121.84	115.15
1	2A	2251	OMG	C2-N3-C4	4.60	120.61	115.36
32	1a	1402	4OC	CM4-N4-C4	-4.59	119.03	122.97
1	2A	2503	2MA	C5-C6-N1	-4.57	118.27	123.06
54	1w	8	4SU	C2-N3-C4	4.53	121.71	115.15
55	1x	8	4SU	C5-C4-N3	-4.49	117.82	123.83
55	2x	8	4SU	C5-C4-N3	-4.47	117.84	123.83
32	2a	1207	2MG	C5-C6-N1	-4.42	117.38	123.43
32	2a	527	7MG	C6-N1-C2	4.42	122.95	115.93
32	1a	527	7MG	C6-N1-C2	4.40	122.92	115.93
55	1x	55	PSU	C5-C6-N1	-4.36	119.08	124.44
54	2y	46	7MG	C6-C5-C4	4.36	119.88	115.20
1	1A	2263	OMG	C6-N1-C2	4.33	122.80	115.93
32	1a	516	PSU	C5-C6-N1	-4.32	119.13	124.44
1	2A	1917	PSU	C5-C6-N1	-4.28	119.18	124.44
1	2A	1920	4OC	C2-N3-C4	4.27	120.67	116.34
1	1A	1942	4OC	C2-N3-C4	4.26	120.66	116.34
1	1A	1939	PSU	C6-N1-C2	4.25	122.37	115.36
54	1y	46	7MG	C5-C6-N1	-4.24	114.42	123.14
1	1A	1933	PSU	C5-C6-N1	-4.24	119.23	124.44
1	2A	2251	OMG	C6-N1-C2	4.23	122.66	115.93
1	2A	2605	PSU	C5-C6-N1	-4.23	119.24	124.44
1	1A	2617	PSU	C6-N1-C2	4.22	122.33	115.36
1	2A	2605	PSU	C6-N1-C2	4.22	122.32	115.36
32	2a	516	PSU	C5-C6-N1	-4.21	119.26	124.44
1	1A	1939	PSU	C5-C6-N1	-4.20	119.28	124.44
32	2a	1207	2MG	C6-N1-C2	4.20	122.69	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	55	PSU	C6-N1-C2	4.18	122.25	115.36
32	2a	516	PSU	C6-N1-C2	4.14	122.19	115.36
54	1y	46	7MG	C6-C5-C4	4.14	119.64	115.20
1	1A	2515	2MA	C5-C6-N1	-4.13	118.73	123.06
54	1y	34	CM0	C7-O5-C5	4.12	125.88	117.76
55	1x	55	PSU	C6-N1-C2	4.11	122.14	115.36
1	1A	2263	OMG	N3-C2-N1	-4.10	121.75	127.22
32	1a	516	PSU	C6-N1-C2	4.09	122.10	115.36
32	1a	527	7MG	C6-C5-C4	4.08	119.58	115.20
1	2A	1911	PSU	C6-N1-C2	4.07	122.08	115.36
56	C	9	IAR	CG-CB-CA	4.06	120.46	113.35
54	1y	55	PSU	C5-C6-N1	-4.06	119.45	124.44
32	1a	1207	2MG	C6-C5-C4	-4.04	116.94	120.80
32	2a	1207	2MG	C6-C5-C4	-4.04	116.94	120.80
1	2A	2251	OMG	C5-C6-N1	-4.02	117.93	123.43
1	1A	1933	PSU	C6-N1-C2	4.02	121.99	115.36
54	1w	46	7MG	C6-C5-C4	3.99	119.48	115.20
1	1A	1939	PSU	C5-C1'-C2'	-3.98	108.21	115.32
54	2w	46	7MG	C6-C5-C4	3.96	119.45	115.20
1	1A	2263	OMG	C6-C5-C4	-3.94	117.04	120.80
1	2A	1911	PSU	C5-C6-N1	-3.94	119.60	124.44
1	1A	2617	PSU	C5-C1'-C2'	-3.93	108.31	115.32
32	1a	1207	2MG	C5-C6-N1	-3.91	118.08	123.43
1	2A	1917	PSU	C6-N1-C2	3.90	121.79	115.36
54	2w	55	PSU	C6-N1-C2	3.89	121.78	115.36
54	2w	55	PSU	C5-C1'-C2'	-3.87	108.41	115.32
54	2y	46	7MG	C5-C6-N1	-3.87	115.19	123.14
54	1w	55	PSU	C6-N1-C2	3.86	121.73	115.36
32	2a	966	M2G	C5-C6-N1	-3.85	118.16	123.43
54	2w	37	6MZ	C9-N6-C6	-3.84	119.56	122.87
54	2w	46	7MG	C5-C6-N1	-3.84	115.25	123.14
1	1A	2263	OMG	C5-C6-N1	-3.83	118.19	123.43
1	2A	2251	OMG	C6-C5-C4	-3.83	117.14	120.80
32	1a	966	M2G	C5-C6-N1	-3.82	118.20	123.43
55	1x	55	PSU	C5-C1'-C2'	-3.82	108.50	115.32
32	2a	527	7MG	C6-C5-C4	3.79	119.27	115.20
54	1w	46	7MG	C5-C6-N1	-3.79	115.36	123.14
32	2a	1518	MA6	C9-N6-C6	-3.78	108.06	119.51
32	2a	1518	MA6	C4-C5-N7	-3.77	105.47	109.40
54	1y	55	PSU	C6-N1-C2	3.76	121.56	115.36
32	1a	1207	2MG	C6-N1-C2	3.75	121.90	115.18
1	2A	1917	PSU	C5-C1'-C2'	-3.73	108.66	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	55	PSU	C6-N1-C2	3.73	121.51	115.36
32	1a	967	5MC	C2-N3-C4	3.71	120.49	116.02
32	1a	527	7MG	C5-C6-N1	-3.70	115.54	123.14
32	2a	1407	5MC	C2-N3-C4	3.67	120.45	116.02
55	2x	32	5MC	C2-N3-C4	3.67	120.45	116.02
32	1a	1404	5MC	C2-N3-C4	3.65	120.42	116.02
32	2a	527	7MG	C5-C6-N1	-3.60	115.73	123.14
32	1a	1400	5MC	C2-N3-C4	3.59	120.34	116.02
32	1a	1207	2MG	C4-C5-N7	-3.57	105.68	109.40
1	1A	1964	5MC	C2-N3-C4	3.57	120.32	116.02
32	1a	966	M2G	C6-C5-C4	-3.56	117.40	120.80
32	1a	1518	MA6	C4-C5-N7	-3.56	105.69	109.40
54	1w	37	6MZ	C9-N6-C6	-3.56	119.81	122.87
32	2a	1519	MA6	C4-C5-N7	-3.51	105.74	109.40
55	1x	32	5MC	C5-C6-N1	-3.47	118.45	122.19
32	2a	1400	5MC	C2-N3-C4	3.44	120.17	116.02
1	2A	2251	OMG	N3-C2-N1	-3.43	122.64	127.22
32	1a	1407	5MC	C2-N3-C4	3.41	120.14	116.02
32	2a	967	5MC	C2-N3-C4	3.41	120.14	116.02
1	2A	1939	5MU	C5-C6-N1	-3.41	118.52	122.19
54	2w	8	4SU	C2-N3-C4	3.41	120.09	115.15
32	1a	1519	MA6	C4-C5-N7	-3.35	105.90	109.40
54	1y	37	6MZ	N3-C2-N1	-3.34	123.45	128.68
32	2a	1404	5MC	C2-N3-C4	3.34	120.05	116.02
32	2a	1207	2MG	C4-C5-N7	-3.32	105.94	109.40
54	2w	55	PSU	C5-C6-N1	-3.32	120.36	124.44
32	1a	1207	2MG	CM2-N2-C2	-3.31	119.60	123.59
1	2A	2605	PSU	C5-C1'-C2'	-3.29	109.44	115.32
54	1y	8	4SU	C5-C4-N3	-3.29	119.43	123.83
54	2y	55	PSU	C5-C1'-C2'	-3.26	109.51	115.32
1	2A	1962	5MC	N4-C4-N3	3.20	121.55	117.03
32	2a	1518	MA6	N3-C2-N1	-3.20	123.68	128.68
54	1w	34	CM0	O5-C5-C4	3.19	119.10	115.19
32	1a	1518	MA6	N3-C2-N1	-3.16	123.73	128.68
1	1A	1984	5MC	C2-N3-C4	3.16	119.83	116.02
32	2a	1519	MA6	C9-N6-C6	-3.15	109.98	119.51
32	2a	966	M2G	C6-C5-C4	-3.12	117.81	120.80
54	2y	8	4SU	C5-C4-N3	-3.12	119.65	123.83
1	2A	1962	5MC	C2-N3-C4	3.12	119.78	116.02
54	2y	55	PSU	C5-C6-N1	-3.12	120.61	124.44
1	1A	1961	5MU	C5-C6-N1	-3.12	118.84	122.19
54	1w	54	5MU	C5-C6-N1	-3.11	118.85	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	32	5MC	C2-N3-C4	3.10	119.76	116.02
54	1w	37	6MZ	N3-C2-N1	-3.10	123.83	128.68
1	2A	1942	5MC	C2-N3-C4	3.10	119.75	116.02
32	2a	1519	MA6	N3-C2-N1	-3.09	123.85	128.68
54	1w	55	PSU	C5-C1'-C2'	-3.04	109.89	115.32
54	2w	37	6MZ	N3-C2-N1	-3.03	123.95	128.68
1	2A	1911	PSU	C5-C1'-C2'	-3.00	109.97	115.32
54	1y	46	7MG	C5-C4-N9	-2.99	102.25	106.44
32	2a	1404	5MC	C5-C6-N1	-2.97	118.99	122.19
32	1a	1519	MA6	N3-C2-N1	-2.94	124.08	128.68
54	1y	46	7MG	N2-C2-N3	2.92	121.79	117.25
54	2y	37	6MZ	C9-N6-C6	-2.91	120.37	122.87
32	1a	1519	MA6	C9-N6-C6	-2.91	110.71	119.51
54	1y	37	6MZ	C9-N6-C6	-2.90	120.38	122.87
32	1a	1518	MA6	C9-N6-C6	-2.90	110.75	119.51
32	2a	1207	2MG	N2-C2-N1	2.89	119.74	116.96
54	2y	37	6MZ	N3-C2-N1	-2.89	124.17	128.68
32	2a	527	7MG	C8-N7-C5	2.88	116.44	108.94
55	1x	32	5MC	CM5-C5-C4	-2.88	118.81	121.72
54	1w	8	4SU	C5-C4-N3	-2.86	120.00	123.83
32	1a	1519	MA6	N1-C6-N6	2.86	120.07	117.06
54	1y	37	6MZ	C4-C5-N7	-2.81	106.47	109.40
1	2A	1942	5MC	N4-C4-N3	2.80	120.99	117.03
54	1w	34	CM0	C5-C4-N3	-2.79	118.83	122.66
54	1w	37	6MZ	C4-C5-N7	-2.79	106.49	109.40
32	1a	966	M2G	C4-C5-N7	-2.75	106.53	109.40
54	2y	34	CM0	O5-C5-C4	2.75	118.56	115.19
54	2y	54	5MU	C5-C6-N1	-2.75	119.23	122.19
54	2w	34	CM0	C5-C4-N3	-2.74	118.90	122.66
32	1a	967	5MC	N4-C4-N3	2.74	120.90	117.03
1	1A	1964	5MC	N4-C4-N3	2.73	120.89	117.03
54	2y	34	CM0	C7-O5-C5	2.73	123.14	117.76
32	1a	527	7MG	C8-N7-C5	2.69	115.93	108.94
54	2w	37	6MZ	C4-C5-N7	-2.68	106.61	109.40
1	1A	1984	5MC	C5-C6-N1	-2.67	119.31	122.19
32	1a	1400	5MC	N4-C4-N3	2.66	120.79	117.03
54	1w	55	PSU	C5-C6-N1	-2.65	121.18	124.44
54	1w	46	7MG	C8-N7-C5	2.65	115.83	108.94
54	1y	55	PSU	C5-C1'-C2'	-2.65	110.59	115.32
1	1A	1933	PSU	C5-C1'-C2'	-2.65	110.60	115.32
1	2A	1942	5MC	C5-C6-N1	-2.64	119.34	122.19
54	2w	34	CM0	O5-C5-C4	2.64	118.43	115.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2263	OMG	C4-C5-N7	-2.63	106.66	109.40
55	2x	55	PSU	C5-C1'-C2'	-2.63	110.63	115.32
55	2x	32	5MC	N4-C4-N3	2.62	120.74	117.03
54	2y	37	6MZ	C4-C5-N7	-2.62	106.67	109.40
32	2a	1407	5MC	N4-C4-N3	2.60	120.71	117.03
56	A	2	EUP	CAN-CAE-CAF	-2.60	107.62	111.77
54	2w	46	7MG	C8-N7-C5	2.59	115.68	108.94
32	2a	967	5MC	C5-C6-N1	-2.58	119.41	122.19
32	1a	1404	5MC	N4-C4-N3	2.56	120.65	117.03
32	2a	1400	5MC	C5-C6-N1	-2.55	119.44	122.19
1	1A	1964	5MC	C5-C6-N1	-2.55	119.45	122.19
54	1y	34	CM0	C5-C4-N3	-2.54	119.17	122.66
55	1x	32	5MC	N4-C4-N3	2.54	120.62	117.03
1	2A	1962	5MC	C5-C6-N1	-2.53	119.47	122.19
32	2a	1207	2MG	CM2-N2-C2	-2.52	120.54	123.59
1	2A	2503	2MA	C4-C5-N7	-2.51	106.79	109.40
55	1x	54	5MU	C5-C6-N1	-2.50	119.50	122.19
54	2y	46	7MG	C8-N7-C5	2.50	115.44	108.94
1	1A	1984	5MC	N4-C4-N3	2.50	120.56	117.03
54	2y	34	CM0	C5-C4-N3	-2.49	119.24	122.66
1	1A	1942	4OC	N4-C4-N3	2.49	120.42	116.49
54	1y	46	7MG	C8-N7-C5	2.48	115.39	108.94
54	2y	46	7MG	C5-C4-N9	-2.46	103.00	106.44
32	1a	1400	5MC	C5-C6-N1	-2.45	119.56	122.19
54	2w	46	7MG	C5-C4-N9	-2.44	103.03	106.44
54	2w	8	4SU	C5-C4-N3	-2.43	120.57	123.83
32	1a	1207	2MG	N2-C2-N1	2.43	119.30	116.96
54	2y	46	7MG	N2-C2-N3	2.41	121.00	117.25
32	1a	966	M2G	CM2-N2-C2	-2.39	119.01	121.29
32	2a	1518	MA6	C10-N6-C9	-2.38	108.44	116.12
55	2x	32	5MC	C5-C6-N1	-2.36	119.65	122.19
32	2a	1407	5MC	C5-C6-N1	-2.36	119.66	122.19
54	1w	34	CM0	C7-O5-C5	2.35	122.40	117.76
32	1a	1407	5MC	N4-C4-N3	2.34	120.35	117.03
1	2A	2251	OMG	C4-C5-N7	-2.34	106.96	109.40
54	1w	46	7MG	C5-C4-N9	-2.34	103.17	106.44
54	2y	46	7MG	C2-N3-C4	2.31	120.28	113.89
54	1y	54	5MU	C5-C6-N1	-2.29	119.73	122.19
55	2x	32	5MC	CM5-C5-C4	-2.28	119.41	121.72
54	2w	54	5MU	C5-C6-N1	-2.27	119.74	122.19
54	1y	46	7MG	N1-C2-N3	-2.27	121.85	125.42
56	C	2	EUP	O-CAF-CAE	-2.26	118.86	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1407	5MC	C5-C6-N1	-2.20	119.83	122.19
32	2a	966	M2G	C4-C5-N7	-2.19	107.11	109.40
54	1y	46	7MG	C2-N3-C4	2.18	119.91	113.89
32	2a	1400	5MC	N4-C4-N3	2.17	120.10	117.03
32	1a	527	7MG	C2-N3-C4	2.17	119.88	113.89
32	2a	966	M2G	N3-C2-N2	2.16	119.38	117.18
54	1w	34	CM0	O3'-C3'-C2'	2.14	118.76	111.82
32	2a	516	PSU	O4'-C1'-C2'	2.14	108.13	104.66
1	2A	1915	5MU	C5-C6-N1	-2.14	119.89	122.19
54	2w	34	CM0	O3'-C3'-C2'	2.13	118.71	111.82
32	2a	1519	MA6	N1-C6-N6	2.12	119.29	117.06
32	2a	516	PSU	C5-C1'-C2'	-2.12	111.54	115.32
32	2a	1519	MA6	C10-N6-C6	-2.11	113.12	119.51
32	2a	967	5MC	N4-C4-N3	2.08	119.97	117.03
32	1a	1207	2MG	C1'-N9-C4	-2.04	123.06	126.64
32	1a	516	PSU	O4'-C1'-C2'	2.04	107.96	104.66
54	1w	46	7MG	C2-N3-C4	2.03	119.51	113.89
32	2a	527	7MG	C2-N3-C4	2.03	119.49	113.89
1	2A	2552	2MU	C5-C4-N3	-2.02	118.85	123.31
54	1y	55	PSU	O4'-C1'-C2'	2.02	107.94	104.66
1	1A	2515	2MA	C4-C5-N7	-2.02	107.30	109.40
54	1y	46	7MG	CM7-N7-C5	2.01	131.75	124.01

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	2w	34	CM0	C4-C5-O5-C7
54	1y	54	5MU	C3'-C4'-C5'-O5'
54	1y	54	5MU	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
54	2w	46	7MG	O4'-C4'-C5'-O5'
54	2w	46	7MG	C3'-C4'-C5'-O5'
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
56	C	9	IAR	C-CA-CB-CG
55	2x	32	5MC	O4'-C1'-N1-C6
32	1a	1518	MA6	C5-C6-N6-C10
1	1A	2263	OMG	C1'-C2'-O2'-CM2
32	1a	1400	5MC	O4'-C4'-C5'-O5'
54	2y	8	4SU	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
1	1A	1942	4OC	C2'-C1'-N1-C6
54	1y	8	4SU	C2'-C1'-N1-C6
54	1y	46	7MG	C4'-C5'-O5'-P
1	2A	1920	4OC	C2'-C1'-N1-C6
56	A	5	ORD	N-CA-CB-CG
56	A	5	ORD	C-CA-CB-CG
54	2y	54	5MU	C3'-C4'-C5'-O5'
54	2y	54	5MU	O4'-C4'-C5'-O5'
56	B	7	IAR	C-CA-CB-CG
32	2a	1518	MA6	C5-C6-N6-C9
1	1A	1984	5MC	O4'-C1'-N1-C6
1	1A	1984	5MC	C2'-C1'-N1-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
56	A	9	IAR	C-CA-CB-CG
56	B	3	ORD	N-CA-CB-CG
56	B	3	ORD	O-C-CA-CB
54	1w	34	CM0	C4-C5-O5-C7
54	1w	46	7MG	C3'-C4'-C5'-O5'
56	C	2	EUP	CAE-CAN-CAP-NAQ
56	C	2	EUP	OAQ-CAN-CAP-NAQ
54	2y	46	7MG	C2'-C1'-N9-C8
1	2A	1939	5MU	O4'-C1'-N1-C6
56	C	5	ORD	N-CA-CB-CG
56	C	5	ORD	C-CA-CB-CG
56	C	5	ORD	O-C-CA-CB
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C2'-C1'-N1-C6
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
56	C	9	IAR	NE-CD-CG-CB
56	A	9	IAR	NE-CD-CG-CB
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	1w	46	7MG	O4'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	2w	34	CM0	C3'-C4'-C5'-O5'
54	2w	34	CM0	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
54	1y	46	7MG	C3'-C4'-C5'-O5'
54	2y	46	7MG	C2'-C1'-N9-C4
32	2a	1518	MA6	N1-C6-N6-C9
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1207	2MG	C3'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
54	2w	34	CM0	C6-C5-O5-C7
32	1a	1518	MA6	C5-C6-N6-C9
54	2y	34	CM0	C4-C5-O5-C7
54	1w	34	CM0	C6-C5-O5-C7
56	B	7	IAR	CA-CB-CG-CD
32	2a	1207	2MG	O4'-C4'-C5'-O5'
54	1w	34	CM0	C8-C7-O5-C5
54	2y	34	CM0	C8-C7-O5-C5
32	2a	527	7MG	C4'-C5'-O5'-P
32	1a	527	7MG	O4'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C4'-C5'-O5'
54	1y	46	7MG	C2'-C1'-N9-C8
54	2y	34	CM0	C6-C5-O5-C7
54	1w	34	CM0	C3'-C4'-C5'-O5'
54	1w	34	CM0	O4'-C4'-C5'-O5'
54	2w	34	CM0	C8-C7-O5-C5
54	2y	37	6MZ	C4'-C5'-O5'-P
32	2a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	C4'-C5'-O5'-P
1	1A	2515	2MA	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
56	A	9	IAR	CG-CD-NE-CZ
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
56	B	3	ORD	C-CA-CB-CG
54	1y	46	7MG	O4'-C1'-N9-C8
56	B	3	ORD	CA-CB-CG-CD
1	1A	2515	2MA	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
54	2y	34	CM0	O4'-C4'-C5'-O5'
56	A	2	EUP	CAN-CAE-CAF-O
56	C	2	EUP	CAN-CAE-CAF-O
32	1a	527	7MG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2842 ligands modelled in this entry, 2840 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	$\# Z > 2$
60	SF4	1d	501	35	0,12,12	0.00	-	-		
60	SF4	2d	501	35	0,12,12	0.00	-	-		

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
60	SF4	1d	501	35	-	-	0/6/5/5
60	SF4	2d	501	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.54	55 (1%) 66 62	21, 37, 96, 109	0
1	2A	2789/2915 (95%)	0.34	52 (1%) 66 62	35, 60, 95, 109	0
2	1B	120/121 (99%)	0.07	0 100 100	31, 51, 63, 88	0
2	2B	120/121 (99%)	-0.12	0 100 100	66, 83, 90, 101	0
3	1D	275/276 (99%)	0.65	6 (2%) 62 56	23, 38, 54, 83	0
3	2D	275/276 (99%)	0.74	8 (2%) 51 45	32, 52, 66, 85	0
4	1E	204/206 (99%)	0.61	0 100 100	20, 41, 62, 80	0
4	2E	204/206 (99%)	0.52	3 (1%) 73 70	36, 61, 75, 89	0
5	1F	203/210 (96%)	0.40	1 (0%) 91 89	21, 43, 70, 85	0
5	2F	203/210 (96%)	0.51	6 (2%) 50 43	37, 72, 84, 89	0
6	1G	181/182 (99%)	0.25	1 (0%) 89 88	42, 64, 78, 88	0
6	2G	181/182 (99%)	1.08	35 (19%) 1 0	77, 86, 93, 98	0
7	1H	174/180 (96%)	0.36	1 (0%) 89 88	39, 56, 69, 79	0
7	2H	174/180 (96%)	0.96	28 (16%) 1 1	72, 85, 93, 97	0
8	1I	146/148 (98%)	0.20	0 100 100	43, 75, 85, 88	0
8	2I	146/148 (98%)	0.40	5 (3%) 45 38	56, 77, 87, 94	0
9	1N	140/140 (100%)	0.46	2 (1%) 75 71	28, 38, 65, 79	0
9	2N	140/140 (100%)	0.67	11 (7%) 12 9	50, 67, 81, 87	0
10	1O	122/122 (100%)	0.59	0 100 100	30, 42, 58, 66	0
10	2O	122/122 (100%)	0.73	2 (1%) 72 68	45, 60, 72, 78	0
11	1P	149/150 (99%)	0.46	1 (0%) 87 86	21, 48, 69, 80	0
11	2P	149/150 (99%)	0.72	14 (9%) 8 5	40, 71, 86, 91	0
12	1Q	141/141 (100%)	0.51	3 (2%) 63 58	27, 43, 59, 79	0
12	2Q	141/141 (100%)	0.94	16 (11%) 5 3	48, 71, 81, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.60	0 100 100	26, 35, 52, 62	0
13	2R	118/118 (100%)	0.58	1 (0%) 86 84	42, 56, 67, 75	0
14	1S	110/112 (98%)	0.30	0 100 100	39, 51, 65, 68	0
14	2S	110/112 (98%)	0.57	11 (10%) 7 4	67, 78, 85, 91	0
15	1T	131/146 (89%)	0.44	0 100 100	34, 45, 73, 83	0
15	2T	131/146 (89%)	0.45	1 (0%) 86 84	52, 63, 80, 85	0
16	1U	116/118 (98%)	0.61	2 (1%) 70 66	22, 31, 46, 69	0
16	2U	116/118 (98%)	0.78	4 (3%) 45 38	48, 65, 80, 88	0
17	1V	101/101 (100%)	0.34	1 (0%) 82 80	22, 41, 57, 71	0
17	2V	101/101 (100%)	0.51	4 (3%) 38 31	47, 76, 84, 88	0
18	1W	112/113 (99%)	0.54	0 100 100	24, 33, 55, 82	0
18	2W	112/113 (99%)	0.69	2 (1%) 68 64	43, 53, 71, 88	0
19	1X	95/96 (98%)	0.64	0 100 100	28, 40, 58, 77	0
19	2X	95/96 (98%)	0.57	3 (3%) 47 40	45, 63, 79, 87	0
20	1Y	107/110 (97%)	0.37	0 100 100	37, 52, 72, 81	0
20	2Y	107/110 (97%)	1.04	16 (14%) 2 1	64, 75, 84, 90	0
21	1Z	154/206 (74%)	0.54	8 (5%) 27 21	41, 67, 93, 100	0
21	2Z	160/206 (77%)	1.12	27 (16%) 1 1	70, 87, 98, 101	0
22	10	83/85 (97%)	0.90	7 (8%) 11 7	30, 40, 63, 78	0
22	20	83/85 (97%)	1.36	14 (16%) 1 1	45, 69, 82, 85	0
23	11	97/98 (98%)	0.64	4 (4%) 37 30	28, 47, 73, 77	0
23	21	97/98 (98%)	0.73	7 (7%) 15 11	40, 57, 78, 84	0
24	12	70/72 (97%)	0.52	2 (2%) 51 45	36, 51, 62, 78	0
24	22	70/72 (97%)	0.41	3 (4%) 35 28	62, 74, 81, 84	0
25	13	59/60 (98%)	0.47	1 (1%) 70 66	28, 37, 65, 85	0
25	23	59/60 (98%)	0.96	8 (13%) 3 1	55, 69, 83, 92	0
26	14	69/71 (97%)	0.23	4 (5%) 23 17	59, 78, 94, 98	0
26	24	69/71 (97%)	1.09	15 (21%) 0 0	80, 91, 97, 98	0
27	15	59/60 (98%)	0.58	1 (1%) 70 66	21, 32, 53, 63	0
27	25	59/60 (98%)	0.52	1 (1%) 70 66	38, 52, 72, 79	0
28	16	53/54 (98%)	0.52	0 100 100	35, 44, 61, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.72	4 (7%) 14 10	55, 63, 74, 77	0
29	17	48/49 (97%)	0.95	4 (8%) 11 8	23, 29, 55, 67	0
29	27	48/49 (97%)	1.25	8 (16%) 1 1	34, 42, 67, 76	0
30	18	64/65 (98%)	0.56	0 100 100	29, 35, 43, 58	0
30	28	64/65 (98%)	0.93	5 (7%) 13 9	51, 59, 66, 71	0
31	19	37/37 (100%)	0.67	0 100 100	31, 42, 60, 62	0
31	29	37/37 (100%)	1.43	9 (24%) 0 0	62, 70, 82, 86	0
32	1a	1488/1521 (97%)	0.21	30 (2%) 65 60	36, 69, 95, 107	0
32	2a	1491/1521 (98%)	0.28	45 (3%) 50 43	50, 80, 99, 109	0
33	1b	231/256 (90%)	0.36	11 (4%) 30 24	66, 82, 93, 98	0
33	2b	231/256 (90%)	1.52	78 (33%) 0 0	76, 90, 96, 101	0
34	1c	206/239 (86%)	0.39	3 (1%) 73 70	64, 76, 85, 91	0
34	2c	206/239 (86%)	1.48	67 (32%) 0 0	79, 89, 94, 98	0
35	1d	208/209 (99%)	0.76	22 (10%) 6 4	59, 74, 85, 90	0
35	2d	208/209 (99%)	0.62	14 (6%) 17 13	63, 74, 83, 91	0
36	1e	148/162 (91%)	0.61	5 (3%) 45 38	51, 66, 77, 84	0
36	2e	148/162 (91%)	0.99	24 (16%) 1 1	72, 80, 88, 95	0
37	1f	100/101 (99%)	0.25	1 (1%) 82 80	57, 70, 79, 82	0
37	2f	100/101 (99%)	0.18	0 100 100	64, 74, 84, 87	0
38	1g	155/156 (99%)	0.44	12 (7%) 13 10	64, 74, 87, 95	0
38	2g	155/156 (99%)	0.91	26 (16%) 1 1	75, 83, 91, 95	0
39	1h	137/138 (99%)	0.38	3 (2%) 62 56	58, 69, 76, 80	0
39	2h	137/138 (99%)	0.69	11 (8%) 12 9	70, 80, 86, 88	0
40	1i	127/128 (99%)	0.60	14 (11%) 5 3	58, 80, 89, 93	0
40	2i	127/128 (99%)	1.79	53 (41%) 0 0	78, 88, 94, 97	0
41	1j	97/105 (92%)	0.71	8 (8%) 11 8	60, 79, 91, 94	0
41	2j	96/105 (91%)	1.80	39 (40%) 0 0	81, 90, 97, 98	0
42	1k	114/129 (88%)	0.64	3 (2%) 56 50	43, 69, 79, 84	0
42	2k	114/129 (88%)	0.65	7 (6%) 21 16	58, 77, 85, 87	0
43	1l	121/132 (91%)	0.58	9 (7%) 14 10	50, 58, 71, 80	0
43	2l	121/132 (91%)	0.96	16 (13%) 3 2	62, 72, 79, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.46	10 (8%) 12 8	62, 75, 86, 94	0
44	2m	122/126 (96%)	1.88	42 (34%) 0 0	78, 88, 96, 102	0
45	1n	60/61 (98%)	1.04	9 (15%) 2 1	62, 72, 79, 81	0
45	2n	60/61 (98%)	2.78	35 (58%) 0 0	81, 89, 94, 97	0
46	1o	88/89 (98%)	0.49	4 (4%) 33 26	50, 67, 78, 83	0
46	2o	88/89 (98%)	0.63	7 (7%) 12 9	66, 76, 86, 91	0
47	1p	82/88 (93%)	1.05	13 (15%) 1 1	59, 74, 84, 86	0
47	2p	82/88 (93%)	0.69	4 (4%) 29 23	61, 71, 80, 83	0
48	1q	99/105 (94%)	0.59	2 (2%) 65 60	57, 70, 79, 84	0
48	2q	99/105 (94%)	0.94	12 (12%) 4 2	66, 76, 85, 86	0
49	1r	68/88 (77%)	0.43	3 (4%) 34 27	61, 70, 80, 86	0
49	2r	68/88 (77%)	0.31	0 100 100	69, 76, 85, 89	0
50	1s	83/93 (89%)	0.18	2 (2%) 59 53	66, 76, 86, 90	0
50	2s	83/93 (89%)	1.90	35 (42%) 0 0	83, 91, 97, 99	0
51	1t	96/106 (90%)	0.79	9 (9%) 8 5	62, 73, 84, 89	0
51	2t	96/106 (90%)	0.59	4 (4%) 36 29	60, 73, 86, 89	0
52	1u	23/27 (85%)	1.23	6 (26%) 0 0	65, 69, 77, 80	0
52	2u	23/27 (85%)	3.12	15 (65%) 0 0	78, 86, 90, 91	0
53	1v	13/27 (48%)	1.76	5 (38%) 0 0	48, 67, 93, 102	0
53	2v	13/27 (48%)	2.41	7 (53%) 0 0	70, 91, 102, 110	0
54	1w	67/76 (88%)	2.56	36 (53%) 0 0	55, 96, 103, 106	0
54	1y	68/76 (89%)	1.56	23 (33%) 0 0	40, 98, 103, 108	0
54	2w	67/76 (88%)	2.57	38 (56%) 0 0	73, 100, 104, 108	0
54	2y	67/76 (88%)	2.38	43 (64%) 0 0	58, 101, 105, 106	0
55	1x	72/77 (93%)	0.22	0 100 100	36, 71, 85, 93	0
55	2x	72/77 (93%)	0.28	3 (4%) 36 29	56, 85, 94, 98	0
56	A	6/9 (66%)	1.47	1 (16%) 1 1	70, 73, 78, 79	0
56	B	5/9 (55%)	3.16	4 (80%) 0 0	70, 75, 79, 79	0
56	C	6/9 (66%)	6.79	6 (100%) 0 0	90, 91, 95, 97	0
All	All	20896/21781 (95%)	0.59	1306 (6%) 20 15	20, 67, 94, 110	0

All (1306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	27.0
44	2m	123	ALA	16.2
56	C	1	LYS	14.8
44	1m	124	PRO	13.9
44	1m	123	ALA	10.8
31	29	37	GLY	9.9
45	2n	34	TYR	9.8
44	2m	122	LYS	9.1
54	2w	71	C	9.0
56	C	4	GLY	8.9
33	2b	165	VAL	8.7
54	1w	56	C	8.4
38	1g	80	VAL	8.3
22	20	7	LEU	8.3
34	2c	124	ILE	8.2
54	1w	70	C	8.0
54	2w	56	C	8.0
44	2m	102	ARG	8.0
22	20	2	ALA	7.6
22	10	7	LEU	7.6
34	2c	155	GLY	7.4
21	2Z	170	THR	7.3
54	1y	20	G	7.2
41	2j	55	LYS	7.2
54	1w	71	C	7.2
21	2Z	149	SER	7.1
23	21	2	SER	7.1
41	2j	47	PHE	7.0
38	2g	80	VAL	7.0
40	2i	102	LEU	7.0
22	10	6	GLY	7.0
40	2i	7	THR	6.9
54	2y	35	A	6.8
26	24	49	PHE	6.8
44	2m	5	ALA	6.8
52	2u	14	TRP	6.7
38	2g	79	ARG	6.6
41	2j	65	LEU	6.5
34	2c	160	ALA	6.5
45	2n	25	VAL	6.4
38	1g	79	ARG	6.4
41	2j	59	SER	6.4
54	2y	36	C	6.3

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Mol	Chain	Res	Type	RSRZ
54	2w	76	A	6.3
44	2m	60	VAL	6.3
38	2g	4	ARG	6.3
52	2u	15	ARG	6.2
54	2w	4	U	6.2
34	2c	196	LEU	6.2
33	2b	122	PHE	6.2
26	24	63	TYR	6.1
56	C	8	LYS	6.1
40	2i	125	TYR	6.0
45	2n	39	LEU	6.0
20	2Y	1	MET	5.9
33	2b	123	ALA	5.9
32	2a	1030(B)	C	5.9
12	2Q	22	LYS	5.9
33	2b	101	MET	5.8
32	2a	1034	G	5.8
50	2s	41	VAL	5.8
21	2Z	144	LEU	5.8
45	2n	42	ILE	5.8
45	2n	35	ARG	5.8
38	2g	82	GLY	5.7
52	2u	6	ARG	5.6
32	1a	1257	U	5.6
54	2w	72	C	5.6
52	2u	16	GLY	5.6
44	2m	121	LYS	5.6
34	2c	206	GLU	5.6
54	1w	69	A	5.5
50	2s	82	GLY	5.5
1	2A	2155	G	5.4
54	1y	36	C	5.4
44	2m	90	LEU	5.4
38	2g	81	GLY	5.4
29	27	48	LYS	5.3
45	2n	29	ARG	5.3
54	1w	3	G	5.3
44	2m	6	GLY	5.3
45	2n	55	GLY	5.3
1	1A	2163	G	5.3
54	2w	3	G	5.2
41	2j	66	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
54	1w	72	C	5.2
34	2c	157	ILE	5.2
45	2n	4	LYS	5.2
42	2k	25	TYR	5.2
29	17	47	ARG	5.2
53	2v	12	A	5.2
1	2A	2112	G	5.2
22	10	3	HIS	5.1
21	2Z	145	GLU	5.1
21	2Z	171	ILE	5.1
34	2c	189	ALA	5.1
45	2n	51	GLY	5.1
53	2v	13	A	5.0
6	2G	19	LEU	5.0
54	2w	31	C	5.0
41	2j	62	HIS	5.0
54	2w	70	C	5.0
22	20	4	LYS	5.0
1	1A	1142	A	5.0
1	2A	2146	C	5.0
22	20	6	GLY	5.0
50	2s	79	THR	5.0
54	2w	1	G	5.0
44	2m	87	TYR	4.9
52	2u	24	ARG	4.9
9	2N	8	GLN	4.9
40	2i	109	VAL	4.9
54	2w	13	C	4.9
6	2G	28	VAL	4.9
45	2n	50	LYS	4.9
50	2s	52	TYR	4.8
33	2b	187	LEU	4.8
53	2v	24	C	4.8
45	1n	2	ALA	4.8
22	20	3	HIS	4.8
26	24	58	ARG	4.8
38	1g	85	TYR	4.8
50	2s	40	ILE	4.8
40	2i	10	ARG	4.8
6	2G	3	LEU	4.7
40	2i	9	ARG	4.7
44	2m	65	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
54	2w	2	G	4.7
50	2s	80	TYR	4.7
54	1w	4	U	4.7
44	2m	88	ARG	4.7
40	2i	127	LYS	4.7
44	2m	4	ILE	4.7
54	2y	18	G	4.7
40	2i	124	GLN	4.7
54	2y	66	A	4.7
12	2Q	6	ARG	4.6
45	2n	58	LYS	4.6
32	1a	1531	A	4.6
1	2A	2115	G	4.6
21	1Z	149	SER	4.6
41	2j	38	ILE	4.6
26	14	55	ARG	4.6
34	2c	197	GLY	4.6
45	2n	41	ARG	4.6
33	2b	70	PHE	4.6
40	2i	36	TYR	4.6
25	23	60	GLU	4.6
20	2Y	106	LEU	4.5
50	2s	15	LEU	4.5
33	2b	152	PHE	4.5
54	2w	32	C	4.5
6	2G	2	PRO	4.5
54	1w	13	C	4.5
45	2n	6	LEU	4.5
26	24	56	VAL	4.5
32	2a	1532	U	4.5
41	2j	85	LEU	4.5
54	1w	5	G	4.5
54	2y	22	G	4.5
45	2n	46	GLU	4.4
54	2y	64	U	4.4
1	2A	652(U)	G	4.4
54	1w	49	G	4.4
40	2i	106	ALA	4.4
34	2c	190	ARG	4.4
53	2v	14	A	4.4
6	2G	140	ILE	4.4
1	2A	2111	C	4.4

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Mol	Chain	Res	Type	RSRZ
32	1a	1002	G	4.4
41	2j	54	PHE	4.4
1	1A	1106	U	4.3
33	2b	214	ILE	4.3
32	2a	1220	G	4.3
50	2s	70	LYS	4.3
27	15	60	VAL	4.3
54	1w	15	G	4.3
1	1A	1103	A	4.3
54	1w	67	U	4.3
38	1g	84	ASN	4.3
40	2i	110	GLU	4.3
40	1i	106	ALA	4.3
33	2b	97	TRP	4.3
33	2b	118	LEU	4.3
54	2y	65	C	4.3
43	2l	18	VAL	4.3
33	2b	81	VAL	4.3
33	2b	232	PRO	4.3
47	1p	19	ILE	4.3
1	2A	2125	G	4.2
1	2A	2145	C	4.2
35	1d	3	ARG	4.2
33	2b	185	ILE	4.2
1	2A	2138	C	4.2
41	2j	48	THR	4.2
1	1A	1140	U	4.2
32	1a	1026	G	4.2
54	1w	76	A	4.2
29	27	1	MET	4.2
32	2a	1035	A	4.2
54	2y	61	C	4.2
32	2a	1033	G	4.2
21	2Z	150	LEU	4.2
1	2A	2119	A	4.2
54	2y	5	G	4.1
1	2A	2113	U	4.1
44	2m	103	THR	4.1
53	1v	13	A	4.1
54	2w	19	G	4.1
54	2y	57	G	4.1
7	2H	35	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
38	2g	78	ARG	4.1
53	1v	24	C	4.1
34	2c	65	ALA	4.1
38	1g	83	ALA	4.1
38	2g	156	TRP	4.1
21	2Z	148	ASP	4.1
14	2S	32	LEU	4.1
33	2b	197	VAL	4.1
8	2I	85	GLU	4.1
32	1a	1003	G	4.1
32	2a	1030(A)	G	4.1
22	10	2	ALA	4.1
21	1Z	119	GLU	4.0
6	2G	152	LEU	4.0
32	2a	1257	U	4.0
45	2n	38	GLY	4.0
45	2n	37	PHE	4.0
51	1t	22	ARG	4.0
34	2c	193	TYR	4.0
22	10	5	LYS	4.0
36	2e	12	LEU	4.0
1	2A	2117	A	4.0
52	2u	22	ARG	4.0
1	2A	2133	G	4.0
54	2y	48	C	4.0
7	2H	48	GLY	4.0
1	2A	2114	A	4.0
21	2Z	125	LEU	4.0
9	2N	9	VAL	4.0
40	2i	15	ALA	4.0
3	2D	276	LYS	4.0
29	27	45	ALA	4.0
47	1p	49	LEU	3.9
52	2u	17	THR	3.9
1	1A	942	A	3.9
1	1A	1139	G	3.9
52	2u	2	GLY	3.9
34	2c	8	ILE	3.9
1	1A	2167	C	3.9
40	2i	126	SER	3.9
44	2m	78	ILE	3.9
50	2s	62	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
5	2F	166	ALA	3.9
11	2P	79	ARG	3.9
44	2m	119	GLY	3.9
32	2a	1286	A	3.9
41	2j	40	LEU	3.9
54	2w	69	A	3.9
39	2h	2	LEU	3.9
52	2u	13	ILE	3.9
40	2i	79	LEU	3.9
34	2c	199	LYS	3.9
54	2y	33	U	3.9
33	2b	201	ILE	3.8
36	2e	45	PHE	3.8
44	2m	94	ARG	3.8
32	2a	1001(A)	G	3.8
35	2d	164	ALA	3.8
54	1w	10	G	3.8
33	2b	34	ALA	3.8
34	2c	185	GLY	3.8
54	1y	24	G	3.8
1	2A	2139	C	3.8
47	1p	6	LEU	3.8
50	2s	69	HIS	3.8
45	2n	57	ARG	3.8
1	1A	1104	G	3.8
39	2h	134	ILE	3.8
41	2j	10	GLY	3.8
41	2j	96	ILE	3.8
21	2Z	139	VAL	3.8
52	2u	10	ARG	3.7
1	2A	2156	G	3.7
3	1D	276	LYS	3.7
34	2c	191	THR	3.7
38	2g	84	ASN	3.7
33	2b	105	PHE	3.7
52	2u	5	ASP	3.7
38	2g	32	ARG	3.7
41	2j	60	ARG	3.7
44	2m	120	LYS	3.7
6	2G	29	TRP	3.7
33	2b	92	TYR	3.7
38	2g	85	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
33	2b	37	ASN	3.7
32	1a	1036	G	3.7
40	2i	105	ASP	3.7
56	C	3	ALA	3.7
21	1Z	168	GLU	3.7
54	1w	14	A	3.7
54	1w	66	A	3.7
54	2y	53	G	3.7
10	2O	1	MET	3.7
56	C	7	HIS	3.7
56	B	1	ALA	3.7
21	2Z	141	VAL	3.7
54	1w	25	C	3.7
1	1A	1114	G	3.7
34	2c	188	LEU	3.6
40	2i	66	ARG	3.6
45	2n	10	ALA	3.6
32	1a	1532	U	3.6
33	2b	163	PHE	3.6
54	2w	6	A	3.6
39	2h	99	GLU	3.6
32	1a	1027	C	3.6
54	1w	61	C	3.6
35	1d	5	ILE	3.6
11	2P	45	LEU	3.6
33	2b	144	ARG	3.6
40	2i	53	VAL	3.6
32	1a	1035	A	3.6
42	1k	25	TYR	3.6
41	2j	71	LEU	3.6
22	20	8	GLY	3.6
32	2a	1036	G	3.6
56	B	5	HIS	3.6
41	2j	29	ARG	3.6
48	2q	100	LYS	3.6
7	2H	36	PRO	3.6
33	2b	164	VAL	3.6
56	C	6	PRO	3.6
54	1w	68	C	3.6
44	2m	23	TYR	3.6
34	2c	158	GLY	3.6
38	2g	86	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
40	1i	126	SER	3.6
33	2b	69	LEU	3.6
50	2s	71	LEU	3.6
20	2Y	5	MET	3.5
40	2i	117	HIS	3.5
7	2H	107	VAL	3.5
1	2A	2116	G	3.5
54	1w	2	G	3.5
54	1y	5	G	3.5
34	2c	5	ILE	3.5
41	2j	49	VAL	3.5
40	2i	83	ARG	3.5
33	2b	33	TYR	3.5
1	1A	1221	G	3.5
47	2p	19	ILE	3.5
1	1A	1133	G	3.5
32	2a	1002	G	3.5
1	2A	888	C	3.5
34	2c	159	GLY	3.5
6	2G	52	ILE	3.5
22	20	5	LYS	3.5
54	2y	47	U	3.5
6	2G	62	LEU	3.5
56	B	4	PRO	3.5
1	2A	2802	G	3.5
54	2w	5	G	3.5
54	2y	39	G	3.5
25	23	26	LEU	3.5
41	2j	63	PHE	3.5
1	1A	1138	C	3.5
54	1w	47	U	3.5
40	2i	112	LYS	3.5
34	2c	200	ALA	3.5
14	2S	35	ILE	3.5
41	2j	74	ILE	3.5
33	2b	177	ALA	3.4
26	24	40	HIS	3.4
38	2g	149	ARG	3.4
20	2Y	45	VAL	3.4
41	2j	6	ILE	3.4
34	2c	4	LYS	3.4
47	1p	1	MET	3.4

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Mol	Chain	Res	Type	RSRZ
54	1y	47	U	3.4
40	2i	28	VAL	3.4
34	2c	57	ILE	3.4
54	2w	73	A	3.4
30	28	29	LYS	3.4
32	1a	1001(A)	G	3.4
50	2s	30	LEU	3.4
43	2l	32	PHE	3.4
1	2A	652(B)	A	3.4
52	1u	6	ARG	3.4
54	1w	73	A	3.4
45	2n	59	ALA	3.4
54	1w	19	G	3.4
38	2g	42	ILE	3.4
34	2c	127	ARG	3.4
50	2s	43	GLU	3.4
1	1A	2162	C	3.4
54	2y	56	C	3.4
21	2Z	155	LEU	3.4
32	1a	1033	G	3.4
50	2s	35	SER	3.4
6	2G	73	ALA	3.4
45	2n	2	ALA	3.4
40	2i	128	ARG	3.4
54	1y	39	G	3.3
32	1a	204	U	3.3
45	2n	13	THR	3.3
54	2y	23	A	3.3
35	2d	179	GLU	3.3
22	20	9	SER	3.3
26	24	51	ASP	3.3
33	2b	143	GLU	3.3
40	2i	82	ALA	3.3
9	2N	116	LEU	3.3
45	2n	44	LEU	3.3
20	2Y	24	VAL	3.3
44	2m	92	HIS	3.3
54	2y	62	C	3.3
45	2n	53	LEU	3.3
5	2F	89	VAL	3.3
1	2A	2147	G	3.3
38	2g	16	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
40	1i	19	LEU	3.3
1	1A	1141	A	3.3
40	2i	14	VAL	3.3
52	2u	23	PRO	3.3
7	2H	115	VAL	3.3
44	2m	104	ARG	3.3
54	2y	38	A	3.2
14	2S	3	ARG	3.2
19	2X	92	LEU	3.2
48	2q	98	LEU	3.2
54	2w	75	C	3.2
54	1w	7	U	3.2
25	23	53	LEU	3.2
1	1A	2135	U	3.2
16	1U	117	GLN	3.2
32	2a	1149	C	3.2
38	2g	7	ALA	3.2
55	2x	47	U	3.2
33	2b	131	PRO	3.2
34	2c	198	VAL	3.2
41	2j	67	THR	3.2
1	2A	896	A	3.2
11	2P	75	ILE	3.2
1	1A	1143	U	3.2
1	2A	883	G	3.2
12	2Q	104	PHE	3.2
29	17	46	VAL	3.2
40	1i	14	VAL	3.2
1	2A	2170	A	3.2
40	2i	123	PRO	3.2
1	1A	2154	U	3.2
54	2w	47	U	3.2
3	2D	273	ARG	3.2
29	27	23	ARG	3.2
34	2c	131	ARG	3.2
44	2m	80	ARG	3.2
44	2m	7	VAL	3.2
34	1c	124	ILE	3.2
36	2e	81	GLU	3.2
56	A	8	LYS	3.2
53	2v	23	U	3.2
45	2n	36	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2127	G	3.2
54	2w	10	G	3.2
38	2g	152	ALA	3.2
43	2l	64	TYR	3.2
22	10	4	LYS	3.2
41	1j	5	ARG	3.2
8	2I	41	GLU	3.1
53	1v	14	A	3.1
6	2G	159	VAL	3.1
34	2c	153	VAL	3.1
54	1w	62	C	3.1
33	2b	31	TYR	3.1
54	2y	52	G	3.1
33	1b	133	LYS	3.1
56	B	6	LYS	3.1
54	2y	21	A	3.1
35	1d	4	TYR	3.1
40	2i	119	ALA	3.1
34	2c	53	ALA	3.1
41	2j	50	ILE	3.1
7	2H	157	TYR	3.1
40	2i	49	PRO	3.1
44	1m	87	TYR	3.1
22	20	69	PHE	3.1
20	2Y	73	ARG	3.1
25	23	59	VAL	3.1
35	2d	49	ARG	3.1
1	1A	1105	G	3.1
22	10	8	GLY	3.1
54	2y	63	G	3.1
12	2Q	63	LYS	3.1
44	1m	121	LYS	3.1
45	1n	7	ILE	3.1
50	1s	12	ASP	3.1
1	2A	1847	A	3.1
36	2e	24	ARG	3.1
40	2i	107	ARG	3.1
9	2N	84	LYS	3.1
23	11	98	LEU	3.1
1	1A	2137	G	3.1
33	2b	26	PRO	3.1
48	2q	95	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
14	2S	20	ARG	3.1
41	2j	51	ARG	3.1
46	2o	68	ARG	3.1
33	2b	48	MET	3.1
54	1y	38	A	3.1
54	2y	13	C	3.1
34	2c	143	GLU	3.1
32	1a	1034	G	3.1
1	1A	932	C	3.1
1	1A	271	U	3.0
1	2A	2132	U	3.0
6	2G	161	THR	3.0
21	2Z	154	ASP	3.0
33	2b	188	ALA	3.0
40	2i	17	VAL	3.0
43	2l	55	VAL	3.0
32	2a	1202	G	3.0
38	1g	82	GLY	3.0
34	2c	6	HIS	3.0
33	2b	94	ASN	3.0
34	2c	120	VAL	3.0
50	2s	36	ARG	3.0
6	2G	146	TYR	3.0
32	1a	1030(C)	G	3.0
41	2j	56	HIS	3.0
40	1i	125	TYR	3.0
1	1A	2160	C	3.0
1	2A	2803	C	3.0
15	2T	108	ARG	3.0
40	2i	93	ARG	3.0
54	1y	56	C	3.0
33	2b	90	MET	3.0
36	2e	90	VAL	3.0
6	2G	135	LEU	3.0
36	2e	86	ALA	3.0
52	1u	16	GLY	3.0
33	2b	19	HIS	3.0
50	2s	14	HIS	3.0
33	2b	114	ARG	3.0
1	2A	2168	G	3.0
50	2s	12	ASP	3.0
54	1w	50	G	3.0

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Mol	Chain	Res	Type	RSRZ
29	17	48	LYS	3.0
1	2A	229	A	3.0
54	2w	67	U	3.0
21	1Z	170	THR	3.0
44	2m	66	LEU	3.0
54	1w	18	G	3.0
1	1A	1124	U	3.0
1	1A	1116	A	3.0
40	2i	5	TYR	3.0
12	2Q	5	ARG	3.0
1	1A	2134	G	2.9
54	1y	33	U	2.9
54	2y	45	G	2.9
7	2H	123	PHE	2.9
32	2a	1363(A)	A	2.9
32	2a	1531	A	2.9
34	2c	44	GLU	2.9
43	1l	64	TYR	2.9
31	29	1	MET	2.9
25	23	29	ARG	2.9
50	2s	49	ILE	2.9
1	1A	1110	C	2.9
21	1Z	169	GLU	2.9
54	2y	2	G	2.9
35	1d	73	ARG	2.9
35	2d	115	ARG	2.9
32	1a	1503	A	2.9
53	1v	12	A	2.9
34	2c	182	ILE	2.9
51	2t	41	ILE	2.9
35	1d	180	GLY	2.9
1	1A	1145	G	2.9
44	2m	97	PRO	2.9
54	2w	45	G	2.9
9	2N	10	GLU	2.9
42	2k	117	ASN	2.9
26	24	42	PHE	2.9
41	1j	45	ARG	2.9
44	2m	100	GLY	2.9
32	2a	1150	U	2.9
26	24	50	VAL	2.9
38	2g	154	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
40	2i	45	ALA	2.9
21	2Z	137	ILE	2.9
40	2i	121	ARG	2.9
54	2w	24	G	2.9
54	2y	1	G	2.9
1	2A	2173	A	2.9
34	2c	13	GLY	2.9
43	2l	60	LEU	2.9
1	2A	2109	U	2.9
41	2j	72	VAL	2.9
54	1w	12	U	2.9
45	2n	11	LYS	2.9
21	1Z	120	ILE	2.9
38	1g	86	GLN	2.9
36	2e	31	LEU	2.9
1	1A	2164	C	2.9
26	14	54	GLY	2.9
33	2b	227	GLY	2.9
12	2Q	34	LEU	2.9
29	27	47	ARG	2.9
48	2q	92	ARG	2.9
34	2c	184	TYR	2.9
54	1y	35	A	2.8
55	2x	76	A	2.8
1	2A	1026	U	2.8
36	2e	27	ARG	2.8
41	2j	58	ASP	2.8
17	2V	72	VAL	2.8
21	2Z	96	VAL	2.8
33	2b	93	VAL	2.8
33	2b	139	LYS	2.8
32	2a	1001	A	2.8
50	1s	71	LEU	2.8
44	2m	101	GLN	2.8
50	2s	77	THR	2.8
48	2q	9	VAL	2.8
40	1i	114	TYR	2.8
50	2s	83	HIS	2.8
1	1A	1112	U	2.8
1	2A	2118	U	2.8
32	2a	1026	G	2.8
54	1w	1	G	2.8

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Mol	Chain	Res	Type	RSRZ
41	2j	61	GLU	2.8
1	1A	933	C	2.8
6	2G	134	GLY	2.8
36	2e	10	MET	2.8
52	2u	21	TYR	2.8
33	2b	111	ARG	2.8
43	2l	46	LYS	2.8
1	1A	1111	U	2.8
33	2b	71	VAL	2.8
36	1e	82	VAL	2.8
54	2y	3	G	2.8
32	2a	1027	C	2.8
42	2k	126	ARG	2.8
50	2s	56	GLN	2.8
22	20	45	PHE	2.8
40	2i	8	GLY	2.8
38	1g	32	ARG	2.8
6	2G	25	TYR	2.8
34	2c	37	GLN	2.8
38	1g	154	TYR	2.8
52	1u	14	TRP	2.8
32	1a	1029	C	2.8
32	1a	1030(B)	C	2.8
12	2Q	37	LEU	2.8
6	2G	165	THR	2.8
26	24	54	GLY	2.8
7	2H	102	ALA	2.8
11	2P	15	ARG	2.8
55	2x	20	U	2.8
36	2e	8	GLU	2.8
45	2n	60	SER	2.8
21	2Z	140	ASP	2.8
32	2a	1221	G	2.8
34	2c	134	ILE	2.8
54	2w	23	A	2.8
54	2y	51	C	2.8
54	2y	70	C	2.8
51	2t	22	ARG	2.8
26	24	67	TYR	2.7
21	2Z	76	LEU	2.7
1	1A	2174	G	2.7
1	2A	2160	G	2.7

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Mol	Chain	Res	Type	RSRZ
45	2n	22	THR	2.7
38	2g	83	ALA	2.7
45	2n	54	PRO	2.7
46	2o	60	VAL	2.7
9	2N	83	LYS	2.7
14	2S	57	LYS	2.7
41	2j	89	ASP	2.7
33	2b	21	ARG	2.7
7	2H	43	VAL	2.7
9	2N	140	VAL	2.7
32	1a	1028	C	2.7
6	2G	34	LEU	2.7
6	2G	95	ARG	2.7
33	2b	66	GLY	2.7
35	1d	2	GLY	2.7
7	2H	105	LEU	2.7
44	2m	91	ARG	2.7
40	2i	114	TYR	2.7
36	2e	109	ILE	2.7
40	2i	63	ILE	2.7
7	2H	106	THR	2.7
28	26	5	VAL	2.7
35	1d	105	VAL	2.7
50	2s	4	SER	2.7
34	2c	21	ARG	2.7
41	2j	64	GLU	2.7
52	2u	9	ARG	2.7
1	1A	1123	A	2.7
1	2A	2161	C	2.7
54	1y	32	C	2.7
9	2N	112	LEU	2.7
35	1d	135	LEU	2.7
34	2c	152	ILE	2.7
51	1t	68	LYS	2.7
7	2H	37	VAL	2.7
36	2e	19	MET	2.7
47	2p	9	PHE	2.7
32	1a	1001	A	2.7
32	2a	1357	A	2.7
35	1d	138	TYR	2.7
33	2b	162	ILE	2.7
54	2y	12	U	2.7

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Mol	Chain	Res	Type	RSRZ
1	1A	2153	G	2.7
54	2w	50	G	2.7
5	2F	161	GLU	2.7
38	2g	77	SER	2.7
41	2j	46	ARG	2.7
26	14	45	GLY	2.7
21	2Z	146	ILE	2.7
1	1A	1127	U	2.7
7	2H	2	SER	2.7
31	29	12	ASP	2.7
1	2A	2159	G	2.7
50	2s	67	VAL	2.7
22	20	55	ARG	2.7
3	2D	5	LYS	2.7
20	2Y	19	LYS	2.7
35	1d	70	ILE	2.7
16	2U	2	PRO	2.6
26	24	45	GLY	2.6
43	2l	101	VAL	2.6
50	2s	66	MET	2.6
25	23	23	LEU	2.6
33	2b	221	LEU	2.6
43	1l	89	ARG	2.6
33	2b	146	GLN	2.6
3	1D	2	ALA	2.6
40	2i	108	VAL	2.6
35	2d	73	ARG	2.6
40	2i	20	ARG	2.6
1	2A	2154	G	2.6
34	2c	39	ILE	2.6
44	2m	84	ILE	2.6
54	1y	45	G	2.6
54	2w	22	G	2.6
11	2P	32	THR	2.6
40	1i	117	HIS	2.6
3	1D	275	LYS	2.6
1	1A	1072	U	2.6
54	1w	60	C	2.6
23	11	2	SER	2.6
6	2G	39	ILE	2.6
12	2Q	66	ILE	2.6
40	2i	4	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
47	1p	59	TRP	2.6
33	2b	40	HIS	2.6
38	2g	76	ARG	2.6
51	1t	72	LEU	2.6
35	1d	110	PHE	2.6
38	2g	110	GLN	2.6
21	2Z	162	GLU	2.6
36	2e	13	ILE	2.6
45	2n	24	CYS	2.6
40	2i	75	ASP	2.6
26	24	59	PHE	2.6
21	2Z	153	SER	2.6
50	2s	84	GLY	2.6
1	1A	696	C	2.6
33	2b	223	ILE	2.6
40	2i	81	ILE	2.6
39	2h	16	ALA	2.6
7	2H	169	VAL	2.6
33	2b	215	LEU	2.6
41	2j	90	LEU	2.6
43	2l	10	LEU	2.6
44	2m	56	LEU	2.6
34	2c	194	GLY	2.6
32	2a	1224	G	2.6
40	2i	42	ARG	2.6
44	1m	103	THR	2.6
45	2n	61	TRP	2.6
16	2U	16	LYS	2.6
51	1t	14	LYS	2.6
31	29	25	VAL	2.6
48	2q	11	VAL	2.6
54	2w	62	C	2.6
12	2Q	33	GLY	2.6
53	2v	15	A	2.6
33	1b	200	ILE	2.5
34	2c	7	PRO	2.5
34	2c	177	THR	2.5
20	2Y	55	TYR	2.5
44	2m	70	LEU	2.5
33	2b	53	ARG	2.5
44	1m	102	ARG	2.5
12	2Q	136	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
43	2l	68	ALA	2.5
48	2q	65	ILE	2.5
6	2G	133	LEU	2.5
7	2H	52	VAL	2.5
8	2I	72	LEU	2.5
46	2o	27	VAL	2.5
6	2G	136	ARG	2.5
32	2a	1003	G	2.5
54	2y	15	G	2.5
50	2s	32	LYS	2.5
51	1t	74	LYS	2.5
7	2H	167	GLU	2.5
30	28	2	PRO	2.5
11	2P	71	VAL	2.5
22	20	11	ARG	2.5
34	2c	179	ARG	2.5
49	1r	78	LEU	2.5
49	1r	85	LEU	2.5
50	2s	28	LYS	2.5
54	2w	14	A	2.5
50	2s	44	MET	2.5
1	1A	2159	C	2.5
23	21	46	LEU	2.5
29	27	46	VAL	2.5
33	2b	135	GLN	2.5
33	2b	50	GLU	2.5
43	1l	16	GLU	2.5
54	2y	6	A	2.5
33	2b	147	LYS	2.5
37	1f	92	LYS	2.5
33	2b	207	ALA	2.5
44	1m	105	THR	2.5
43	1l	29	GLY	2.5
14	2S	58	LEU	2.5
35	1d	157	LEU	2.5
43	1l	60	LEU	2.5
6	2G	109	VAL	2.5
53	2v	21	U	2.5
14	2S	33	LYS	2.5
33	2b	96	ARG	2.5
35	2d	168	ARG	2.5
45	1n	3	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
17	2V	42	GLY	2.5
6	2G	88	ILE	2.5
33	2b	77	ALA	2.5
54	1y	13	C	2.5
14	2S	92	TYR	2.5
26	14	59	PHE	2.5
45	1n	23	ARG	2.5
50	2s	13	ASP	2.5
38	1g	81	GLY	2.5
26	24	52	THR	2.5
1	2A	899	A	2.5
33	2b	200	ILE	2.5
3	2D	38	LYS	2.5
24	22	60	LEU	2.5
47	2p	6	LEU	2.5
36	2e	55	VAL	2.5
41	1j	72	VAL	2.5
13	2R	68	ARG	2.5
32	2a	1116	C	2.5
54	2y	32	C	2.5
54	2w	15	G	2.5
7	2H	159	GLU	2.4
36	2e	22	GLY	2.4
44	1m	120	LYS	2.4
4	2E	195	LEU	2.4
35	1d	21	LEU	2.4
35	1d	120	LEU	2.4
18	2W	20	VAL	2.4
40	2i	65	VAL	2.4
54	2y	28	C	2.4
32	2a	202	U	2.4
54	2w	57	G	2.4
6	2G	91	ARG	2.4
12	1Q	81	VAL	2.4
3	2D	275	LYS	2.4
34	2c	28	GLN	2.4
35	2d	2	GLY	2.4
50	2s	6	LYS	2.4
54	1w	23	A	2.4
54	2w	66	A	2.4
14	2S	17	ARG	2.4
33	1b	21	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
35	2d	3	ARG	2.4
46	2o	54	ARG	2.4
32	1a	1031	G	2.4
50	2s	11	VAL	2.4
47	1p	76	GLN	2.4
33	2b	18	GLY	2.4
1	1A	2195	A	2.4
1	2A	2169	A	2.4
32	1a	161	A	2.4
34	2c	54	ARG	2.4
7	2H	72	ILE	2.4
41	1j	97	GLU	2.4
54	2y	72	C	2.4
40	1i	109	VAL	2.4
44	2m	98	VAL	2.4
38	2g	151	TYR	2.4
24	12	13	ALA	2.4
33	2b	133	LYS	2.4
34	2c	129	ALA	2.4
43	1l	23	LYS	2.4
43	2l	56	ALA	2.4
49	1r	79	LEU	2.4
20	2Y	44	ILE	2.4
34	2c	170	GLN	2.4
1	1A	1555	C	2.4
6	2G	70	VAL	2.4
8	2I	92	VAL	2.4
50	2s	53	ASN	2.4
6	2G	155	MET	2.4
33	1b	130	ARG	2.4
8	2I	117	GLU	2.4
32	2a	1032	G	2.4
45	2n	49	HIS	2.4
6	2G	49	ASP	2.4
41	2j	34	VAL	2.4
54	1y	21	A	2.4
1	2A	2128	C	2.4
42	2k	75	TYR	2.4
7	2H	71	LEU	2.4
44	2m	105	THR	2.4
46	2o	57	LEU	2.4
51	1t	13	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
7	2H	113	VAL	2.4
33	1b	93	VAL	2.4
33	2b	129	GLU	2.4
43	2l	41	ARG	2.4
51	1t	80	ARG	2.4
32	1a	172	A	2.3
44	2m	76	ALA	2.3
7	2H	82	GLY	2.3
4	2E	134	ILE	2.3
25	23	30	ARG	2.3
33	2b	41	ILE	2.3
35	2d	122	ARG	2.3
6	2G	160	VAL	2.3
34	2c	173	VAL	2.3
54	2w	39	G	2.3
32	2a	1219	U	2.3
43	2l	13	LYS	2.3
34	2c	33	LEU	2.3
33	2b	228	GLY	2.3
6	2G	157	ILE	2.3
5	1F	89	VAL	2.3
34	2c	150	LYS	2.3
19	2X	1	MET	2.3
1	1A	2155	G	2.3
11	1P	59	LEU	2.3
21	2Z	147	GLY	2.3
35	2d	157	LEU	2.3
48	2q	12	SER	2.3
54	1y	50	G	2.3
22	20	10	THR	2.3
21	2Z	124	ILE	2.3
32	2a	1030	C	2.3
40	2i	41	VAL	2.3
41	2j	80	LYS	2.3
7	2H	103	LEU	2.3
12	2Q	2	LEU	2.3
34	2c	47	LEU	2.3
39	1h	112	LEU	2.3
45	2n	31	ARG	2.3
51	2t	20	LEU	2.3
22	20	12	ASN	2.3
50	2s	39	THR	2.3

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Mol	Chain	Res	Type	RSRZ
54	2w	7	U	2.3
31	29	15	LYS	2.3
47	2p	76	GLN	2.3
1	2A	2174	C	2.3
32	2a	1325	C	2.3
33	1b	165	VAL	2.3
36	2e	105	VAL	2.3
43	1l	43	VAL	2.3
12	2Q	10	ARG	2.3
33	2b	195	ASP	2.3
46	1o	64	ARG	2.3
34	2c	145	GLY	2.3
41	2j	36	GLY	2.3
6	2G	173	LEU	2.3
11	2P	115	LEU	2.3
20	2Y	90	LEU	2.3
39	1h	133	LEU	2.3
46	1o	57	LEU	2.3
48	1q	98	LEU	2.3
28	26	2	ALA	2.3
24	12	70	GLN	2.3
17	1V	52	VAL	2.3
20	2Y	60	PHE	2.3
1	2A	2157	G	2.3
32	1a	1032	G	2.3
1	1A	2130	C	2.3
34	2c	167	TRP	2.3
35	1d	167	GLY	2.3
40	2i	21	PRO	2.3
35	2d	194	LEU	2.3
39	1h	2	LEU	2.3
35	2d	160	GLN	2.3
44	2m	21	TYR	2.3
47	1p	7	ALA	2.3
3	2D	181	GLU	2.3
7	2H	124	GLU	2.3
1	1A	2518	U	2.3
1	2A	2167	U	2.3
26	24	61	ARG	2.3
39	2h	19	VAL	2.3
52	1u	15	ARG	2.3
6	2G	42	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
34	2c	81	GLY	2.3
41	2j	93	GLY	2.3
9	2N	44	PRO	2.3
47	1p	16	HIS	2.3
32	2a	1114	C	2.3
34	2c	180	ALA	2.3
32	1a	1286	A	2.3
32	1a	1447	A	2.3
54	1y	23	A	2.3
54	2y	73	A	2.3
7	2H	95	ARG	2.3
23	21	26	ARG	2.3
39	2h	84	ARG	2.3
35	2d	166	LYS	2.3
40	1i	113	LYS	2.3
25	13	60	GLU	2.2
35	1d	147	ALA	2.2
32	2a	1030(C)	G	2.2
35	1d	166	LYS	2.2
38	1g	155	ARG	2.2
38	2g	3	ARG	2.2
40	1i	112	LYS	2.2
40	2i	120	ARG	2.2
41	1j	60	ARG	2.2
45	1n	29	ARG	2.2
11	2P	51	PHE	2.2
33	2b	55	PHE	2.2
1	1A	1144	A	2.2
1	1A	2084	A	2.2
1	1A	2180	A	2.2
36	1e	89	ILE	2.2
40	2i	115	GLY	2.2
52	2u	11	GLY	2.2
54	1w	9	A	2.2
51	1t	18	GLN	2.2
16	2U	20	LEU	2.2
43	2l	5	PRO	2.2
12	2Q	103	MET	2.2
31	29	19	ARG	2.2
33	1b	188	ALA	2.2
41	1j	58	ASP	2.2
10	2O	19	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
32	2a	1131	G	2.2
54	1w	24	G	2.2
1	1A	2141	A	2.2
14	2S	54	LEU	2.2
12	2Q	1	MET	2.2
18	2W	92	ARG	2.2
38	2g	41	ARG	2.2
54	1y	12	U	2.2
33	2b	120	ALA	2.2
6	1G	146	TYR	2.2
16	2U	89	GLU	2.2
38	2g	26	PHE	2.2
12	2Q	102	VAL	2.2
21	1Z	171	ILE	2.2
33	2b	211	ILE	2.2
46	2o	47	LYS	2.2
54	2w	74	C	2.2
7	2H	29	PRO	2.2
12	1Q	79	LEU	2.2
33	2b	196	LEU	2.2
34	1c	87	LEU	2.2
36	2e	75	THR	2.2
54	1w	41	A	2.2
42	2k	51	LYS	2.2
45	2n	12	ARG	2.2
1	1A	931	C	2.2
1	2A	2188	C	2.2
32	2a	1018	C	2.2
54	1w	74	C	2.2
1	1A	2173	G	2.2
1	2A	2166	G	2.2
33	1b	126	GLU	2.2
34	2c	105	GLU	2.2
42	2k	57	THR	2.2
5	2F	64	ILE	2.2
6	2G	113	ARG	2.2
14	2S	14	VAL	2.2
33	2b	98	LEU	2.2
40	2i	19	LEU	2.2
3	1D	38	LYS	2.2
34	2c	149	ALA	2.2
40	2i	30	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
44	2m	95	GLY	2.2
50	2s	24	ALA	2.2
54	1y	48	C	2.2
5	2F	62	ARG	2.2
54	2w	12	U	2.2
54	2y	59	U	2.2
32	2a	1353	G	2.2
43	2l	69	TYR	2.2
54	1y	2	G	2.2
28	26	7	ILE	2.2
32	2a	1030(D)	A	2.2
32	2a	1092	A	2.2
54	2y	14	A	2.2
26	24	46	GLN	2.2
33	2b	140	HIS	2.2
38	1g	153	HIS	2.2
44	2m	19	LEU	2.2
48	2q	6	LEU	2.2
33	2b	218	ALA	2.2
43	1l	63	GLY	2.2
44	1m	107	ALA	2.2
41	2j	15	THR	2.2
7	2H	97	ARG	2.2
33	2b	36	ARG	2.2
48	2q	71	PHE	2.2
53	1v	23	U	2.1
20	2Y	42	VAL	2.1
20	2Y	75	ILE	2.1
21	1Z	39	VAL	2.1
35	2d	5	ILE	2.1
34	1c	196	LEU	2.1
1	2A	2149	G	2.1
32	2a	1021	G	2.1
32	2a	1064	G	2.1
54	1y	3	G	2.1
11	2P	77	ARG	2.1
7	1H	25	LYS	2.1
44	2m	13	LYS	2.1
32	2a	1354	C	2.1
1	2A	2172	U	2.1
6	2G	15	VAL	2.1
9	1N	140	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
33	2b	229	VAL	2.1
39	2h	129	VAL	2.1
45	1n	18	VAL	2.1
24	22	35	LEU	2.1
36	2e	71	LEU	2.1
9	2N	12	ARG	2.1
20	2Y	50	ARG	2.1
43	1l	97	ARG	2.1
32	2a	1061	G	2.1
42	1k	123	LYS	2.1
40	2i	18	PHE	2.1
25	23	9	VAL	2.1
39	2h	95	VAL	2.1
3	2D	177	LEU	2.1
23	21	98	LEU	2.1
1	2A	2585	U	2.1
3	1D	176	ARG	2.1
32	2a	962	C	2.1
54	2y	71	C	2.1
48	2q	37	LYS	2.1
3	2D	2	ALA	2.1
34	2c	19	GLU	2.1
36	1e	17	ALA	2.1
36	2e	21	ALA	2.1
32	1a	1030(A)	G	2.1
12	2Q	125	LEU	2.1
21	2Z	122	ARG	2.1
28	26	52	VAL	2.1
30	28	41	ILE	2.1
31	29	31	LYS	2.1
33	2b	130	ARG	2.1
36	1e	64	ARG	2.1
43	2l	27	LEU	2.1
23	21	68	PRO	2.1
33	2b	202	PRO	2.1
1	1A	1220	U	2.1
1	2A	652(V)	C	2.1
54	1y	59	U	2.1
44	2m	42	ALA	2.1
54	2w	25	C	2.1
11	2P	70	GLN	2.1
20	2Y	43	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
34	2c	17	ASP	2.1
51	2t	86	ARG	2.1
5	2F	181	LEU	2.1
11	2P	6	LEU	2.1
17	2V	5	VAL	2.1
20	2Y	72	VAL	2.1
17	2V	81	TYR	2.1
21	2Z	102	LEU	2.1
35	1d	112	VAL	2.1
36	2e	33	VAL	2.1
39	2h	111	ILE	2.1
44	2m	15	VAL	2.1
46	2o	87	ILE	2.1
34	2c	162	GLN	2.1
32	2a	1020	U	2.1
1	1A	2196	C	2.1
7	2H	41	MET	2.1
6	2G	51	ARG	2.1
9	1N	61	ARG	2.1
36	2e	28	PHE	2.1
33	2b	99	GLY	2.1
40	2i	6	GLY	2.1
36	1e	81	GLU	2.1
33	2b	32	ILE	2.1
35	1d	8	VAL	2.1
35	1d	136	PRO	2.1
42	2k	21	ILE	2.1
46	1o	36	ILE	2.1
46	1o	69	TYR	2.1
47	1p	38	TYR	2.1
34	2c	169	ALA	2.1
44	2m	27	LYS	2.1
54	1y	1	G	2.1
54	1y	14	A	2.1
54	2w	9	A	2.1
54	2y	24	G	2.1
12	1Q	5	ARG	2.1
44	2m	99	ARG	2.1
45	2n	26	ARG	2.1
33	2b	17	PHE	2.1
1	1A	2165	C	2.1
7	2H	58	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
36	2e	29	GLY	2.1
21	2Z	57	ILE	2.1
21	2Z	161	VAL	2.1
23	11	82	LEU	2.1
24	22	63	VAL	2.1
33	2b	102	LEU	2.1
39	2h	83	ILE	2.1
39	2h	93	VAL	2.1
48	1q	31	LEU	2.1
41	2j	53	PRO	2.1
41	2j	98	ILE	2.1
45	2n	7	ILE	2.1
21	2Z	156	LYS	2.1
47	1p	39	TYR	2.1
33	1b	37	ASN	2.1
33	1b	233	SER	2.1
40	2i	27	THR	2.1
42	1k	92	GLU	2.1
1	2A	2110	G	2.0
32	1a	344	A	2.1
32	1a	975	A	2.1
38	2g	33	ASP	2.1
40	1i	59	PHE	2.1
54	2w	49	G	2.0
29	27	42	LEU	2.0
32	2a	1039	C	2.0
34	2c	101	LEU	2.0
4	2E	167	VAL	2.0
45	1n	56	VAL	2.0
19	2X	8	ILE	2.0
47	1p	15	PRO	2.0
23	11	26	ARG	2.0
29	17	45	ALA	2.0
29	27	41	ARG	2.0
40	1i	120	ARG	2.0
45	1n	10	ALA	2.0
48	2q	25	ARG	2.0
27	25	29	THR	2.0
33	2b	233	SER	2.0
45	1n	51	GLY	2.0
11	2P	39	LYS	2.0
34	2c	186	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
35	1d	184	LYS	2.0
40	2i	70	LYS	2.0
40	1i	47	LEU	2.0
44	1m	19	LEU	2.0
1	2A	2310	A	2.0
1	1A	2179	G	2.0
3	1D	205	VAL	2.0
9	2N	46	VAL	2.0
11	2P	50	ARG	2.0
16	1U	17	ILE	2.0
30	28	16	ILE	2.0
54	1w	57	G	2.0
32	1a	1030	C	2.0
36	2e	14	ARG	2.0
54	2y	60	C	2.0
41	1j	20	ALA	2.0
41	2j	27	ALA	2.0
51	1t	9	ASN	2.0
31	29	33	LYS	2.0
52	1u	2	GLY	2.0
52	1u	17	THR	2.0
33	1b	48	MET	2.0
47	1p	48	TRP	2.0
11	2P	59	LEU	2.0
34	2c	87	LEU	2.0
34	2c	204	LEU	2.0
34	2c	207	VAL	2.0
35	1d	118	ARG	2.0
54	2y	67	U	2.0
32	1a	1030(D)	A	2.0
32	2a	1250	A	2.0
1	1A	2147	G	2.0
40	1i	15	ALA	2.0
47	1p	17	TYR	2.0
21	2Z	93	ASP	2.0
23	21	28	GLY	2.0
50	2s	68	GLY	2.0
54	2y	27	C	2.0
30	28	61	LEU	2.0
41	1j	65	LEU	2.0
34	2c	69	HIS	2.0
43	2l	59	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
23	21	4	VAL	2.0
31	29	23	VAL	2.0
36	2e	9	LYS	2.0

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	0.33	0.38	95,102,111,112	0
56	IAR	B	7	12/12	0.39	0.64	76,91,98,99	0
54	PSU	1w	55	20/21	0.44	0.46	71,97,102,104	0
56	IAR	C	9	12/12	0.60	0.56	81,88,101,103	0
54	CM0	2y	34	25/26	0.66	0.59	85,102,110,128	0
54	4SU	2y	8	20/21	0.68	0.27	99,104,116,125	0
54	PSU	2y	55	20/21	0.69	0.36	94,101,106,117	0
54	CM0	1y	34	25/26	0.74	0.35	84,94,101,121	0
56	IAR	A	9	12/12	0.75	0.53	67,79,91,94	0
54	7MG	1y	46	24/25	0.75	0.28	90,101,105,118	0
54	7MG	1w	46	24/25	0.76	0.22	88,96,107,117	0
54	4SU	2w	8	20/21	0.76	0.29	97,102,109,122	0
54	4SU	1y	8	20/21	0.79	0.27	95,99,109,118	0
54	5MU	2y	54	21/22	0.79	0.48	93,102,109,126	0
54	PSU	1y	55	20/21	0.79	0.34	93,98,104,117	0
54	5MU	2w	54	21/22	0.80	0.21	87,92,100,102	0
54	7MG	2y	46	24/25	0.81	0.31	94,104,109,114	0
56	EUP	A	2	8/9	0.81	0.27	59,75,76,78	0
56	ORD	C	5	8/9	0.82	0.31	90,95,96,98	0
56	ORD	B	3	8/9	0.82	0.39	72,75,81,82	0
54	CM0	2w	34	25/26	0.83	0.30	83,92,98,110	0
54	7MG	2w	46	24/25	0.83	0.27	92,102,108,119	0
56	EUP	C	2	8/9	0.84	0.51	87,92,94,94	0
54	4SU	1w	8	20/21	0.85	0.27	93,97,110,113	0
54	5MU	1y	54	21/22	0.85	0.32	90,95,100,110	0
54	6MZ	2y	37	23/24	0.85	0.39	89,99,106,125	0
54	6MZ	1y	37	23/24	0.86	0.33	85,94,103,117	0
32	2MG	2a	1207	24/25	0.87	0.18	84,94,98,101	0
55	4SU	2x	8	20/21	0.88	0.18	83,89,97,98	0
32	M2G	2a	966	25/26	0.88	0.21	63,73,89,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	5MU	1w	54	21/22	0.88	0.21	69,85,91,95	0
55	PSU	2x	55	20/21	0.89	0.14	78,86,93,99	0
32	PSU	2a	516	20/21	0.89	0.20	78,81,88,90	0
43	0TD	2l	92	10/11	0.90	0.18	70,70,74,88	0
54	CM0	1w	34	25/26	0.91	0.19	74,78,85,93	0
43	0TD	1l	92	10/11	0.92	0.19	50,54,58,79	0
54	6MZ	2w	37	23/24	0.92	0.27	82,87,91,96	0
55	5MU	2x	54	21/22	0.92	0.19	82,88,92,102	0
56	ORD	A	5	8/9	0.92	0.37	72,74,77,77	0
32	5MC	2a	967	21/22	0.92	0.17	67,75,84,91	0
55	5MC	2x	32	21/22	0.93	0.22	74,79,84,85	0
1	5MU	2A	1915	21/22	0.93	0.14	74,77,85,90	0
32	5MC	2a	1404	21/22	0.94	0.21	52,61,70,76	0
55	4SU	1x	8	20/21	0.94	0.17	61,68,82,83	0
1	PSU	2A	1917	20/21	0.94	0.15	64,69,82,86	0
32	4OC	2a	1402	22/23	0.94	0.20	57,67,73,79	0
32	7MG	2a	527	24/25	0.94	0.17	64,72,81,89	0
54	6MZ	1w	37	23/24	0.95	0.24	59,65,70,71	0
1	4OC	2A	1920	21/23	0.95	0.17	57,66,69,70	0
1	5MU	1A	1937	21/22	0.95	0.19	56,62,67,74	0
55	PSU	1x	55	20/21	0.95	0.18	64,70,77,78	0
32	MA6	2a	1519	24/25	0.95	0.30	56,68,70,73	0
1	PSU	1A	1939	20/21	0.96	0.18	52,56,63,70	0
32	MA6	2a	1518	24/25	0.96	0.25	58,67,72,75	0
32	UR3	2a	1498	21/22	0.96	0.23	52,60,69,72	0
1	PSU	2A	1911	20/21	0.96	0.14	64,68,75,79	0
32	5MC	2a	1400	21/22	0.96	0.24	67,72,76,82	0
55	5MU	1x	54	21/22	0.96	0.15	63,72,76,83	0
32	PSU	1a	516	20/21	0.96	0.18	61,68,71,72	0
32	7MG	1a	527	24/25	0.97	0.19	46,52,57,59	0
32	2MG	1a	1207	24/25	0.97	0.17	70,74,80,80	0
32	5MC	1a	1400	21/22	0.97	0.21	46,54,59,62	0
1	2MU	2A	2552	21/23	0.97	0.23	38,42,49,54	0
1	2MA	2A	2503	23/24	0.97	0.22	31,39,43,53	0
55	5MC	1x	32	21/22	0.97	0.23	47,57,61,67	0
1	5MC	2A	1942	21/22	0.97	0.19	56,63,67,79	0
32	5MC	1a	1404	21/22	0.97	0.20	35,40,47,51	0
32	5MC	2a	1407	21/22	0.97	0.19	49,60,64,76	0
32	5MC	1a	967	21/22	0.97	0.20	52,59,67,70	0
1	5MC	2A	1962	21/22	0.97	0.21	43,53,59,75	0
1	5MC	1A	1964	21/22	0.98	0.22	40,43,47,53	0
1	5MC	1A	1984	21/22	0.98	0.22	22,36,41,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MA6	1a	1519	24/25	0.98	0.24	40,43,47,49	0
32	M2G	1a	966	25/26	0.98	0.20	51,57,63,72	0
32	MA6	1a	1518	24/25	0.98	0.22	35,42,46,47	0
1	2MU	1A	2564	21/23	0.98	0.22	24,30,35,36	0
1	OMG	1A	2263	24/25	0.98	0.23	23,27,31,35	0
32	4OC	1a	1402	22/23	0.98	0.23	42,47,55,57	0
32	5MC	1a	1407	21/22	0.98	0.23	35,41,44,46	0
1	5MU	2A	1939	21/22	0.98	0.21	37,40,46,48	0
1	OMG	2A	2251	24/25	0.98	0.25	38,43,47,57	0
1	PSU	1A	1933	20/21	0.98	0.19	45,49,53,59	0
1	PSU	2A	2605	20/21	0.98	0.20	38,43,46,49	0
1	2MA	1A	2515	23/24	0.98	0.24	21,24,28,31	0
1	4OC	1A	1942	21/23	0.98	0.21	38,47,50,55	0
1	PSU	1A	2617	20/21	0.98	0.22	23,29,33,33	0
1	5MU	1A	1961	21/22	0.99	0.24	24,28,33,35	0
32	UR3	1a	1498	21/22	0.99	0.23	34,41,47,50	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	18	101	1/1	0.01	0.34	80,80,80,80	0
57	MG	2x	103	1/1	0.14	0.21	92,92,92,92	0
57	MG	2A	3767	1/1	0.22	0.27	95,95,95,95	0
57	MG	1a	1765	1/1	0.23	0.30	87,87,87,87	0
57	MG	1a	1794	1/1	0.27	0.14	79,79,79,79	0
57	MG	2A	3698	1/1	0.28	0.08	93,93,93,93	0
57	MG	1A	4108	1/1	0.30	0.33	76,76,76,76	0
57	MG	1a	1659	1/1	0.35	0.42	85,85,85,85	0
57	MG	2A	3320	1/1	0.36	0.25	81,81,81,81	0
57	MG	2A	3817	1/1	0.40	0.10	64,64,64,64	0
57	MG	C	8002	1/1	0.41	1.27	98,98,98,98	0
57	MG	2A	3300	1/1	0.41	0.16	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1B	229	1/1	0.42	0.21	77,77,77,77	0
57	MG	1A	3924	1/1	0.43	0.37	63,63,63,63	0
57	MG	1a	1805	1/1	0.43	0.10	73,73,73,73	0
57	MG	2A	3416	1/1	0.43	0.15	70,70,70,70	0
57	MG	1a	1808	1/1	0.45	0.18	86,86,86,86	0
57	MG	1w	106	1/1	0.45	0.45	89,89,89,89	0
57	MG	2A	3669	1/1	0.46	0.26	62,62,62,62	0
57	MG	2A	3101	1/1	0.46	0.20	73,73,73,73	0
57	MG	2A	3397	1/1	0.48	0.16	72,72,72,72	0
57	MG	2A	3198	1/1	0.49	0.27	76,76,76,76	0
57	MG	1a	1691	1/1	0.50	0.26	68,68,68,68	0
57	MG	1a	1834	1/1	0.51	0.23	70,70,70,70	0
57	MG	2A	3521	1/1	0.51	0.15	66,66,66,66	0
57	MG	2A	3350	1/1	0.52	0.16	76,76,76,76	0
57	MG	1A	3421	1/1	0.52	0.24	74,74,74,74	0
57	MG	2A	3654	1/1	0.53	0.12	83,83,83,83	0
57	MG	1a	1734	1/1	0.53	0.14	63,63,63,63	0
57	MG	1A	3473	1/1	0.53	0.59	62,62,62,62	0
57	MG	2A	3301	1/1	0.53	0.20	88,88,88,88	0
57	MG	2A	3770	1/1	0.54	0.10	78,78,78,78	0
57	MG	2A	3832	1/1	0.54	0.81	67,67,67,67	0
57	MG	2a	1724	1/1	0.55	0.09	84,84,84,84	0
57	MG	2A	3292	1/1	0.55	0.81	62,62,62,62	0
57	MG	2A	3843	1/1	0.56	0.60	86,86,86,86	0
57	MG	2A	3556	1/1	0.57	0.15	56,56,56,56	0
57	MG	1A	3975	1/1	0.57	0.25	74,74,74,74	0
57	MG	1a	1842	1/1	0.57	0.19	74,74,74,74	0
57	MG	2A	3769	1/1	0.58	0.20	83,83,83,83	0
57	MG	2B	3013	1/1	0.58	0.18	70,70,70,70	0
57	MG	1A	3973	1/1	0.58	0.11	72,72,72,72	0
57	MG	1A	3875	1/1	0.58	0.11	60,60,60,60	0
57	MG	1A	3995	1/1	0.58	0.17	52,52,52,52	0
57	MG	1Y	203	1/1	0.58	0.11	80,80,80,80	0
57	MG	1A	3786	1/1	0.59	0.23	74,74,74,74	0
57	MG	1a	1806	1/1	0.59	0.10	80,80,80,80	0
57	MG	2A	3347	1/1	0.59	0.17	72,72,72,72	0
57	MG	1a	1762	1/1	0.59	0.12	77,77,77,77	0
57	MG	2A	3522	1/1	0.59	0.08	73,73,73,73	0
57	MG	2y	3003	1/1	0.59	1.20	102,102,102,102	0
57	MG	2A	3329	1/1	0.60	0.26	67,67,67,67	0
57	MG	1a	1692	1/1	0.60	0.23	73,73,73,73	0
57	MG	1A	3893	1/1	0.60	0.20	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1693	1/1	0.61	0.41	87,87,87,87	0
57	MG	1A	3381	1/1	0.61	0.29	68,68,68,68	0
57	MG	2A	3797	1/1	0.61	0.19	72,72,72,72	0
57	MG	2A	3341	1/1	0.62	0.30	71,71,71,71	0
57	MG	2A	3194	1/1	0.62	0.26	73,73,73,73	0
57	MG	1A	3601	1/1	0.62	0.26	68,68,68,68	0
57	MG	2A	3720	1/1	0.62	0.16	81,81,81,81	0
57	MG	2A	3696	1/1	0.62	0.32	80,80,80,80	0
57	MG	1A	3365	1/1	0.62	0.22	59,59,59,59	0
57	MG	2A	3773	1/1	0.62	0.35	83,83,83,83	0
57	MG	2A	3214	1/1	0.62	0.19	56,56,56,56	0
57	MG	2a	1689	1/1	0.63	0.11	83,83,83,83	0
57	MG	1A	3459	1/1	0.63	0.29	71,71,71,71	0
57	MG	2A	3299	1/1	0.63	0.12	79,79,79,79	0
57	MG	2A	3309	1/1	0.63	0.36	85,85,85,85	0
57	MG	1a	1655	1/1	0.63	0.15	74,74,74,74	0
57	MG	2y	3007	1/1	0.63	0.16	92,92,92,92	0
57	MG	2A	3213	1/1	0.63	0.47	65,65,65,65	0
57	MG	2A	3707	1/1	0.63	0.14	69,69,69,69	0
57	MG	1a	1727	1/1	0.63	0.17	79,79,79,79	0
57	MG	2a	1624	1/1	0.64	0.13	81,81,81,81	0
57	MG	2A	3209	1/1	0.64	0.43	70,70,70,70	0
57	MG	2A	3249	1/1	0.64	0.33	81,81,81,81	0
57	MG	2A	3344	1/1	0.64	0.37	85,85,85,85	0
57	MG	2A	3407	1/1	0.64	0.28	75,75,75,75	0
57	MG	2A	3327	1/1	0.64	1.16	73,73,73,73	0
57	MG	1B	202	1/1	0.65	0.24	62,62,62,62	0
57	MG	1A	3256	1/1	0.65	0.32	65,65,65,65	0
57	MG	2A	3726	1/1	0.65	0.07	71,71,71,71	0
57	MG	2A	3291	1/1	0.65	0.28	69,69,69,69	0
57	MG	1A	3453	1/1	0.65	0.28	70,70,70,70	0
57	MG	1a	1876	1/1	0.65	0.15	83,83,83,83	0
57	MG	1a	1673	1/1	0.65	0.25	78,78,78,78	0
57	MG	2A	3053	1/1	0.65	0.24	75,75,75,75	0
57	MG	2a	1686	1/1	0.66	0.27	65,65,65,65	0
57	MG	2a	1757	1/1	0.66	0.25	77,77,77,77	0
57	MG	2a	1626	1/1	0.66	0.14	74,74,74,74	0
57	MG	1a	1773	1/1	0.66	0.22	89,89,89,89	0
57	MG	1a	1882	1/1	0.66	0.34	67,67,67,67	0
57	MG	2Z	8001	1/1	0.66	0.14	89,89,89,89	0
57	MG	1A	4064	1/1	0.66	0.22	78,78,78,78	0
57	MG	2x	102	1/1	0.66	0.15	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3354	1/1	0.66	0.26	71,71,71,71	0
57	MG	2W	3001	1/1	0.66	0.15	62,62,62,62	0
57	MG	1A	3594	1/1	0.66	0.19	35,35,35,35	0
57	MG	1x	3003	1/1	0.67	0.18	77,77,77,77	0
57	MG	2A	3281	1/1	0.67	0.46	69,69,69,69	0
57	MG	1s	3001	1/1	0.67	0.28	71,71,71,71	0
57	MG	1A	3040	1/1	0.67	0.30	55,55,55,55	0
57	MG	1a	1898	1/1	0.67	0.18	89,89,89,89	0
57	MG	1a	1801	1/1	0.67	0.10	77,77,77,77	0
57	MG	2a	1687	1/1	0.67	0.21	78,78,78,78	0
57	MG	2A	3268	1/1	0.67	0.26	68,68,68,68	0
57	MG	2A	3074	1/1	0.68	0.36	67,67,67,67	0
57	MG	1a	1665	1/1	0.68	0.32	67,67,67,67	0
57	MG	2A	3528	1/1	0.68	0.37	58,58,58,58	0
57	MG	2A	3235	1/1	0.68	0.20	79,79,79,79	0
57	MG	2A	3197	1/1	0.68	0.14	71,71,71,71	0
57	MG	2A	3001	1/1	0.68	0.20	78,78,78,78	0
57	MG	2A	3252	1/1	0.68	0.21	70,70,70,70	0
57	MG	2O	8002	1/1	0.68	0.12	82,82,82,82	0
57	MG	2a	1695	1/1	0.68	0.15	69,69,69,69	0
57	MG	1a	1811	1/1	0.68	0.10	73,73,73,73	0
57	MG	1A	3286	1/1	0.69	0.25	66,66,66,66	0
57	MG	1y	103	1/1	0.69	0.15	86,86,86,86	0
57	MG	1a	1795	1/1	0.69	0.34	71,71,71,71	0
57	MG	1A	3529	1/1	0.69	0.21	62,62,62,62	0
57	MG	1A	3068	1/1	0.69	0.21	46,46,46,46	0
57	MG	2A	3587	1/1	0.69	0.39	64,64,64,64	0
57	MG	1a	1755	1/1	0.69	0.07	71,71,71,71	0
57	MG	18	102	1/1	0.69	0.10	63,63,63,63	0
57	MG	2F	301	1/1	0.69	0.36	57,57,57,57	0
57	MG	1B	212	1/1	0.69	0.10	69,69,69,69	0
57	MG	1a	1900	1/1	0.69	0.17	70,70,70,70	0
57	MG	2A	3089	1/1	0.69	0.17	65,65,65,65	0
57	MG	1A	4073	1/1	0.69	0.24	63,63,63,63	0
57	MG	1A	4046	1/1	0.69	0.17	70,70,70,70	0
57	MG	2A	3242	1/1	0.70	0.14	63,63,63,63	0
57	MG	2A	3082	1/1	0.70	1.11	56,56,56,56	0
57	MG	1a	1802	1/1	0.70	0.25	92,92,92,92	0
57	MG	2A	3664	1/1	0.70	0.16	69,69,69,69	0
57	MG	1a	1656	1/1	0.70	0.25	69,69,69,69	0
57	MG	2A	3026	1/1	0.70	0.16	63,63,63,63	0
57	MG	1A	3319	1/1	0.70	0.25	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3266	1/1	0.70	0.32	78,78,78,78	0
57	MG	2A	3287	1/1	0.70	0.36	70,70,70,70	0
57	MG	2A	3270	1/1	0.70	0.15	64,64,64,64	0
57	MG	2A	3243	1/1	0.70	0.36	69,69,69,69	0
57	MG	2A	3627	1/1	0.70	0.18	45,45,45,45	0
57	MG	2y	3006	1/1	0.71	0.39	106,106,106,106	0
57	MG	1A	3805	1/1	0.71	0.13	61,61,61,61	0
57	MG	2a	1607	1/1	0.71	0.13	81,81,81,81	0
57	MG	2a	1705	1/1	0.71	0.15	75,75,75,75	0
57	MG	2A	3850	1/1	0.71	0.70	56,56,56,56	0
57	MG	2A	3444	1/1	0.71	0.27	71,71,71,71	0
57	MG	1a	1724	1/1	0.71	0.17	71,71,71,71	0
57	MG	2A	3312	1/1	0.71	0.52	71,71,71,71	0
57	MG	1A	3961	1/1	0.71	0.18	49,49,49,49	0
57	MG	1A	3813	1/1	0.71	0.12	58,58,58,58	0
57	MG	2A	3455	1/1	0.71	0.12	66,66,66,66	0
57	MG	2A	3106	1/1	0.71	0.16	58,58,58,58	0
57	MG	1x	3014	1/1	0.71	0.55	82,82,82,82	0
57	MG	1A	3398	1/1	0.71	0.21	64,64,64,64	0
57	MG	23	101	1/1	0.71	0.50	64,64,64,64	0
57	MG	1A	3532	1/1	0.71	0.14	69,69,69,69	0
57	MG	2A	3303	1/1	0.71	0.22	77,77,77,77	0
57	MG	2X	3001	1/1	0.72	0.68	86,86,86,86	0
57	MG	2A	3104	1/1	0.72	0.19	73,73,73,73	0
57	MG	2a	1610	1/1	0.72	0.12	78,78,78,78	0
57	MG	2a	1640	1/1	0.72	0.20	77,77,77,77	0
57	MG	1A	3458	1/1	0.72	0.15	47,47,47,47	0
57	MG	1A	3428	1/1	0.72	0.14	72,72,72,72	0
57	MG	2a	1793	1/1	0.72	0.09	75,75,75,75	0
57	MG	1y	104	1/1	0.72	0.28	79,79,79,79	0
57	MG	2A	3753	1/1	0.72	0.08	65,65,65,65	0
57	MG	1A	3897	1/1	0.72	0.15	47,47,47,47	0
57	MG	2A	3387	1/1	0.72	0.24	52,52,52,52	0
57	MG	2a	1653	1/1	0.72	0.18	75,75,75,75	0
57	MG	2A	3665	1/1	0.72	0.22	66,66,66,66	0
57	MG	1b	3002	1/1	0.72	0.12	87,87,87,87	0
57	MG	2a	1609	1/1	0.72	0.24	68,68,68,68	0
57	MG	2A	3182	1/1	0.72	0.30	67,67,67,67	0
57	MG	1a	1759	1/1	0.72	0.11	60,60,60,60	0
57	MG	2A	3742	1/1	0.72	0.15	50,50,50,50	0
57	MG	1A	3084	1/1	0.72	0.64	47,47,47,47	0
57	MG	2A	3311	1/1	0.72	0.19	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3782	1/1	0.73	0.07	66,66,66,66	0
57	MG	1A	3912	1/1	0.73	0.18	56,56,56,56	0
57	MG	2a	1649	1/1	0.73	0.24	85,85,85,85	0
57	MG	2A	3579	1/1	0.73	0.15	62,62,62,62	0
57	MG	2A	3342	1/1	0.73	0.62	65,65,65,65	0
57	MG	2A	3776	1/1	0.73	0.24	70,70,70,70	0
57	MG	1A	3465	1/1	0.73	0.23	72,72,72,72	0
57	MG	1a	1616	1/1	0.73	0.19	68,68,68,68	0
57	MG	25	104	1/1	0.73	0.15	62,62,62,62	0
57	MG	2A	3325	1/1	0.73	0.33	74,74,74,74	0
57	MG	2a	1615	1/1	0.73	0.23	73,73,73,73	0
57	MG	2A	3704	1/1	0.73	0.24	89,89,89,89	0
57	MG	2A	3713	1/1	0.73	0.18	68,68,68,68	0
57	MG	2A	3047	1/1	0.73	0.18	64,64,64,64	0
57	MG	2A	3675	1/1	0.74	0.53	74,74,74,74	0
57	MG	1A	3289	1/1	0.74	0.39	60,60,60,60	0
57	MG	2E	309	1/1	0.74	0.17	62,62,62,62	0
57	MG	2A	3219	1/1	0.74	0.50	67,67,67,67	0
57	MG	1A	3446	1/1	0.74	0.52	67,67,67,67	0
57	MG	2A	3395	1/1	0.74	0.18	61,61,61,61	0
57	MG	2a	1733	1/1	0.74	0.28	82,82,82,82	0
57	MG	2B	3005	1/1	0.74	0.10	76,76,76,76	0
57	MG	1a	1849	1/1	0.74	0.19	95,95,95,95	0
57	MG	2A	3185	1/1	0.74	0.27	69,69,69,69	0
57	MG	1A	4079	1/1	0.74	0.15	73,73,73,73	0
57	MG	2v	101	1/1	0.74	1.40	85,85,85,85	0
57	MG	1A	3757	1/1	0.74	0.29	46,46,46,46	0
57	MG	2a	1683	1/1	0.74	0.13	76,76,76,76	0
57	MG	2a	1685	1/1	0.74	0.09	67,67,67,67	0
57	MG	2A	3317	1/1	0.74	0.41	71,71,71,71	0
57	MG	2A	3636	1/1	0.74	0.13	60,60,60,60	0
57	MG	2A	3337	1/1	0.74	0.14	74,74,74,74	0
57	MG	2A	3642	1/1	0.74	0.12	45,45,45,45	0
57	MG	1A	3363	1/1	0.74	0.49	50,50,50,50	0
57	MG	2A	3260	1/1	0.74	0.19	77,77,77,77	0
57	MG	1A	3451	1/1	0.74	0.33	66,66,66,66	0
57	MG	1A	4054	1/1	0.74	0.18	79,79,79,79	0
57	MG	1a	1866	1/1	0.74	0.18	76,76,76,76	0
57	MG	1A	3721	1/1	0.74	0.34	59,59,59,59	0
57	MG	1a	1756	1/1	0.74	0.18	72,72,72,72	0
57	MG	1A	3273	1/1	0.74	0.29	62,62,62,62	0
57	MG	1A	3359	1/1	0.74	0.31	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3557	1/1	0.75	0.48	57,57,57,57	0
57	MG	2a	1709	1/1	0.75	0.08	69,69,69,69	0
57	MG	2a	1728	1/1	0.75	0.13	65,65,65,65	0
57	MG	1A	4024	1/1	0.75	0.09	60,60,60,60	0
57	MG	2A	3594	1/1	0.75	0.10	75,75,75,75	0
57	MG	29	101	1/1	0.75	1.44	79,79,79,79	0
57	MG	2A	3334	1/1	0.75	0.27	63,63,63,63	0
57	MG	2A	3094	1/1	0.75	0.29	83,83,83,83	0
57	MG	2A	3371	1/1	0.75	0.20	70,70,70,70	0
57	MG	2A	3191	1/1	0.75	0.35	74,74,74,74	0
57	MG	1a	1684	1/1	0.75	0.12	79,79,79,79	0
57	MG	1A	3725	1/1	0.75	0.12	61,61,61,61	0
57	MG	1A	3542	1/1	0.75	0.20	44,44,44,44	0
57	MG	1A	3038	1/1	0.75	0.38	52,52,52,52	0
57	MG	1A	3596	1/1	0.75	0.16	44,44,44,44	0
57	MG	1A	3713	1/1	0.75	0.18	72,72,72,72	0
57	MG	2A	3211	1/1	0.75	0.28	71,71,71,71	0
57	MG	1A	3114	1/1	0.75	0.31	41,41,41,41	0
57	MG	1a	1761	1/1	0.75	0.20	59,59,59,59	0
57	MG	2A	3708	1/1	0.75	0.22	81,81,81,81	0
57	MG	2A	3240	1/1	0.76	0.75	69,69,69,69	0
57	MG	1A	3371	1/1	0.76	0.14	58,58,58,58	0
57	MG	1a	1671	1/1	0.76	0.42	57,57,57,57	0
57	MG	1A	3020	1/1	0.76	0.21	45,45,45,45	0
57	MG	1A	3086	1/1	0.76	0.72	49,49,49,49	0
57	MG	1A	3235	1/1	0.76	0.16	55,55,55,55	0
57	MG	1A	3819	1/1	0.76	0.15	48,48,48,48	0
57	MG	2a	1678	1/1	0.76	0.09	76,76,76,76	0
57	MG	1B	231	1/1	0.76	0.24	70,70,70,70	0
57	MG	2A	3660	1/1	0.76	0.26	69,69,69,69	0
57	MG	1a	1880	1/1	0.76	0.14	72,72,72,72	0
57	MG	1A	3452	1/1	0.76	0.22	53,53,53,53	0
57	MG	2A	3498	1/1	0.76	0.17	62,62,62,62	0
57	MG	2A	3090	1/1	0.76	0.18	89,89,89,89	0
57	MG	2A	3204	1/1	0.76	0.12	75,75,75,75	0
57	MG	2A	3177	1/1	0.76	0.15	65,65,65,65	0
57	MG	2B	3012	1/1	0.76	0.12	102,102,102,102	0
57	MG	1a	1654	1/1	0.76	0.30	72,72,72,72	0
57	MG	2R	8001	1/1	0.76	0.26	83,83,83,83	0
57	MG	2A	3719	1/1	0.76	0.19	78,78,78,78	0
57	MG	19	101	1/1	0.76	0.18	52,52,52,52	0
57	MG	2a	1800	1/1	0.76	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1628	1/1	0.76	0.16	68,68,68,68	0
57	MG	2a	1676	1/1	0.76	0.19	73,73,73,73	0
57	MG	2A	3576	1/1	0.76	0.12	84,84,84,84	0
57	MG	1A	3373	1/1	0.76	0.24	69,69,69,69	0
57	MG	1a	1815	1/1	0.76	0.17	87,87,87,87	0
57	MG	2A	3701	1/1	0.76	0.10	61,61,61,61	0
57	MG	2a	1795	1/1	0.76	0.12	83,83,83,83	0
57	MG	1E	306	1/1	0.76	0.34	74,74,74,74	0
57	MG	2A	3553	1/1	0.76	0.19	52,52,52,52	0
57	MG	1A	3521	1/1	0.76	0.18	34,34,34,34	0
57	MG	1a	1799	1/1	0.76	0.20	70,70,70,70	0
57	MG	2A	3205	1/1	0.76	0.20	66,66,66,66	0
57	MG	2A	3731	1/1	0.76	0.13	63,63,63,63	0
57	MG	2g	8001	1/1	0.76	0.16	76,76,76,76	0
57	MG	2a	1664	1/1	0.76	0.17	71,71,71,71	0
57	MG	1A	3360	1/1	0.77	0.12	58,58,58,58	0
57	MG	2a	1679	1/1	0.77	0.24	75,75,75,75	0
57	MG	1A	3250	1/1	0.77	0.21	62,62,62,62	0
57	MG	1a	1758	1/1	0.77	0.06	85,85,85,85	0
57	MG	2A	3122	1/1	0.77	0.56	86,86,86,86	0
57	MG	1A	3195	1/1	0.77	0.19	67,67,67,67	0
57	MG	2A	3103	1/1	0.77	0.12	70,70,70,70	0
57	MG	2A	3598	1/1	0.77	0.39	71,71,71,71	0
57	MG	1a	1678	1/1	0.77	0.13	62,62,62,62	0
57	MG	1B	203	1/1	0.77	0.20	51,51,51,51	0
57	MG	1a	1785	1/1	0.77	0.18	71,71,71,71	0
57	MG	1a	1911	1/1	0.77	0.29	79,79,79,79	0
57	MG	2a	1666	1/1	0.77	0.10	87,87,87,87	0
57	MG	1A	3744	1/1	0.77	0.15	56,56,56,56	0
57	MG	1A	3249	1/1	0.77	0.17	56,56,56,56	0
57	MG	1A	3984	1/1	0.77	0.16	55,55,55,55	0
57	MG	1A	3945	1/1	0.77	0.55	69,69,69,69	0
57	MG	2a	1608	1/1	0.77	0.13	77,77,77,77	0
57	MG	2A	3236	1/1	0.77	0.14	84,84,84,84	0
57	MG	2A	3829	1/1	0.77	0.23	75,75,75,75	0
57	MG	2A	3199	1/1	0.77	0.17	62,62,62,62	0
57	MG	1E	308	1/1	0.77	0.18	73,73,73,73	0
57	MG	2a	1786	1/1	0.77	0.15	85,85,85,85	0
57	MG	2A	3188	1/1	0.77	0.22	73,73,73,73	0
57	MG	1A	3169	1/1	0.77	0.17	53,53,53,53	0
57	MG	2A	3638	1/1	0.77	0.28	77,77,77,77	0
57	MG	1A	3401	1/1	0.77	0.28	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3386	1/1	0.77	0.18	56,56,56,56	0
57	MG	1A	3931	1/1	0.77	0.43	69,69,69,69	0
57	MG	2A	3765	1/1	0.77	0.08	66,66,66,66	0
57	MG	1A	3433	1/1	0.77	0.15	60,60,60,60	0
57	MG	2A	3160	1/1	0.77	0.17	85,85,85,85	0
57	MG	2A	3789	1/1	0.77	0.08	68,68,68,68	0
57	MG	1a	1870	1/1	0.77	0.86	80,80,80,80	0
57	MG	1A	3841	1/1	0.77	0.07	57,57,57,57	0
57	MG	2A	3318	1/1	0.77	0.16	70,70,70,70	0
57	MG	1a	1648	1/1	0.77	0.43	58,58,58,58	0
57	MG	2A	3070	1/1	0.78	0.22	57,57,57,57	0
57	MG	2A	3227	1/1	0.78	0.69	69,69,69,69	0
57	MG	1A	3340	1/1	0.78	0.39	53,53,53,53	0
57	MG	2A	3615	1/1	0.78	0.14	92,92,92,92	0
57	MG	1a	1625	1/1	0.78	0.17	68,68,68,68	0
57	MG	2A	3799	1/1	0.78	0.30	77,77,77,77	0
57	MG	2A	3657	1/1	0.78	0.11	70,70,70,70	0
57	MG	1A	3374	1/1	0.78	0.33	68,68,68,68	0
57	MG	1A	3955	1/1	0.78	0.23	54,54,54,54	0
57	MG	1A	3801	1/1	0.78	0.07	65,65,65,65	0
57	MG	2A	3093	1/1	0.78	0.27	71,71,71,71	0
57	MG	1A	4034	1/1	0.78	0.14	34,34,34,34	0
57	MG	1a	1897	1/1	0.78	0.11	83,83,83,83	0
57	MG	2A	3689	1/1	0.78	0.29	72,72,72,72	0
57	MG	1A	4060	1/1	0.78	0.22	69,69,69,69	0
57	MG	1A	3998	1/1	0.78	0.24	71,71,71,71	0
57	MG	2A	3018	1/1	0.78	0.19	78,78,78,78	0
57	MG	2A	3245	1/1	0.78	0.13	79,79,79,79	0
57	MG	2A	3487	1/1	0.78	0.14	44,44,44,44	0
57	MG	2A	3045	1/1	0.78	0.21	78,78,78,78	0
57	MG	2A	3063	1/1	0.78	0.14	60,60,60,60	0
57	MG	1A	3297	1/1	0.78	0.66	44,44,44,44	0
57	MG	2A	3667	1/1	0.78	0.30	63,63,63,63	0
57	MG	2a	1802	1/1	0.78	0.85	100,100,100,100	0
57	MG	2Q	3003	1/1	0.78	0.21	55,55,55,55	0
57	MG	1a	1731	1/1	0.78	0.22	90,90,90,90	0
57	MG	1A	3165	1/1	0.78	0.21	62,62,62,62	0
57	MG	2a	1638	1/1	0.78	0.12	64,64,64,64	0
57	MG	2A	3038	1/1	0.78	0.18	63,63,63,63	0
57	MG	2A	3724	1/1	0.78	0.20	88,88,88,88	0
57	MG	2a	1630	1/1	0.78	0.19	64,64,64,64	0
57	MG	1A	4053	1/1	0.78	0.18	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3222	1/1	0.78	0.53	61,61,61,61	0
57	MG	1A	3205	1/1	0.78	0.11	76,76,76,76	0
57	MG	2a	1667	1/1	0.78	0.14	83,83,83,83	0
57	MG	2A	3709	1/1	0.78	0.05	76,76,76,76	0
57	MG	1A	3422	1/1	0.78	0.19	50,50,50,50	0
57	MG	1a	1686	1/1	0.78	0.14	69,69,69,69	0
57	MG	1w	103	1/1	0.78	0.24	85,85,85,85	0
57	MG	1A	3795	1/1	0.78	0.15	60,60,60,60	0
57	MG	1A	3375	1/1	0.79	0.19	66,66,66,66	0
57	MG	1A	3417	1/1	0.79	0.15	69,69,69,69	0
57	MG	2A	3644	1/1	0.79	0.13	82,82,82,82	0
57	MG	1T	202	1/1	0.79	0.10	70,70,70,70	0
57	MG	1A	3326	1/1	0.79	0.10	64,64,64,64	0
57	MG	2A	3688	1/1	0.79	0.10	61,61,61,61	0
57	MG	1a	1695	1/1	0.79	0.28	69,69,69,69	0
57	MG	1v	3001	1/1	0.79	0.32	85,85,85,85	0
57	MG	2A	3737	1/1	0.79	0.22	67,67,67,67	0
57	MG	1A	3097	1/1	0.79	0.16	65,65,65,65	0
57	MG	1A	3185	1/1	0.79	0.22	64,64,64,64	0
57	MG	1a	1770	1/1	0.79	0.26	74,74,74,74	0
57	MG	2A	3694	1/1	0.79	0.12	58,58,58,58	0
57	MG	1a	1749	1/1	0.79	0.12	85,85,85,85	0
57	MG	2A	3179	1/1	0.79	0.51	79,79,79,79	0
57	MG	1A	3754	1/1	0.79	0.17	75,75,75,75	0
57	MG	1A	3581	1/1	0.79	0.12	73,73,73,73	0
57	MG	2A	3080	1/1	0.79	0.28	72,72,72,72	0
57	MG	2A	3606	1/1	0.79	0.11	53,53,53,53	0
57	MG	1A	3952	1/1	0.79	0.18	52,52,52,52	0
57	MG	2A	3402	1/1	0.79	0.15	68,68,68,68	0
57	MG	1A	3415	1/1	0.79	0.15	56,56,56,56	0
57	MG	1A	3232	1/1	0.79	0.46	64,64,64,64	0
57	MG	1a	1852	1/1	0.79	0.10	67,67,67,67	0
57	MG	1A	3970	1/1	0.79	0.10	55,55,55,55	0
57	MG	2a	1673	1/1	0.79	0.09	83,83,83,83	0
57	MG	1E	301	1/1	0.79	0.50	42,42,42,42	0
57	MG	1a	1748	1/1	0.79	0.16	68,68,68,68	0
57	MG	2A	3845	1/1	0.79	0.72	69,69,69,69	0
57	MG	1A	3329	1/1	0.79	0.19	59,59,59,59	0
57	MG	2a	1722	1/1	0.79	0.22	87,87,87,87	0
57	MG	1A	3388	1/1	0.79	0.17	61,61,61,61	0
57	MG	2A	3481	1/1	0.79	0.14	52,52,52,52	0
57	MG	2A	3107	1/1	0.79	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4011	1/1	0.79	0.16	58,58,58,58	0
57	MG	1A	3796	1/1	0.79	0.11	55,55,55,55	0
57	MG	1A	4030	1/1	0.79	0.24	59,59,59,59	0
57	MG	2B	3017	1/1	0.79	0.10	75,75,75,75	0
57	MG	1a	1774	1/1	0.79	0.19	78,78,78,78	0
57	MG	1A	3553	1/1	0.79	0.16	44,44,44,44	0
57	MG	2A	3224	1/1	0.79	1.51	72,72,72,72	0
57	MG	1a	1645	1/1	0.79	0.52	65,65,65,65	0
57	MG	1a	1857	1/1	0.79	0.17	74,74,74,74	0
57	MG	1A	3789	1/1	0.79	0.12	49,49,49,49	0
57	MG	28	101	1/1	0.80	0.41	78,78,78,78	0
57	MG	1V	202	1/1	0.80	0.21	78,78,78,78	0
57	MG	1A	3170	1/1	0.80	0.20	59,59,59,59	0
57	MG	2U	202	1/1	0.80	0.63	65,65,65,65	0
57	MG	2A	3159	1/1	0.80	0.20	86,86,86,86	0
57	MG	1A	4009	1/1	0.80	0.21	38,38,38,38	0
57	MG	2A	3469	1/1	0.80	0.10	49,49,49,49	0
57	MG	2a	1796	1/1	0.80	0.20	79,79,79,79	0
57	MG	2A	3165	1/1	0.80	0.14	59,59,59,59	0
57	MG	2A	3504	1/1	0.80	0.13	67,67,67,67	0
57	MG	1Q	204	1/1	0.80	0.20	61,61,61,61	0
57	MG	1A	3817	1/1	0.80	0.14	55,55,55,55	0
57	MG	1A	3382	1/1	0.80	0.35	56,56,56,56	0
57	MG	2A	3278	1/1	0.80	0.21	63,63,63,63	0
57	MG	2A	3059	1/1	0.80	0.28	68,68,68,68	0
57	MG	2A	3267	1/1	0.80	0.35	71,71,71,71	0
57	MG	2f	3002	1/1	0.80	0.10	76,76,76,76	0
57	MG	2A	3834	1/1	0.80	0.68	68,68,68,68	0
57	MG	2a	1699	1/1	0.80	0.10	68,68,68,68	0
57	MG	1A	4001	1/1	0.80	0.23	49,49,49,49	0
57	MG	2A	3370	1/1	0.80	0.16	63,63,63,63	0
57	MG	2D	304	1/1	0.80	0.51	73,73,73,73	0
57	MG	2a	1601	1/1	0.80	0.16	67,67,67,67	0
59	ZN	24	501	1/1	0.80	0.06	125,125,125,125	0
57	MG	2B	3002	1/1	0.80	0.80	81,81,81,81	0
57	MG	1A	4037	1/1	0.80	0.23	43,43,43,43	0
57	MG	1x	3010	1/1	0.80	0.12	80,80,80,80	0
57	MG	2B	3014	1/1	0.80	0.14	74,74,74,74	0
57	MG	2a	1713	1/1	0.80	0.11	74,74,74,74	0
57	MG	1a	1657	1/1	0.80	0.12	61,61,61,61	0
57	MG	2A	3237	1/1	0.80	0.68	70,70,70,70	0
57	MG	2A	3413	1/1	0.80	0.10	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3942	1/1	0.80	0.14	64,64,64,64	0
57	MG	1A	3477	1/1	0.80	0.17	26,26,26,26	0
57	MG	2A	3715	1/1	0.80	0.21	55,55,55,55	0
57	MG	1w	104	1/1	0.80	0.81	87,87,87,87	0
57	MG	1A	3260	1/1	0.80	0.30	55,55,55,55	0
57	MG	2A	3836	1/1	0.80	0.15	72,72,72,72	0
57	MG	1A	4076	1/1	0.80	0.56	64,64,64,64	0
57	MG	1P	203	1/1	0.80	0.56	47,47,47,47	0
57	MG	1A	4003	1/1	0.80	0.16	58,58,58,58	0
57	MG	2A	3766	1/1	0.80	0.09	67,67,67,67	0
57	MG	1a	1608	1/1	0.80	0.23	68,68,68,68	0
57	MG	2x	104	1/1	0.80	0.14	77,77,77,77	0
57	MG	2A	3493	1/1	0.80	0.13	65,65,65,65	0
57	MG	2A	3046	1/1	0.80	0.10	57,57,57,57	0
57	MG	2a	1675	1/1	0.80	0.13	76,76,76,76	0
57	MG	1a	1826	1/1	0.80	0.14	60,60,60,60	0
57	MG	1A	3538	1/1	0.80	0.09	68,68,68,68	0
57	MG	2A	3322	1/1	0.80	0.75	71,71,71,71	0
57	MG	2A	3733	1/1	0.80	0.14	65,65,65,65	0
57	MG	1a	1869	1/1	0.81	0.35	70,70,70,70	0
57	MG	1A	3345	1/1	0.81	0.38	72,72,72,72	0
57	MG	1B	227	1/1	0.81	0.22	73,73,73,73	0
57	MG	1A	3907	1/1	0.81	0.14	25,25,25,25	0
57	MG	2A	3812	1/1	0.81	0.15	80,80,80,80	0
57	MG	2A	3833	1/1	0.81	0.14	70,70,70,70	0
57	MG	2a	1712	1/1	0.81	0.08	71,71,71,71	0
57	MG	2A	3536	1/1	0.81	0.21	66,66,66,66	0
57	MG	1a	1817	1/1	0.81	0.17	65,65,65,65	0
57	MG	1A	3940	1/1	0.81	0.15	56,56,56,56	0
57	MG	1A	3906	1/1	0.81	0.42	47,47,47,47	0
57	MG	2A	3384	1/1	0.81	0.28	64,64,64,64	0
57	MG	1a	1687	1/1	0.81	0.17	68,68,68,68	0
57	MG	1A	3305	1/1	0.81	0.24	52,52,52,52	0
57	MG	2A	3599	1/1	0.81	0.15	57,57,57,57	0
57	MG	1A	3671	1/1	0.81	0.10	41,41,41,41	0
57	MG	1a	1841	1/1	0.81	0.27	58,58,58,58	0
57	MG	2a	1674	1/1	0.81	0.14	69,69,69,69	0
57	MG	1a	1905	1/1	0.81	0.33	75,75,75,75	0
57	MG	1A	3747	1/1	0.81	0.27	43,43,43,43	0
57	MG	2A	3324	1/1	0.81	0.25	57,57,57,57	0
57	MG	1a	1690	1/1	0.81	0.17	60,60,60,60	0
57	MG	2A	3519	1/1	0.81	0.21	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4068	1/1	0.81	0.20	36,36,36,36	0
57	MG	2A	3471	1/1	0.81	0.22	45,45,45,45	0
57	MG	1a	1669	1/1	0.81	0.12	93,93,93,93	0
57	MG	2A	3691	1/1	0.81	0.10	64,64,64,64	0
57	MG	1a	1635	1/1	0.81	0.29	64,64,64,64	0
57	MG	1a	1652	1/1	0.81	0.26	70,70,70,70	0
57	MG	1A	3290	1/1	0.81	0.41	63,63,63,63	0
57	MG	2A	3218	1/1	0.81	0.67	62,62,62,62	0
57	MG	2A	3140	1/1	0.81	0.25	72,72,72,72	0
57	MG	1N	202	1/1	0.81	0.21	53,53,53,53	0
57	MG	1a	1859	1/1	0.81	0.09	72,72,72,72	0
57	MG	2A	3494	1/1	0.81	0.20	73,73,73,73	0
57	MG	1A	3782	1/1	0.81	0.31	60,60,60,60	0
57	MG	2q	203	1/1	0.81	0.09	87,87,87,87	0
57	MG	1A	3310	1/1	0.81	0.16	64,64,64,64	0
57	MG	1A	4055	1/1	0.81	0.23	72,72,72,72	0
57	MG	1A	3741	1/1	0.81	0.20	70,70,70,70	0
57	MG	2A	3588	1/1	0.81	0.39	67,67,67,67	0
57	MG	1a	1791	1/1	0.81	0.13	82,82,82,82	0
57	MG	1a	1607	1/1	0.81	0.22	69,69,69,69	0
57	MG	1F	306	1/1	0.81	0.30	55,55,55,55	0
57	MG	2A	3515	1/1	0.81	0.15	37,37,37,37	0
57	MG	1l	8001	1/1	0.81	0.22	84,84,84,84	0
57	MG	1A	3834	1/1	0.81	0.16	41,41,41,41	0
57	MG	1A	3829	1/1	0.81	0.11	56,56,56,56	0
57	MG	2a	1783	1/1	0.81	0.17	85,85,85,85	0
57	MG	2a	1727	1/1	0.81	0.12	82,82,82,82	0
57	MG	2a	1652	1/1	0.81	0.13	72,72,72,72	0
57	MG	1A	3739	1/1	0.81	0.14	66,66,66,66	0
57	MG	1a	1844	1/1	0.81	0.10	92,92,92,92	0
57	MG	1a	1899	1/1	0.81	0.09	73,73,73,73	0
57	MG	1A	3318	1/1	0.81	0.49	45,45,45,45	0
57	MG	1A	3544	1/1	0.81	0.14	56,56,56,56	0
57	MG	1a	1868	1/1	0.81	0.33	71,71,71,71	0
57	MG	2A	3290	1/1	0.81	0.21	57,57,57,57	0
57	MG	2A	3100	1/1	0.81	0.13	51,51,51,51	0
57	MG	1A	3291	1/1	0.82	0.75	61,61,61,61	0
57	MG	2A	3403	1/1	0.82	0.17	63,63,63,63	0
57	MG	2A	3087	1/1	0.82	0.14	59,59,59,59	0
57	MG	2A	3602	1/1	0.82	0.09	69,69,69,69	0
57	MG	2U	201	1/1	0.82	0.20	59,59,59,59	0
57	MG	2A	3794	1/1	0.82	0.14	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4095	1/1	0.82	0.49	44,44,44,44	0
57	MG	1a	1632	1/1	0.82	0.20	72,72,72,72	0
57	MG	1A	3500	1/1	0.82	0.21	55,55,55,55	0
57	MG	1A	3263	1/1	0.82	0.34	61,61,61,61	0
57	MG	1A	3632	1/1	0.82	0.15	66,66,66,66	0
57	MG	1A	3887	1/1	0.82	0.10	58,58,58,58	0
57	MG	2A	3734	1/1	0.82	0.08	60,60,60,60	0
57	MG	1A	3749	1/1	0.82	0.53	55,55,55,55	0
57	MG	1F	304	1/1	0.82	0.14	54,54,54,54	0
57	MG	2t	3001	1/1	0.82	0.14	58,58,58,58	0
57	MG	2A	3051	1/1	0.82	0.30	80,80,80,80	0
57	MG	2A	3663	1/1	0.82	0.18	53,53,53,53	0
57	MG	1A	3957	1/1	0.82	0.14	70,70,70,70	0
57	MG	2T	3002	1/1	0.82	0.16	61,61,61,61	0
57	MG	2A	3114	1/1	0.82	0.31	63,63,63,63	0
57	MG	1a	1653	1/1	0.82	0.32	65,65,65,65	0
57	MG	2a	1661	1/1	0.82	0.14	71,71,71,71	0
57	MG	2A	3559	1/1	0.82	0.50	67,67,67,67	0
57	MG	1A	3559	1/1	0.82	0.11	39,39,39,39	0
57	MG	2A	3672	1/1	0.82	0.14	66,66,66,66	0
57	MG	1A	3616	1/1	0.82	0.18	72,72,72,72	0
57	MG	1a	1689	1/1	0.82	0.22	70,70,70,70	0
57	MG	2y	3001	1/1	0.82	0.14	65,65,65,65	0
57	MG	2a	1632	1/1	0.82	0.11	78,78,78,78	0
57	MG	1a	1714	1/1	0.82	0.15	76,76,76,76	0
57	MG	2a	1647	1/1	0.82	0.21	64,64,64,64	0
57	MG	2a	1708	1/1	0.82	0.09	95,95,95,95	0
57	MG	2A	3421	1/1	0.82	0.23	44,44,44,44	0
57	MG	2A	3376	1/1	0.82	0.14	55,55,55,55	0
57	MG	1A	3988	1/1	0.82	0.11	67,67,67,67	0
57	MG	2A	3203	1/1	0.82	0.13	73,73,73,73	0
57	MG	1e	202	1/1	0.82	0.16	77,77,77,77	0
57	MG	2a	1767	1/1	0.82	0.08	76,76,76,76	0
57	MG	1S	3003	1/1	0.82	0.18	73,73,73,73	0
57	MG	2A	3105	1/1	0.82	0.14	54,54,54,54	0
57	MG	1a	1725	1/1	0.82	0.22	62,62,62,62	0
57	MG	2A	3801	1/1	0.82	0.65	69,69,69,69	0
57	MG	2A	3178	1/1	0.82	0.52	74,74,74,74	0
57	MG	2A	3352	1/1	0.82	0.63	70,70,70,70	0
57	MG	1A	3331	1/1	0.82	0.18	57,57,57,57	0
57	MG	2A	3285	1/1	0.82	0.20	66,66,66,66	0
57	MG	2A	3193	1/1	0.82	0.11	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3480	1/1	0.82	0.17	44,44,44,44	0
57	MG	2A	3098	1/1	0.82	0.14	76,76,76,76	0
57	MG	1A	4093	1/1	0.82	0.12	73,73,73,73	0
57	MG	2A	3346	1/1	0.82	0.22	65,65,65,65	0
57	MG	1A	3148	1/1	0.82	0.57	38,38,38,38	0
57	MG	1A	3974	1/1	0.82	0.11	76,76,76,76	0
57	MG	2I	102	1/1	0.82	0.30	63,63,63,63	0
57	MG	1a	1879	1/1	0.82	0.12	89,89,89,89	0
57	MG	2A	3393	1/1	0.82	0.17	69,69,69,69	0
57	MG	1A	3997	1/1	0.82	0.16	61,61,61,61	0
57	MG	2A	3363	1/1	0.82	0.18	64,64,64,64	0
57	MG	2A	3286	1/1	0.82	0.23	63,63,63,63	0
57	MG	1A	3321	1/1	0.82	0.28	63,63,63,63	0
57	MG	1A	3277	1/1	0.82	0.64	43,43,43,43	0
57	MG	2A	3394	1/1	0.82	0.33	46,46,46,46	0
57	MG	2A	3690	1/1	0.82	0.10	87,87,87,87	0
57	MG	2X	3002	1/1	0.83	1.86	78,78,78,78	0
57	MG	2A	3848	1/1	0.83	0.10	70,70,70,70	0
57	MG	1a	1827	1/1	0.83	0.22	58,58,58,58	0
57	MG	2A	3354	1/1	0.83	0.18	71,71,71,71	0
57	MG	1A	4021	1/1	0.83	0.24	60,60,60,60	0
57	MG	1A	3667	1/1	0.83	0.06	78,78,78,78	0
57	MG	1A	3268	1/1	0.83	0.12	51,51,51,51	0
57	MG	2B	3009	1/1	0.83	0.14	75,75,75,75	0
57	MG	2a	1616	1/1	0.83	0.16	71,71,71,71	0
57	MG	1A	3043	1/1	0.83	0.20	37,37,37,37	0
57	MG	2A	3524	1/1	0.83	0.19	59,59,59,59	0
57	MG	2I	101	1/1	0.83	0.11	73,73,73,73	0
57	MG	1A	4097	1/1	0.83	0.12	68,68,68,68	0
57	MG	1G	3003	1/1	0.83	0.12	71,71,71,71	0
57	MG	1a	1614	1/1	0.83	0.10	60,60,60,60	0
57	MG	2A	3144	1/1	0.83	0.26	67,67,67,67	0
57	MG	1A	3216	1/1	0.83	0.22	55,55,55,55	0
57	MG	1A	3774	1/1	0.83	0.11	49,49,49,49	0
57	MG	1A	3871	1/1	0.83	0.16	50,50,50,50	0
57	MG	1A	3571	1/1	0.83	0.17	62,62,62,62	0
57	MG	2A	3231	1/1	0.83	0.24	67,67,67,67	0
57	MG	2A	3377	1/1	0.83	0.41	79,79,79,79	0
57	MG	1a	1660	1/1	0.83	0.23	73,73,73,73	0
57	MG	1A	3403	1/1	0.83	0.57	63,63,63,63	0
57	MG	2a	1779	1/1	0.83	0.08	75,75,75,75	0
57	MG	1U	204	1/1	0.83	0.34	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3965	1/1	0.83	0.19	59,59,59,59	0
57	MG	2A	3049	1/1	0.83	0.53	75,75,75,75	0
57	MG	2A	3326	1/1	0.83	0.19	72,72,72,72	0
57	MG	2a	1701	1/1	0.83	0.11	76,76,76,76	0
57	MG	2A	3099	1/1	0.83	0.23	62,62,62,62	0
57	MG	2A	3256	1/1	0.83	0.22	74,74,74,74	0
57	MG	1a	1713	1/1	0.83	0.25	77,77,77,77	0
57	MG	2E	303	1/1	0.83	0.12	71,71,71,71	0
57	MG	2R	8002	1/1	0.83	0.14	60,60,60,60	0
57	MG	1A	3279	1/1	0.83	0.13	65,65,65,65	0
57	MG	2A	3005	1/1	0.83	0.14	64,64,64,64	0
57	MG	1A	4061	1/1	0.83	0.14	47,47,47,47	0
57	MG	2A	3187	1/1	0.83	0.18	68,68,68,68	0
57	MG	2A	3732	1/1	0.83	0.06	59,59,59,59	0
57	MG	1A	3208	1/1	0.83	0.21	48,48,48,48	0
57	MG	2A	3151	1/1	0.83	0.24	69,69,69,69	0
57	MG	1A	3809	1/1	0.83	0.18	23,23,23,23	0
57	MG	2A	3184	1/1	0.83	0.31	68,68,68,68	0
57	MG	2A	3339	1/1	0.83	0.11	73,73,73,73	0
57	MG	1A	3117	1/1	0.83	0.41	40,40,40,40	0
57	MG	2y	3005	1/1	0.83	0.07	101,101,101,101	0
57	MG	1A	3578	1/1	0.83	0.19	27,27,27,27	0
57	MG	1A	3946	1/1	0.83	0.12	64,64,64,64	0
57	MG	1A	3918	1/1	0.83	0.31	65,65,65,65	0
57	MG	1A	3332	1/1	0.83	0.35	54,54,54,54	0
57	MG	2A	3573	1/1	0.83	0.47	67,67,67,67	0
57	MG	1A	3328	1/1	0.83	0.15	53,53,53,53	0
57	MG	1A	3212	1/1	0.83	0.14	50,50,50,50	0
57	MG	2A	3646	1/1	0.83	0.35	78,78,78,78	0
57	MG	2A	3328	1/1	0.83	0.12	82,82,82,82	0
57	MG	1A	3842	1/1	0.83	0.20	30,30,30,30	0
57	MG	1A	3869	1/1	0.83	0.11	44,44,44,44	0
57	MG	2j	8002	1/1	0.83	0.07	79,79,79,79	0
57	MG	2A	3604	1/1	0.83	0.16	55,55,55,55	0
57	MG	1y	106	1/1	0.84	0.50	84,84,84,84	0
57	MG	2a	1671	1/1	0.84	0.11	66,66,66,66	0
57	MG	2Q	3002	1/1	0.84	0.26	61,61,61,61	0
57	MG	1a	1602	1/1	0.84	0.31	65,65,65,65	0
57	MG	2A	3168	1/1	0.84	0.09	61,61,61,61	0
57	MG	1A	3503	1/1	0.84	0.11	54,54,54,54	0
57	MG	1A	3154	1/1	0.84	0.15	59,59,59,59	0
57	MG	1A	3411	1/1	0.84	0.21	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3392	1/1	0.84	0.38	34,34,34,34	0
57	MG	1A	3264	1/1	0.84	0.22	49,49,49,49	0
57	MG	15	102	1/1	0.84	0.75	66,66,66,66	0
57	MG	1A	3344	1/1	0.84	0.21	64,64,64,64	0
57	MG	1A	3101	1/1	0.84	0.32	44,44,44,44	0
57	MG	1A	3848	1/1	0.84	0.12	66,66,66,66	0
57	MG	1A	3797	1/1	0.84	0.16	51,51,51,51	0
57	MG	1A	3349	1/1	0.84	0.28	59,59,59,59	0
57	MG	1a	1771	1/1	0.84	0.07	60,60,60,60	0
57	MG	1a	1824	1/1	0.84	0.17	74,74,74,74	0
57	MG	1A	4122	1/1	0.84	0.15	54,54,54,54	0
57	MG	2A	3163	1/1	0.84	0.52	78,78,78,78	0
57	MG	1y	105	1/1	0.84	0.18	93,93,93,93	0
57	MG	1A	3353	1/1	0.84	0.19	38,38,38,38	0
57	MG	2A	3427	1/1	0.84	0.13	71,71,71,71	0
57	MG	1B	206	1/1	0.84	0.13	74,74,74,74	0
57	MG	2A	3162	1/1	0.84	0.18	58,58,58,58	0
57	MG	1A	3301	1/1	0.84	0.33	51,51,51,51	0
57	MG	1A	3928	1/1	0.84	0.38	41,41,41,41	0
57	MG	1B	208	1/1	0.84	0.39	53,53,53,53	0
57	MG	1A	3209	1/1	0.84	0.14	61,61,61,61	0
57	MG	2T	3001	1/1	0.84	0.23	68,68,68,68	0
57	MG	2A	3516	1/1	0.84	0.12	70,70,70,70	0
57	MG	1A	4040	1/1	0.84	0.13	82,82,82,82	0
57	MG	C	8001	1/1	0.84	0.87	95,95,95,95	0
57	MG	2A	3749	1/1	0.84	0.10	54,54,54,54	0
57	MG	2A	3825	1/1	0.84	0.07	73,73,73,73	0
57	MG	2A	3706	1/1	0.84	0.08	57,57,57,57	0
57	MG	2A	3323	1/1	0.84	0.27	63,63,63,63	0
57	MG	1A	3204	1/1	0.84	0.25	61,61,61,61	0
57	MG	2A	3614	1/1	0.84	0.14	80,80,80,80	0
57	MG	2A	3338	1/1	0.84	0.23	73,73,73,73	0
57	MG	2A	3279	1/1	0.84	0.09	67,67,67,67	0
57	MG	1A	3347	1/1	0.84	0.61	40,40,40,40	0
57	MG	2A	3189	1/1	0.84	0.50	70,70,70,70	0
57	MG	1a	1710	1/1	0.84	0.16	73,73,73,73	0
57	MG	2a	1744	1/1	0.84	0.17	51,51,51,51	0
57	MG	1a	1855	1/1	0.84	0.30	80,80,80,80	0
57	MG	2a	1784	1/1	0.84	0.12	77,77,77,77	0
57	MG	2A	3666	1/1	0.84	0.17	46,46,46,46	0
57	MG	1a	1812	1/1	0.84	0.14	66,66,66,66	0
57	MG	1A	3039	1/1	0.84	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1672	1/1	0.84	0.10	74,74,74,74	0
57	MG	2A	3662	1/1	0.84	0.13	63,63,63,63	0
57	MG	1A	3853	1/1	0.84	0.12	52,52,52,52	0
57	MG	1A	3093	1/1	0.84	0.31	40,40,40,40	0
57	MG	1a	1860	1/1	0.84	0.14	83,83,83,83	0
57	MG	2A	3296	1/1	0.84	0.37	73,73,73,73	0
57	MG	2A	3383	1/1	0.84	0.18	56,56,56,56	0
57	MG	2A	3121	1/1	0.84	0.11	80,80,80,80	0
57	MG	1A	3966	1/1	0.84	0.08	55,55,55,55	0
57	MG	1A	3890	1/1	0.84	0.09	46,46,46,46	0
57	MG	1A	4109	1/1	0.84	0.18	62,62,62,62	0
57	MG	2i	8001	1/1	0.84	0.12	72,72,72,72	0
57	MG	2A	3409	1/1	0.84	0.32	75,75,75,75	0
57	MG	2E	304	1/1	0.84	0.16	69,69,69,69	0
57	MG	2A	3751	1/1	0.84	0.13	47,47,47,47	0
57	MG	1A	3740	1/1	0.84	0.13	57,57,57,57	0
57	MG	1a	1875	1/1	0.84	0.87	90,90,90,90	0
57	MG	2a	1798	1/1	0.84	0.09	69,69,69,69	0
57	MG	2A	3225	1/1	0.84	0.57	54,54,54,54	0
57	MG	1A	3625	1/1	0.84	0.14	42,42,42,42	0
57	MG	1R	201	1/1	0.84	0.21	42,42,42,42	0
57	MG	2a	1769	1/1	0.84	0.25	72,72,72,72	0
57	MG	1A	3261	1/1	0.84	0.12	58,58,58,58	0
57	MG	1A	3304	1/1	0.84	0.13	57,57,57,57	0
57	MG	1A	3546	1/1	0.84	0.18	59,59,59,59	0
57	MG	1A	3920	1/1	0.84	0.45	50,50,50,50	0
57	MG	2A	3473	1/1	0.84	0.16	37,37,37,37	0
57	MG	2A	3451	1/1	0.84	0.11	78,78,78,78	0
57	MG	2A	3173	1/1	0.84	0.19	58,58,58,58	0
57	MG	1A	3395	1/1	0.84	0.17	66,66,66,66	0
57	MG	2a	1772	1/1	0.85	0.19	66,66,66,66	0
57	MG	1a	1816	1/1	0.85	0.11	84,84,84,84	0
57	MG	1A	4057	1/1	0.85	0.10	73,73,73,73	0
57	MG	1A	4017	1/1	0.85	0.09	56,56,56,56	0
57	MG	10	105	1/1	0.85	0.12	66,66,66,66	0
57	MG	2A	3307	1/1	0.85	0.34	54,54,54,54	0
57	MG	1A	3037	1/1	0.85	0.15	52,52,52,52	0
57	MG	2q	201	1/1	0.85	0.15	64,64,64,64	0
57	MG	2A	3248	1/1	0.85	0.25	56,56,56,56	0
57	MG	2A	3705	1/1	0.85	0.24	83,83,83,83	0
57	MG	1A	3570	1/1	0.85	0.15	31,31,31,31	0
57	MG	1B	214	1/1	0.85	0.19	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3501	1/1	0.85	0.17	40,40,40,40	0
57	MG	1A	3491	1/1	0.85	0.17	45,45,45,45	0
57	MG	1a	1839	1/1	0.85	0.09	77,77,77,77	0
57	MG	2A	3703	1/1	0.85	0.08	79,79,79,79	0
57	MG	2B	3019	1/1	0.85	0.17	85,85,85,85	0
57	MG	2A	3807	1/1	0.85	0.21	84,84,84,84	0
57	MG	1a	1603	1/1	0.85	0.22	58,58,58,58	0
57	MG	15	103	1/1	0.85	0.16	68,68,68,68	0
57	MG	1A	3025	1/1	0.85	0.21	46,46,46,46	0
57	MG	2A	3809	1/1	0.85	0.06	73,73,73,73	0
57	MG	2A	3847	1/1	0.85	0.15	59,59,59,59	0
57	MG	1A	3845	1/1	0.85	0.18	23,23,23,23	0
57	MG	2x	101	1/1	0.85	0.23	89,89,89,89	0
57	MG	1A	3850	1/1	0.85	0.26	58,58,58,58	0
57	MG	1A	3790	1/1	0.85	0.07	38,38,38,38	0
57	MG	1a	1873	1/1	0.85	0.11	79,79,79,79	0
57	MG	1A	3180	1/1	0.85	0.43	49,49,49,49	0
57	MG	2A	3255	1/1	0.85	0.22	58,58,58,58	0
57	MG	1A	3241	1/1	0.85	0.23	52,52,52,52	0
57	MG	1A	3515	1/1	0.85	0.16	69,69,69,69	0
57	MG	2A	3777	1/1	0.85	0.15	69,69,69,69	0
57	MG	1a	1867	1/1	0.85	0.31	80,80,80,80	0
57	MG	2A	3725	1/1	0.85	0.13	58,58,58,58	0
57	MG	1d	503	1/1	0.85	0.12	69,69,69,69	0
57	MG	1A	3003	1/1	0.85	0.14	41,41,41,41	0
57	MG	1A	3166	1/1	0.85	0.17	70,70,70,70	0
57	MG	2A	3263	1/1	0.85	0.23	50,50,50,50	0
57	MG	1A	3849	1/1	0.85	0.30	46,46,46,46	0
57	MG	1x	3009	1/1	0.85	0.14	76,76,76,76	0
57	MG	2A	3273	1/1	0.85	0.17	82,82,82,82	0
57	MG	1A	3307	1/1	0.85	0.17	48,48,48,48	0
57	MG	2A	3282	1/1	0.85	0.29	74,74,74,74	0
57	MG	2A	3265	1/1	0.85	0.17	67,67,67,67	0
57	MG	1a	1854	1/1	0.85	0.23	68,68,68,68	0
57	MG	1A	3287	1/1	0.85	0.25	64,64,64,64	0
57	MG	1B	223	1/1	0.85	0.14	80,80,80,80	0
57	MG	1A	3127	1/1	0.85	0.11	65,65,65,65	0
57	MG	1F	308	1/1	0.85	0.22	57,57,57,57	0
57	MG	1A	3111	1/1	0.85	0.31	48,48,48,48	0
57	MG	1A	3184	1/1	0.85	0.12	47,47,47,47	0
57	MG	1A	3793	1/1	0.85	0.13	55,55,55,55	0
57	MG	1A	3519	1/1	0.85	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3282	1/1	0.85	0.24	67,67,67,67	0
57	MG	1A	4008	1/1	0.85	0.17	54,54,54,54	0
57	MG	1A	3440	1/1	0.85	0.25	48,48,48,48	0
57	MG	1A	3463	1/1	0.85	0.21	58,58,58,58	0
57	MG	2A	3693	1/1	0.85	0.38	75,75,75,75	0
57	MG	2A	3166	1/1	0.85	0.17	72,72,72,72	0
57	MG	1a	1803	1/1	0.85	0.09	61,61,61,61	0
57	MG	1A	3300	1/1	0.85	0.29	48,48,48,48	0
57	MG	2A	3251	1/1	0.85	0.20	75,75,75,75	0
57	MG	2a	1730	1/1	0.85	0.14	72,72,72,72	0
57	MG	1Z	303	1/1	0.85	0.46	74,74,74,74	0
57	MG	1a	1832	1/1	0.85	0.17	81,81,81,81	0
57	MG	2A	3259	1/1	0.85	0.18	83,83,83,83	0
57	MG	1A	3564	1/1	0.85	0.17	29,29,29,29	0
57	MG	2A	3010	1/1	0.85	0.22	41,41,41,41	0
57	MG	1a	1693	1/1	0.85	0.09	58,58,58,58	0
57	MG	1a	1865	1/1	0.85	0.15	85,85,85,85	0
57	MG	1a	1735	1/1	0.85	0.16	53,53,53,53	0
57	MG	2A	3228	1/1	0.85	0.46	57,57,57,57	0
57	MG	1A	3259	1/1	0.85	0.13	59,59,59,59	0
57	MG	1A	3054	1/1	0.85	0.29	65,65,65,65	0
57	MG	1A	3865	1/1	0.85	0.20	34,34,34,34	0
57	MG	2A	3234	1/1	0.85	0.20	71,71,71,71	0
57	MG	1A	3929	1/1	0.85	0.57	85,85,85,85	0
57	MG	1A	3628	1/1	0.85	0.11	41,41,41,41	0
57	MG	2a	1617	1/1	0.85	0.20	68,68,68,68	0
57	MG	1N	201	1/1	0.85	0.34	52,52,52,52	0
57	MG	1A	3311	1/1	0.85	0.26	38,38,38,38	0
57	MG	2A	3388	1/1	0.85	0.13	67,67,67,67	0
57	MG	1a	1694	1/1	0.85	0.11	63,63,63,63	0
57	MG	26	502	1/1	0.85	0.14	73,73,73,73	0
57	MG	1a	1697	1/1	0.85	0.38	60,60,60,60	0
57	MG	1a	1838	1/1	0.85	0.09	71,71,71,71	0
57	MG	1A	3118	1/1	0.86	0.52	47,47,47,47	0
57	MG	2A	3617	1/1	0.86	0.10	64,64,64,64	0
57	MG	2A	3078	1/1	0.86	0.33	51,51,51,51	0
57	MG	2A	3514	1/1	0.86	0.21	67,67,67,67	0
57	MG	2A	3489	1/1	0.86	0.12	41,41,41,41	0
57	MG	2A	3860	1/1	0.86	0.95	64,64,64,64	0
57	MG	1A	3211	1/1	0.86	0.14	55,55,55,55	0
57	MG	1A	3497	1/1	0.86	0.21	21,21,21,21	0
57	MG	10	102	1/1	0.86	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3022	1/1	0.86	0.11	44,44,44,44	0
57	MG	2E	305	1/1	0.86	0.12	65,65,65,65	0
57	MG	1A	3408	1/1	0.86	0.69	39,39,39,39	0
57	MG	1x	3007	1/1	0.86	0.12	72,72,72,72	0
57	MG	2A	3117	1/1	0.86	0.29	54,54,54,54	0
57	MG	1A	3407	1/1	0.86	0.58	41,41,41,41	0
57	MG	2a	1710	1/1	0.86	0.07	83,83,83,83	0
57	MG	1A	3724	1/1	0.86	0.21	67,67,67,67	0
57	MG	1A	3390	1/1	0.86	0.69	56,56,56,56	0
57	MG	1A	4045	1/1	0.86	0.36	72,72,72,72	0
57	MG	2a	1711	1/1	0.86	0.26	80,80,80,80	0
57	MG	2A	3806	1/1	0.86	0.16	76,76,76,76	0
57	MG	1A	3384	1/1	0.86	0.52	44,44,44,44	0
57	MG	1A	3128	1/1	0.86	0.29	45,45,45,45	0
57	MG	1a	1631	1/1	0.86	0.21	63,63,63,63	0
57	MG	23	102	1/1	0.86	0.42	68,68,68,68	0
57	MG	1a	1892	1/1	0.86	0.11	69,69,69,69	0
57	MG	1R	203	1/1	0.86	0.22	46,46,46,46	0
57	MG	1A	3852	1/1	0.86	0.14	43,43,43,43	0
57	MG	2A	3786	1/1	0.86	0.07	59,59,59,59	0
57	MG	2A	3298	1/1	0.86	0.16	55,55,55,55	0
57	MG	1A	3991	1/1	0.86	0.10	54,54,54,54	0
57	MG	13	101	1/1	0.86	0.25	76,76,76,76	0
57	MG	1A	3091	1/1	0.86	0.33	43,43,43,43	0
57	MG	1A	3426	1/1	0.86	0.13	63,63,63,63	0
57	MG	2A	3823	1/1	0.86	0.15	51,51,51,51	0
57	MG	1a	1611	1/1	0.86	0.08	68,68,68,68	0
57	MG	10	101	1/1	0.86	0.14	42,42,42,42	0
57	MG	1A	3296	1/1	0.86	0.80	52,52,52,52	0
57	MG	2A	3319	1/1	0.86	0.17	70,70,70,70	0
57	MG	1a	1688	1/1	0.86	0.14	76,76,76,76	0
57	MG	2A	3158	1/1	0.86	0.09	63,63,63,63	0
57	MG	2A	3747	1/1	0.86	0.16	45,45,45,45	0
57	MG	2a	1791	1/1	0.86	0.21	72,72,72,72	0
57	MG	2A	3079	1/1	0.86	0.20	82,82,82,82	0
57	MG	2A	3280	1/1	0.86	0.42	50,50,50,50	0
57	MG	1a	1753	1/1	0.86	0.11	71,71,71,71	0
57	MG	2A	3284	1/1	0.86	0.40	63,63,63,63	0
57	MG	1A	3683	1/1	0.86	0.11	52,52,52,52	0
57	MG	1A	3361	1/1	0.86	0.21	46,46,46,46	0
57	MG	1A	3092	1/1	0.86	0.52	48,48,48,48	0
57	MG	1A	3953	1/1	0.86	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3447	1/1	0.86	0.13	82,82,82,82	0
57	MG	1N	204	1/1	0.86	0.76	53,53,53,53	0
57	MG	2a	1792	1/1	0.86	0.12	75,75,75,75	0
57	MG	2A	3684	1/1	0.86	0.12	82,82,82,82	0
57	MG	1A	3574	1/1	0.86	0.20	29,29,29,29	0
57	MG	1A	3816	1/1	0.86	0.22	60,60,60,60	0
57	MG	1A	3281	1/1	0.86	0.10	79,79,79,79	0
57	MG	1A	3822	1/1	0.86	0.11	40,40,40,40	0
57	MG	1A	3990	1/1	0.86	0.25	63,63,63,63	0
57	MG	2A	3412	1/1	0.86	0.08	75,75,75,75	0
57	MG	1A	3164	1/1	0.86	0.57	44,44,44,44	0
57	MG	2A	3349	1/1	0.86	0.17	74,74,74,74	0
57	MG	2A	3406	1/1	0.86	0.29	72,72,72,72	0
57	MG	1A	3770	1/1	0.86	0.24	52,52,52,52	0
57	MG	2A	3790	1/1	0.86	0.08	58,58,58,58	0
57	MG	2A	3003	1/1	0.86	0.16	67,67,67,67	0
57	MG	2A	3601	1/1	0.86	0.14	75,75,75,75	0
57	MG	1A	3933	1/1	0.86	0.12	75,75,75,75	0
57	MG	2A	3215	1/1	0.86	0.30	46,46,46,46	0
57	MG	2A	3257	1/1	0.86	0.37	59,59,59,59	0
57	MG	1a	1601	1/1	0.86	0.10	53,53,53,53	0
57	MG	1A	3267	1/1	0.86	0.14	57,57,57,57	0
57	MG	2a	1637	1/1	0.86	0.16	67,67,67,67	0
57	MG	2A	3250	1/1	0.86	0.50	73,73,73,73	0
57	MG	1A	3985	1/1	0.86	0.14	59,59,59,59	0
57	MG	2A	3775	1/1	0.86	0.15	47,47,47,47	0
57	MG	2A	3086	1/1	0.86	0.11	73,73,73,73	0
57	MG	1A	3292	1/1	0.86	0.41	49,49,49,49	0
57	MG	1a	1813	1/1	0.86	0.15	72,72,72,72	0
57	MG	2A	3119	1/1	0.86	0.13	53,53,53,53	0
57	MG	2a	1785	1/1	0.86	0.13	73,73,73,73	0
57	MG	2a	1755	1/1	0.86	0.28	75,75,75,75	0
57	MG	2a	1788	1/1	0.86	0.13	76,76,76,76	0
57	MG	2A	3305	1/1	0.86	0.32	76,76,76,76	0
57	MG	1X	3005	1/1	0.86	0.34	52,52,52,52	0
57	MG	2A	3616	1/1	0.86	0.33	82,82,82,82	0
57	MG	1A	3369	1/1	0.86	0.41	62,62,62,62	0
57	MG	17	102	1/1	0.86	0.12	51,51,51,51	0
57	MG	2A	3057	1/1	0.86	0.15	66,66,66,66	0
57	MG	2A	3401	1/1	0.86	0.14	62,62,62,62	0
57	MG	1A	3723	1/1	0.86	0.09	67,67,67,67	0
57	MG	1A	3246	1/1	0.86	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3294	1/1	0.86	0.11	53,53,53,53	0
57	MG	2A	3574	1/1	0.86	0.08	69,69,69,69	0
57	MG	1A	3186	1/1	0.86	0.16	53,53,53,53	0
57	MG	2A	3123	1/1	0.86	0.12	46,46,46,46	0
57	MG	1n	502	1/1	0.86	0.26	66,66,66,66	0
57	MG	2A	3541	1/1	0.86	0.25	62,62,62,62	0
57	MG	1x	3002	1/1	0.86	0.29	74,74,74,74	0
57	MG	1A	3299	1/1	0.86	0.36	39,39,39,39	0
57	MG	25	103	1/1	0.86	0.50	68,68,68,68	0
57	MG	1A	3449	1/1	0.86	0.31	66,66,66,66	0
57	MG	1A	3327	1/1	0.86	0.43	46,46,46,46	0
57	MG	2A	3239	1/1	0.86	0.21	67,67,67,67	0
57	MG	1a	1853	1/1	0.86	0.12	63,63,63,63	0
57	MG	1f	3001	1/1	0.86	0.23	61,61,61,61	0
57	MG	18	104	1/1	0.86	0.23	58,58,58,58	0
57	MG	1B	204	1/1	0.87	0.13	70,70,70,70	0
57	MG	2A	3423	1/1	0.87	0.10	77,77,77,77	0
57	MG	2v	102	1/1	0.87	0.13	87,87,87,87	0
57	MG	1A	3935	1/1	0.87	0.10	57,57,57,57	0
57	MG	1A	3276	1/1	0.87	0.97	55,55,55,55	0
57	MG	2a	1620	1/1	0.87	0.22	73,73,73,73	0
57	MG	2a	1635	1/1	0.87	0.17	60,60,60,60	0
57	MG	2A	3036	1/1	0.87	0.18	72,72,72,72	0
57	MG	1A	3298	1/1	0.87	0.26	57,57,57,57	0
57	MG	1A	3979	1/1	0.87	0.10	53,53,53,53	0
57	MG	1a	1681	1/1	0.87	0.12	64,64,64,64	0
57	MG	2A	3621	1/1	0.87	0.12	86,86,86,86	0
57	MG	1A	3552	1/1	0.87	0.16	59,59,59,59	0
57	MG	1A	3062	1/1	0.87	0.25	36,36,36,36	0
57	MG	1a	1830	1/1	0.87	0.08	62,62,62,62	0
57	MG	2A	3316	1/1	0.87	0.09	62,62,62,62	0
57	MG	1A	3626	1/1	0.87	0.21	20,20,20,20	0
57	MG	1a	1809	1/1	0.87	0.13	69,69,69,69	0
57	MG	2r	3001	1/1	0.87	0.23	84,84,84,84	0
57	MG	1A	3372	1/1	0.87	0.14	65,65,65,65	0
57	MG	11	102	1/1	0.87	0.42	76,76,76,76	0
57	MG	2A	3641	1/1	0.87	0.07	69,69,69,69	0
57	MG	1A	3891	1/1	0.87	0.09	46,46,46,46	0
57	MG	2A	3077	1/1	0.87	0.11	71,71,71,71	0
57	MG	2A	3502	1/1	0.87	0.17	74,74,74,74	0
57	MG	1a	1629	1/1	0.87	0.15	69,69,69,69	0
57	MG	1A	3174	1/1	0.87	0.36	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3577	1/1	0.87	0.19	41,41,41,41	0
59	ZN	2n	501	1/1	0.87	0.10	106,106,106,106	0
57	MG	1A	3803	1/1	0.87	0.14	36,36,36,36	0
57	MG	2A	3071	1/1	0.87	0.15	62,62,62,62	0
57	MG	1a	1778	1/1	0.87	0.10	60,60,60,60	0
57	MG	2a	1762	1/1	0.87	0.15	75,75,75,75	0
57	MG	1A	3963	1/1	0.87	0.11	44,44,44,44	0
57	MG	1A	3171	1/1	0.87	0.37	44,44,44,44	0
57	MG	1A	3648	1/1	0.87	0.17	29,29,29,29	0
57	MG	1A	3050	1/1	0.87	0.11	59,59,59,59	0
57	MG	2A	3716	1/1	0.87	0.38	79,79,79,79	0
57	MG	2A	3575	1/1	0.87	0.07	82,82,82,82	0
57	MG	1A	3949	1/1	0.87	0.17	68,68,68,68	0
57	MG	2A	3180	1/1	0.87	0.20	59,59,59,59	0
57	MG	1a	1751	1/1	0.87	0.36	65,65,65,65	0
57	MG	1a	1728	1/1	0.87	0.18	52,52,52,52	0
57	MG	1A	4063	1/1	0.87	0.10	54,54,54,54	0
57	MG	1A	3266	1/1	0.87	0.16	60,60,60,60	0
57	MG	1a	1908	1/1	0.87	0.19	75,75,75,75	0
57	MG	2A	3254	1/1	0.87	0.27	69,69,69,69	0
57	MG	2A	3011	1/1	0.87	0.10	64,64,64,64	0
57	MG	1x	3006	1/1	0.87	0.12	62,62,62,62	0
57	MG	1A	3759	1/1	0.87	0.16	41,41,41,41	0
57	MG	2a	1774	1/1	0.87	0.21	68,68,68,68	0
57	MG	1a	1682	1/1	0.87	0.10	65,65,65,65	0
57	MG	2A	3258	1/1	0.87	0.43	67,67,67,67	0
57	MG	1A	3357	1/1	0.87	0.24	71,71,71,71	0
57	MG	2A	3283	1/1	0.87	0.42	61,61,61,61	0
57	MG	1a	1779	1/1	0.87	0.08	68,68,68,68	0
57	MG	2D	303	1/1	0.87	1.08	51,51,51,51	0
57	MG	1A	3656	1/1	0.87	0.14	33,33,33,33	0
57	MG	2a	1766	1/1	0.87	0.13	69,69,69,69	0
57	MG	2B	3001	1/1	0.87	0.26	80,80,80,80	0
57	MG	2B	3020	1/1	0.87	0.23	72,72,72,72	0
57	MG	2A	3505	1/1	0.87	0.11	67,67,67,67	0
57	MG	2A	3484	1/1	0.87	0.17	84,84,84,84	0
57	MG	2A	3816	1/1	0.87	0.09	80,80,80,80	0
57	MG	2j	8001	1/1	0.87	0.08	86,86,86,86	0
57	MG	2a	1776	1/1	0.87	0.17	67,67,67,67	0
57	MG	1A	3135	1/1	0.87	0.17	43,43,43,43	0
57	MG	1I	3001	1/1	0.87	0.12	80,80,80,80	0
57	MG	1A	3468	1/1	0.87	0.18	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1840	1/1	0.87	0.23	74,74,74,74	0
57	MG	1A	3736	1/1	0.87	0.27	69,69,69,69	0
57	MG	2A	3647	1/1	0.87	0.11	81,81,81,81	0
57	MG	2a	1736	1/1	0.87	0.17	67,67,67,67	0
57	MG	2A	3818	1/1	0.87	0.14	76,76,76,76	0
57	MG	2A	3207	1/1	0.87	0.15	73,73,73,73	0
57	MG	1D	3004	1/1	0.87	0.23	42,42,42,42	0
57	MG	2A	3052	1/1	0.87	0.15	62,62,62,62	0
57	MG	1B	226	1/1	0.87	0.18	46,46,46,46	0
57	MG	12	3001	1/1	0.87	0.14	52,52,52,52	0
57	MG	1A	3860	1/1	0.87	0.15	80,80,80,80	0
57	MG	1A	3659	1/1	0.87	0.12	61,61,61,61	0
57	MG	2A	3542	1/1	0.87	0.19	45,45,45,45	0
57	MG	2A	3302	1/1	0.87	0.23	90,90,90,90	0
57	MG	1V	201	1/1	0.87	0.30	47,47,47,47	0
57	MG	1A	3556	1/1	0.87	0.18	27,27,27,27	0
57	MG	2A	3565	1/1	0.87	0.14	69,69,69,69	0
57	MG	2A	3648	1/1	0.87	0.09	69,69,69,69	0
57	MG	1A	3368	1/1	0.87	0.29	51,51,51,51	0
57	MG	1A	3141	1/1	0.87	0.39	37,37,37,37	0
57	MG	1A	3285	1/1	0.87	0.17	55,55,55,55	0
57	MG	2A	3580	1/1	0.87	0.23	57,57,57,57	0
57	MG	2a	1778	1/1	0.88	0.14	91,91,91,91	0
57	MG	1A	4065	1/1	0.88	0.10	66,66,66,66	0
57	MG	1A	3499	1/1	0.88	0.15	24,24,24,24	0
57	MG	2A	3459	1/1	0.88	0.23	58,58,58,58	0
57	MG	1A	3364	1/1	0.88	0.14	66,66,66,66	0
57	MG	2A	3722	1/1	0.88	0.26	75,75,75,75	0
57	MG	2a	1688	1/1	0.88	0.12	62,62,62,62	0
57	MG	1A	3142	1/1	0.88	0.16	55,55,55,55	0
57	MG	1Z	304	1/1	0.88	0.16	58,58,58,58	0
57	MG	1A	3173	1/1	0.88	0.14	44,44,44,44	0
57	MG	2A	3138	1/1	0.88	0.22	70,70,70,70	0
57	MG	1A	3785	1/1	0.88	0.06	82,82,82,82	0
57	MG	2A	3331	1/1	0.88	0.26	64,64,64,64	0
57	MG	2A	3027	1/1	0.88	0.12	43,43,43,43	0
57	MG	2A	3075	1/1	0.88	0.18	56,56,56,56	0
57	MG	1A	3178	1/1	0.88	0.14	54,54,54,54	0
57	MG	2A	3539	1/1	0.88	0.20	83,83,83,83	0
57	MG	2A	3830	1/1	0.88	0.18	41,41,41,41	0
57	MG	1P	202	1/1	0.88	0.10	35,35,35,35	0
57	MG	2A	3622	1/1	0.88	0.11	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3031	1/1	0.88	0.14	62,62,62,62	0
57	MG	1A	3804	1/1	0.88	0.12	29,29,29,29	0
57	MG	2A	3781	1/1	0.88	0.14	59,59,59,59	0
57	MG	1A	3100	1/1	0.88	0.55	42,42,42,42	0
57	MG	2E	307	1/1	0.88	0.18	64,64,64,64	0
57	MG	2A	3226	1/1	0.88	0.27	73,73,73,73	0
57	MG	1A	3474	1/1	0.88	0.35	42,42,42,42	0
57	MG	2a	1641	1/1	0.88	0.20	62,62,62,62	0
57	MG	2A	3417	1/1	0.88	0.09	58,58,58,58	0
57	MG	2A	3819	1/1	0.88	0.13	57,57,57,57	0
57	MG	1a	1833	1/1	0.88	0.14	69,69,69,69	0
57	MG	1a	1644	1/1	0.88	0.25	74,74,74,74	0
57	MG	1A	3831	1/1	0.88	0.10	48,48,48,48	0
57	MG	1A	3335	1/1	0.88	0.10	55,55,55,55	0
57	MG	2A	3389	1/1	0.88	0.57	54,54,54,54	0
57	MG	1A	3315	1/1	0.88	0.13	61,61,61,61	0
57	MG	1A	3156	1/1	0.88	0.16	47,47,47,47	0
57	MG	2A	3019	1/1	0.88	0.26	75,75,75,75	0
57	MG	2A	3446	1/1	0.88	0.13	69,69,69,69	0
57	MG	1A	4028	1/1	0.88	0.14	60,60,60,60	0
57	MG	1A	3650	1/1	0.88	0.22	25,25,25,25	0
57	MG	2A	3091	1/1	0.88	0.09	75,75,75,75	0
57	MG	2A	3062	1/1	0.88	0.93	64,64,64,64	0
57	MG	1a	1818	1/1	0.88	0.06	74,74,74,74	0
57	MG	2A	3796	1/1	0.88	0.18	72,72,72,72	0
57	MG	1A	3455	1/1	0.88	0.12	50,50,50,50	0
57	MG	1a	1638	1/1	0.88	0.18	46,46,46,46	0
57	MG	1A	4015	1/1	0.88	0.26	56,56,56,56	0
57	MG	1A	4042	1/1	0.88	0.20	69,69,69,69	0
57	MG	1A	3944	1/1	0.88	0.31	62,62,62,62	0
57	MG	2A	3061	1/1	0.88	0.10	41,41,41,41	0
57	MG	1a	1780	1/1	0.88	0.05	65,65,65,65	0
57	MG	2a	1761	1/1	0.88	0.12	86,86,86,86	0
57	MG	2a	1648	1/1	0.88	0.09	74,74,74,74	0
57	MG	1A	4029	1/1	0.88	0.08	58,58,58,58	0
57	MG	2A	3067	1/1	0.88	0.94	52,52,52,52	0
57	MG	2A	3851	1/1	0.88	0.19	36,36,36,36	0
57	MG	2A	3449	1/1	0.88	0.23	54,54,54,54	0
57	MG	1a	1683	1/1	0.88	0.16	86,86,86,86	0
57	MG	1a	1646	1/1	0.88	0.12	70,70,70,70	0
57	MG	1A	3172	1/1	0.88	0.74	45,45,45,45	0
57	MG	2E	302	1/1	0.88	0.25	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3723	1/1	0.88	0.25	60,60,60,60	0
57	MG	1A	3586	1/1	0.88	0.19	41,41,41,41	0
57	MG	2V	202	1/1	0.88	0.16	58,58,58,58	0
57	MG	2A	3220	1/1	0.88	0.23	65,65,65,65	0
57	MG	2A	3520	1/1	0.88	0.24	62,62,62,62	0
57	MG	1A	3448	1/1	0.88	0.19	62,62,62,62	0
57	MG	1A	3316	1/1	0.88	0.28	52,52,52,52	0
57	MG	2A	3661	1/1	0.88	0.44	84,84,84,84	0
57	MG	2A	3253	1/1	0.88	0.46	79,79,79,79	0
57	MG	1w	102	1/1	0.88	0.14	73,73,73,73	0
57	MG	1A	4025	1/1	0.88	0.06	73,73,73,73	0
57	MG	1F	301	1/1	0.88	0.11	44,44,44,44	0
57	MG	1B	210	1/1	0.88	0.34	47,47,47,47	0
57	MG	1N	207	1/1	0.88	0.27	33,33,33,33	0
57	MG	2A	3135	1/1	0.88	0.15	63,63,63,63	0
57	MG	2A	3009	1/1	0.88	0.23	50,50,50,50	0
57	MG	1a	1672	1/1	0.88	0.21	62,62,62,62	0
57	MG	1A	3456	1/1	0.88	0.20	37,37,37,37	0
57	MG	1A	3454	1/1	0.88	0.17	67,67,67,67	0
57	MG	28	103	1/1	0.88	0.19	65,65,65,65	0
57	MG	2A	3343	1/1	0.88	0.24	57,57,57,57	0
57	MG	1a	1736	1/1	0.88	0.08	62,62,62,62	0
57	MG	2A	3540	1/1	0.88	0.11	59,59,59,59	0
57	MG	1A	4031	1/1	0.88	0.14	67,67,67,67	0
57	MG	1A	3237	1/1	0.88	0.15	64,64,64,64	0
57	MG	1A	3783	1/1	0.88	0.30	62,62,62,62	0
57	MG	1A	3245	1/1	0.88	0.27	60,60,60,60	0
57	MG	1a	1699	1/1	0.88	0.16	56,56,56,56	0
57	MG	1a	1784	1/1	0.88	0.12	67,67,67,67	0
57	MG	1A	3657	1/1	0.88	0.16	26,26,26,26	0
57	MG	1a	1606	1/1	0.88	0.07	62,62,62,62	0
57	MG	2a	1747	1/1	0.88	0.11	76,76,76,76	0
57	MG	1A	3743	1/1	0.88	0.17	58,58,58,58	0
57	MG	2A	3700	1/1	0.88	0.20	76,76,76,76	0
57	MG	2A	3630	1/1	0.88	0.32	50,50,50,50	0
57	MG	2A	3147	1/1	0.88	0.17	68,68,68,68	0
57	MG	1A	3583	1/1	0.88	0.14	42,42,42,42	0
57	MG	1A	4113	1/1	0.88	0.15	29,29,29,29	0
57	MG	1Z	302	1/1	0.88	0.15	60,60,60,60	0
57	MG	2A	3171	1/1	0.88	0.23	63,63,63,63	0
57	MG	1a	1871	1/1	0.88	0.10	96,96,96,96	0
57	MG	1A	3735	1/1	0.88	0.32	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1814	1/1	0.88	0.23	89,89,89,89	0
57	MG	28	102	1/1	0.88	0.09	73,73,73,73	0
57	MG	2A	3064	1/1	0.88	0.31	54,54,54,54	0
57	MG	1B	233	1/1	0.88	0.36	73,73,73,73	0
57	MG	1B	232	1/1	0.88	0.10	57,57,57,57	0
57	MG	2A	3202	1/1	0.88	0.15	61,61,61,61	0
57	MG	1A	3923	1/1	0.88	0.12	62,62,62,62	0
57	MG	1E	304	1/1	0.88	0.39	57,57,57,57	0
57	MG	1a	1848	1/1	0.88	0.29	82,82,82,82	0
57	MG	1A	3962	1/1	0.88	0.14	56,56,56,56	0
57	MG	2B	3018	1/1	0.88	0.17	80,80,80,80	0
57	MG	1A	3652	1/1	0.88	0.18	37,37,37,37	0
57	MG	1y	102	1/1	0.88	0.07	80,80,80,80	0
57	MG	1A	3280	1/1	0.88	0.15	57,57,57,57	0
57	MG	2a	1703	1/1	0.88	0.14	67,67,67,67	0
57	MG	1a	1605	1/1	0.88	0.13	66,66,66,66	0
57	MG	2A	3554	1/1	0.88	0.11	58,58,58,58	0
57	MG	1W	202	1/1	0.88	0.16	51,51,51,51	0
57	MG	1A	3781	1/1	0.88	0.17	26,26,26,26	0
57	MG	1A	3765	1/1	0.88	0.20	65,65,65,65	0
57	MG	1A	3681	1/1	0.88	0.16	37,37,37,37	0
57	MG	2A	3513	1/1	0.88	0.17	68,68,68,68	0
57	MG	1A	3647	1/1	0.88	0.16	35,35,35,35	0
57	MG	2a	1680	1/1	0.89	0.11	88,88,88,88	0
57	MG	1a	1901	1/1	0.89	0.23	64,64,64,64	0
57	MG	1A	3063	1/1	0.89	0.74	50,50,50,50	0
57	MG	2A	3591	1/1	0.89	0.13	76,76,76,76	0
57	MG	1A	3217	1/1	0.89	0.53	46,46,46,46	0
57	MG	1a	1792	1/1	0.89	0.11	69,69,69,69	0
57	MG	1A	3653	1/1	0.89	0.17	33,33,33,33	0
57	MG	1A	3356	1/1	0.89	0.23	36,36,36,36	0
57	MG	2A	3652	1/1	0.89	0.19	72,72,72,72	0
57	MG	1A	4020	1/1	0.89	0.10	57,57,57,57	0
57	MG	1A	3763	1/1	0.89	0.15	35,35,35,35	0
57	MG	2A	3637	1/1	0.89	0.13	47,47,47,47	0
57	MG	1a	1716	1/1	0.89	0.12	74,74,74,74	0
57	MG	2A	3561	1/1	0.89	0.32	80,80,80,80	0
57	MG	1S	3002	1/1	0.89	0.17	47,47,47,47	0
57	MG	1A	3346	1/1	0.89	0.22	56,56,56,56	0
57	MG	1A	3444	1/1	0.89	0.24	53,53,53,53	0
57	MG	1A	3196	1/1	0.89	0.47	56,56,56,56	0
57	MG	2A	3718	1/1	0.89	0.55	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1754	1/1	0.89	0.08	67,67,67,67	0
57	MG	1U	202	1/1	0.89	0.19	58,58,58,58	0
57	MG	1A	3642	1/1	0.89	0.18	54,54,54,54	0
57	MG	2A	3853	1/1	0.89	0.21	57,57,57,57	0
57	MG	1A	3387	1/1	0.89	0.13	63,63,63,63	0
57	MG	2a	1623	1/1	0.89	0.23	78,78,78,78	0
57	MG	1A	3325	1/1	0.89	0.38	47,47,47,47	0
57	MG	2A	3304	1/1	0.89	0.23	87,87,87,87	0
57	MG	1A	3768	1/1	0.89	0.10	60,60,60,60	0
57	MG	1a	1883	1/1	0.89	0.22	69,69,69,69	0
57	MG	1A	3420	1/1	0.89	0.29	39,39,39,39	0
57	MG	2a	1771	1/1	0.89	0.24	78,78,78,78	0
57	MG	2A	3792	1/1	0.89	0.17	72,72,72,72	0
57	MG	1a	1797	1/1	0.89	0.07	72,72,72,72	0
57	MG	1A	3618	1/1	0.89	0.14	56,56,56,56	0
57	MG	1A	3855	1/1	0.89	0.19	27,27,27,27	0
57	MG	2d	502	1/1	0.89	0.12	75,75,75,75	0
57	MG	2A	3778	1/1	0.89	0.16	75,75,75,75	0
57	MG	1a	1825	1/1	0.89	0.16	76,76,76,76	0
57	MG	1A	3234	1/1	0.89	0.10	38,38,38,38	0
57	MG	2A	3674	1/1	0.89	0.11	63,63,63,63	0
57	MG	1a	1829	1/1	0.89	0.16	50,50,50,50	0
57	MG	2a	1614	1/1	0.89	0.23	70,70,70,70	0
57	MG	1a	1772	1/1	0.89	0.13	85,85,85,85	0
57	MG	2a	1764	1/1	0.89	0.15	65,65,65,65	0
57	MG	1A	4071	1/1	0.89	0.11	82,82,82,82	0
57	MG	1A	4044	1/1	0.89	0.19	57,57,57,57	0
57	MG	1A	3787	1/1	0.89	0.20	75,75,75,75	0
57	MG	2A	3396	1/1	0.89	0.34	61,61,61,61	0
57	MG	2A	3592	1/1	0.89	0.14	77,77,77,77	0
57	MG	1A	4022	1/1	0.89	0.12	63,63,63,63	0
57	MG	1A	3167	1/1	0.89	0.19	46,46,46,46	0
57	MG	1A	3144	1/1	0.89	0.09	72,72,72,72	0
57	MG	1F	305	1/1	0.89	0.17	47,47,47,47	0
57	MG	1A	3999	1/1	0.89	0.09	66,66,66,66	0
57	MG	2A	3157	1/1	0.89	0.10	70,70,70,70	0
57	MG	1A	3746	1/1	0.89	0.10	36,36,36,36	0
57	MG	1A	3674	1/1	0.89	0.10	61,61,61,61	0
57	MG	1A	3134	1/1	0.89	0.23	51,51,51,51	0
57	MG	10	104	1/1	0.89	0.18	61,61,61,61	0
57	MG	2a	1665	1/1	0.89	0.21	70,70,70,70	0
57	MG	1A	3769	1/1	0.89	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3468	1/1	0.89	0.18	73,73,73,73	0
57	MG	1a	1658	1/1	0.89	0.15	52,52,52,52	0
57	MG	1A	3200	1/1	0.89	0.15	53,53,53,53	0
57	MG	2a	1719	1/1	0.89	0.06	82,82,82,82	0
57	MG	1A	3380	1/1	0.89	0.35	37,37,37,37	0
57	MG	2A	3136	1/1	0.89	0.23	48,48,48,48	0
57	MG	1A	3132	1/1	0.89	0.12	50,50,50,50	0
57	MG	2A	3609	1/1	0.89	0.07	72,72,72,72	0
57	MG	1A	3199	1/1	0.89	0.11	70,70,70,70	0
57	MG	1A	3911	1/1	0.89	0.12	48,48,48,48	0
57	MG	1A	3269	1/1	0.89	0.15	62,62,62,62	0
57	MG	1A	4075	1/1	0.89	0.92	51,51,51,51	0
57	MG	2A	3462	1/1	0.89	0.15	47,47,47,47	0
57	MG	2a	1655	1/1	0.89	0.12	67,67,67,67	0
57	MG	1A	3719	1/1	0.89	0.14	66,66,66,66	0
57	MG	2E	308	1/1	0.89	0.15	73,73,73,73	0
57	MG	2a	1611	1/1	0.89	0.27	67,67,67,67	0
57	MG	1A	3215	1/1	0.89	0.19	66,66,66,66	0
57	MG	1A	3379	1/1	0.89	0.39	49,49,49,49	0
57	MG	2A	3547	1/1	0.89	0.15	40,40,40,40	0
57	MG	1A	3404	1/1	0.89	0.29	51,51,51,51	0
57	MG	2A	3314	1/1	0.89	0.08	68,68,68,68	0
57	MG	1A	3464	1/1	0.89	0.29	70,70,70,70	0
57	MG	1A	3646	1/1	0.89	0.21	21,21,21,21	0
57	MG	2A	3112	1/1	0.89	0.18	57,57,57,57	0
57	MG	2A	3544	1/1	0.89	0.18	42,42,42,42	0
57	MG	2A	3721	1/1	0.89	0.22	62,62,62,62	0
57	MG	2A	3385	1/1	0.89	0.12	69,69,69,69	0
57	MG	2A	3458	1/1	0.89	0.16	38,38,38,38	0
57	MG	2A	3414	1/1	0.89	0.07	64,64,64,64	0
57	MG	1A	3179	1/1	0.89	0.39	47,47,47,47	0
57	MG	1a	1804	1/1	0.89	0.07	53,53,53,53	0
57	MG	1r	3001	1/1	0.89	0.28	66,66,66,66	0
57	MG	1A	3194	1/1	0.89	0.38	61,61,61,61	0
57	MG	1A	3265	1/1	0.89	0.25	56,56,56,56	0
57	MG	2A	3230	1/1	0.89	0.28	67,67,67,67	0
57	MG	2A	3479	1/1	0.89	0.15	48,48,48,48	0
57	MG	1A	3772	1/1	0.89	0.33	45,45,45,45	0
57	MG	1A	3695	1/1	0.89	0.14	35,35,35,35	0
57	MG	2A	3146	1/1	0.89	0.34	59,59,59,59	0
57	MG	2a	1714	1/1	0.89	0.13	58,58,58,58	0
57	MG	2a	1775	1/1	0.89	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3649	1/1	0.89	0.07	61,61,61,61	0
57	MG	1A	3941	1/1	0.89	0.10	50,50,50,50	0
57	MG	2A	3340	1/1	0.89	0.14	77,77,77,77	0
57	MG	1A	3885	1/1	0.89	0.18	55,55,55,55	0
57	MG	1a	1685	1/1	0.89	0.13	74,74,74,74	0
57	MG	1A	3597	1/1	0.89	0.10	56,56,56,56	0
57	MG	2A	3728	1/1	0.89	0.40	71,71,71,71	0
57	MG	2a	1642	1/1	0.89	0.07	74,74,74,74	0
57	MG	1A	3930	1/1	0.89	0.23	59,59,59,59	0
57	MG	2A	3025	1/1	0.89	0.08	53,53,53,53	0
57	MG	1A	3788	1/1	0.89	0.21	76,76,76,76	0
57	MG	2a	1742	1/1	0.89	0.17	83,83,83,83	0
57	MG	2a	1612	1/1	0.89	0.14	65,65,65,65	0
57	MG	1a	1668	1/1	0.89	0.28	67,67,67,67	0
57	MG	1A	3396	1/1	0.89	0.20	55,55,55,55	0
57	MG	1m	201	1/1	0.89	0.10	72,72,72,72	0
57	MG	1A	3351	1/1	0.89	0.47	45,45,45,45	0
57	MG	1A	3950	1/1	0.89	0.23	62,62,62,62	0
57	MG	1A	4104	1/1	0.89	0.17	53,53,53,53	0
57	MG	2A	3846	1/1	0.89	0.15	80,80,80,80	0
57	MG	1A	3472	1/1	0.89	0.18	50,50,50,50	0
57	MG	1A	4002	1/1	0.89	0.11	77,77,77,77	0
57	MG	1A	3163	1/1	0.89	0.09	55,55,55,55	0
57	MG	1A	3729	1/1	0.89	0.16	62,62,62,62	0
57	MG	2A	3310	1/1	0.89	0.19	65,65,65,65	0
57	MG	2A	3828	1/1	0.89	0.07	74,74,74,74	0
57	MG	2a	1717	1/1	0.89	0.11	85,85,85,85	0
57	MG	1A	3839	1/1	0.89	0.36	76,76,76,76	0
57	MG	2A	3457	1/1	0.89	0.21	52,52,52,52	0
57	MG	2A	3181	1/1	0.89	0.36	62,62,62,62	0
57	MG	1A	3046	1/1	0.89	0.17	52,52,52,52	0
57	MG	1A	3758	1/1	0.89	0.13	44,44,44,44	0
57	MG	1A	3324	1/1	0.89	0.17	50,50,50,50	0
57	MG	2A	3856	1/1	0.89	0.40	49,49,49,49	0
57	MG	1A	3568	1/1	0.89	0.20	57,57,57,57	0
57	MG	1A	3643	1/1	0.89	0.20	23,23,23,23	0
57	MG	1A	3862	1/1	0.89	0.14	37,37,37,37	0
57	MG	1A	3313	1/1	0.89	0.54	52,52,52,52	0
57	MG	1A	3882	1/1	0.89	0.09	37,37,37,37	0
57	MG	1A	3358	1/1	0.90	0.56	50,50,50,50	0
57	MG	2A	3612	1/1	0.90	0.18	56,56,56,56	0
57	MG	1A	4036	1/1	0.90	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3590	1/1	0.90	0.17	22,22,22,22	0
57	MG	2A	3534	1/1	0.90	0.12	72,72,72,72	0
57	MG	1A	3226	1/1	0.90	0.73	39,39,39,39	0
57	MG	1a	1709	1/1	0.90	0.32	61,61,61,61	0
57	MG	1A	3221	1/1	0.90	0.46	42,42,42,42	0
57	MG	2A	3128	1/1	0.90	0.12	62,62,62,62	0
57	MG	1A	3121	1/1	0.90	0.20	52,52,52,52	0
57	MG	2A	3854	1/1	0.90	0.25	53,53,53,53	0
57	MG	1A	3980	1/1	0.90	0.16	57,57,57,57	0
57	MG	1A	3925	1/1	0.90	0.21	68,68,68,68	0
57	MG	1a	1845	1/1	0.90	0.19	79,79,79,79	0
57	MG	2A	3607	1/1	0.90	0.10	68,68,68,68	0
57	MG	1a	1886	1/1	0.90	0.15	83,83,83,83	0
57	MG	2A	3784	1/1	0.90	0.14	56,56,56,56	0
57	MG	1A	3967	1/1	0.90	0.15	65,65,65,65	0
57	MG	1O	3001	1/1	0.90	0.30	70,70,70,70	0
57	MG	1a	1670	1/1	0.90	0.20	64,64,64,64	0
57	MG	1A	3076	1/1	0.90	0.22	32,32,32,32	0
57	MG	1A	3727	1/1	0.90	0.18	16,16,16,16	0
57	MG	1a	1863	1/1	0.90	0.17	73,73,73,73	0
57	MG	1A	3257	1/1	0.90	0.13	61,61,61,61	0
57	MG	1A	4119	1/1	0.90	0.29	39,39,39,39	0
57	MG	1A	4127	1/1	0.90	0.21	33,33,33,33	0
57	MG	2A	3134	1/1	0.90	0.21	63,63,63,63	0
57	MG	1A	4110	1/1	0.90	0.45	69,69,69,69	0
57	MG	1A	3690	1/1	0.90	0.45	62,62,62,62	0
57	MG	1A	3240	1/1	0.90	0.15	35,35,35,35	0
57	MG	1A	3994	1/1	0.90	0.27	54,54,54,54	0
57	MG	1A	4070	1/1	0.90	0.42	66,66,66,66	0
57	MG	2A	3040	1/1	0.90	0.17	62,62,62,62	0
57	MG	1B	211	1/1	0.90	0.16	51,51,51,51	0
57	MG	2a	1662	1/1	0.90	0.11	66,66,66,66	0
57	MG	2B	3008	1/1	0.90	0.16	70,70,70,70	0
57	MG	2a	1627	1/1	0.90	0.11	71,71,71,71	0
57	MG	1A	3323	1/1	0.90	0.19	56,56,56,56	0
57	MG	2a	1625	1/1	0.90	0.27	67,67,67,67	0
57	MG	1A	3760	1/1	0.90	0.23	25,25,25,25	0
57	MG	2A	3497	1/1	0.90	0.14	63,63,63,63	0
57	MG	2A	3739	1/1	0.90	0.18	73,73,73,73	0
57	MG	1A	3703	1/1	0.90	0.10	43,43,43,43	0
57	MG	1A	3818	1/1	0.90	0.23	72,72,72,72	0
57	MG	1A	3670	1/1	0.90	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1751	1/1	0.90	0.08	77,77,77,77	0
57	MG	1A	3476	1/1	0.90	0.73	33,33,33,33	0
57	MG	2A	3271	1/1	0.90	0.16	69,69,69,69	0
57	MG	2B	3004	1/1	0.90	0.17	79,79,79,79	0
57	MG	2A	3643	1/1	0.90	0.23	64,64,64,64	0
57	MG	2A	3746	1/1	0.90	0.10	79,79,79,79	0
57	MG	1A	3236	1/1	0.90	0.14	58,58,58,58	0
57	MG	1A	3309	1/1	0.90	0.49	39,39,39,39	0
57	MG	2A	3550	1/1	0.90	0.11	40,40,40,40	0
57	MG	1A	3244	1/1	0.90	0.19	52,52,52,52	0
57	MG	1A	3779	1/1	0.90	0.17	29,29,29,29	0
57	MG	2A	3139	1/1	0.90	0.41	46,46,46,46	0
57	MG	1B	207	1/1	0.90	0.11	71,71,71,71	0
57	MG	2A	3677	1/1	0.90	0.16	64,64,64,64	0
57	MG	1A	3362	1/1	0.90	0.27	54,54,54,54	0
57	MG	1A	3416	1/1	0.90	0.23	36,36,36,36	0
57	MG	2A	3088	1/1	0.90	0.10	51,51,51,51	0
57	MG	2a	1752	1/1	0.90	0.15	74,74,74,74	0
57	MG	1A	3498	1/1	0.90	0.20	48,48,48,48	0
57	MG	2A	3118	1/1	0.90	0.12	71,71,71,71	0
57	MG	1A	3077	1/1	0.90	0.45	39,39,39,39	0
57	MG	2A	3126	1/1	0.90	0.43	49,49,49,49	0
57	MG	1A	3445	1/1	0.90	0.24	61,61,61,61	0
57	MG	2a	1691	1/1	0.90	0.22	68,68,68,68	0
57	MG	2A	3464	1/1	0.90	0.14	67,67,67,67	0
57	MG	2T	3003	1/1	0.90	0.21	57,57,57,57	0
57	MG	2A	3332	1/1	0.90	0.13	77,77,77,77	0
57	MG	2A	3569	1/1	0.90	0.36	68,68,68,68	0
57	MG	2A	3195	1/1	0.90	0.45	67,67,67,67	0
57	MG	1A	3709	1/1	0.90	0.12	56,56,56,56	0
57	MG	1a	1741	1/1	0.90	0.16	83,83,83,83	0
57	MG	2A	3241	1/1	0.90	0.12	60,60,60,60	0
57	MG	2A	3398	1/1	0.90	0.14	58,58,58,58	0
57	MG	1A	3248	1/1	0.90	0.13	51,51,51,51	0
57	MG	2A	3692	1/1	0.90	0.07	69,69,69,69	0
57	MG	1A	3799	1/1	0.90	0.14	14,14,14,14	0
57	MG	1U	201	1/1	0.90	0.29	38,38,38,38	0
57	MG	1a	1793	1/1	0.90	0.11	61,61,61,61	0
57	MG	1A	3393	1/1	0.90	0.21	55,55,55,55	0
57	MG	1A	3558	1/1	0.90	0.18	26,26,26,26	0
57	MG	1a	1627	1/1	0.90	0.32	62,62,62,62	0
57	MG	1A	3486	1/1	0.90	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1843	1/1	0.90	0.05	84,84,84,84	0
57	MG	2A	3308	1/1	0.90	0.89	62,62,62,62	0
57	MG	2A	3172	1/1	0.90	0.37	72,72,72,72	0
57	MG	1A	3017	1/1	0.90	0.21	56,56,56,56	0
57	MG	1A	3598	1/1	0.90	0.16	50,50,50,50	0
57	MG	1A	3649	1/1	0.90	0.11	31,31,31,31	0
57	MG	2A	3472	1/1	0.90	0.14	44,44,44,44	0
57	MG	2A	3535	1/1	0.90	0.14	57,57,57,57	0
57	MG	2A	3633	1/1	0.90	0.08	55,55,55,55	0
57	MG	1A	3254	1/1	0.90	0.26	41,41,41,41	0
57	MG	2A	3570	1/1	0.90	0.18	55,55,55,55	0
57	MG	2a	1644	1/1	0.90	0.09	58,58,58,58	0
57	MG	1A	3528	1/1	0.90	0.19	42,42,42,42	0
57	MG	1O	3003	1/1	0.90	0.19	71,71,71,71	0
57	MG	2A	3774	1/1	0.90	0.07	65,65,65,65	0
57	MG	1A	3129	1/1	0.90	0.20	46,46,46,46	0
57	MG	2A	3408	1/1	0.90	0.17	56,56,56,56	0
57	MG	2a	1760	1/1	0.90	0.13	77,77,77,77	0
57	MG	2A	3758	1/1	0.90	0.07	77,77,77,77	0
57	MG	2A	3410	1/1	0.90	0.41	46,46,46,46	0
57	MG	2A	3420	1/1	0.90	0.09	60,60,60,60	0
57	MG	2A	3120	1/1	0.90	0.19	47,47,47,47	0
57	MG	2A	3735	1/1	0.90	0.10	62,62,62,62	0
57	MG	1a	1890	1/1	0.90	0.17	63,63,63,63	0
57	MG	1A	3355	1/1	0.90	0.22	60,60,60,60	0
57	MG	2X	3003	1/1	0.90	0.14	60,60,60,60	0
57	MG	1a	1822	1/1	0.90	0.20	55,55,55,55	0
57	MG	2a	1746	1/1	0.90	0.15	70,70,70,70	0
57	MG	1x	3005	1/1	0.90	0.15	68,68,68,68	0
57	MG	2A	3274	1/1	0.90	0.60	79,79,79,79	0
57	MG	2A	3673	1/1	0.90	0.06	62,62,62,62	0
57	MG	2A	3233	1/1	0.90	0.22	75,75,75,75	0
57	MG	2A	3380	1/1	0.90	0.15	71,71,71,71	0
57	MG	1a	1641	1/1	0.90	0.16	76,76,76,76	0
57	MG	1A	3197	1/1	0.90	0.12	61,61,61,61	0
57	MG	1A	3637	1/1	0.90	0.12	46,46,46,46	0
57	MG	2A	3364	1/1	0.90	0.30	58,58,58,58	0
57	MG	1A	3868	1/1	0.90	0.12	41,41,41,41	0
57	MG	1A	3460	1/1	0.90	0.35	34,34,34,34	0
57	MG	1X	3002	1/1	0.90	0.31	39,39,39,39	0
57	MG	1A	4038	1/1	0.90	0.12	59,59,59,59	0
57	MG	1A	3176	1/1	0.90	0.61	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3682	1/1	0.90	0.13	51,51,51,51	0
57	MG	2A	3353	1/1	0.90	0.10	78,78,78,78	0
57	MG	2A	3628	1/1	0.90	0.16	55,55,55,55	0
57	MG	1a	1776	1/1	0.90	0.16	74,74,74,74	0
57	MG	1A	4090	1/1	0.90	0.41	52,52,52,52	0
57	MG	2G	3001	1/1	0.90	0.20	81,81,81,81	0
57	MG	1A	3042	1/1	0.90	0.18	57,57,57,57	0
57	MG	1A	3702	1/1	0.90	0.32	71,71,71,71	0
57	MG	2A	3115	1/1	0.90	0.09	63,63,63,63	0
57	MG	1B	217	1/1	0.90	0.17	37,37,37,37	0
57	MG	2a	1799	1/1	0.90	0.25	78,78,78,78	0
57	MG	1A	3595	1/1	0.91	0.34	52,52,52,52	0
57	MG	2A	3116	1/1	0.91	0.08	75,75,75,75	0
57	MG	2A	3586	1/1	0.91	0.14	54,54,54,54	0
57	MG	1A	3412	1/1	0.91	0.95	54,54,54,54	0
57	MG	1a	1763	1/1	0.91	0.08	65,65,65,65	0
57	MG	2B	3015	1/1	0.91	0.12	81,81,81,81	0
57	MG	2A	3276	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3207	1/1	0.91	0.22	48,48,48,48	0
57	MG	1A	4091	1/1	0.91	1.10	50,50,50,50	0
57	MG	1A	3206	1/1	0.91	0.43	32,32,32,32	0
57	MG	2A	3568	1/1	0.91	0.10	88,88,88,88	0
57	MG	1A	3339	1/1	0.91	0.21	52,52,52,52	0
57	MG	2A	3041	1/1	0.91	0.26	67,67,67,67	0
57	MG	2A	3699	1/1	0.91	0.15	73,73,73,73	0
57	MG	1a	1889	1/1	0.91	0.23	75,75,75,75	0
57	MG	1A	3106	1/1	0.91	0.49	38,38,38,38	0
57	MG	1A	3716	1/1	0.91	0.17	39,39,39,39	0
57	MG	1a	1760	1/1	0.91	0.17	66,66,66,66	0
57	MG	2A	3793	1/1	0.91	0.16	79,79,79,79	0
57	MG	1A	3430	1/1	0.91	0.52	51,51,51,51	0
57	MG	2A	3216	1/1	0.91	0.61	44,44,44,44	0
57	MG	1a	1703	1/1	0.91	0.29	60,60,60,60	0
57	MG	1A	3609	1/1	0.91	0.10	49,49,49,49	0
57	MG	1A	3018	1/1	0.91	0.14	76,76,76,76	0
57	MG	1A	4035	1/1	0.91	0.11	76,76,76,76	0
57	MG	1A	3386	1/1	0.91	0.14	55,55,55,55	0
57	MG	1D	3008	1/1	0.91	0.34	47,47,47,47	0
57	MG	2A	3668	1/1	0.91	0.60	50,50,50,50	0
57	MG	1A	3645	1/1	0.91	0.18	44,44,44,44	0
57	MG	1A	3098	1/1	0.91	0.11	35,35,35,35	0
57	MG	2A	3686	1/1	0.91	0.19	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1846	1/1	0.91	0.13	73,73,73,73	0
57	MG	1a	1613	1/1	0.91	0.09	58,58,58,58	0
57	MG	1A	3734	1/1	0.91	0.13	64,64,64,64	0
57	MG	2A	3196	1/1	0.91	0.99	60,60,60,60	0
57	MG	1A	3160	1/1	0.91	0.15	42,42,42,42	0
57	MG	1A	3275	1/1	0.91	0.18	61,61,61,61	0
57	MG	2a	1739	1/1	0.91	0.11	59,59,59,59	0
57	MG	1A	3745	1/1	0.91	0.23	44,44,44,44	0
57	MG	2A	3670	1/1	0.91	0.16	54,54,54,54	0
57	MG	2A	3034	1/1	0.91	0.14	69,69,69,69	0
57	MG	1A	3303	1/1	0.91	0.66	47,47,47,47	0
57	MG	2A	3313	1/1	0.91	0.15	75,75,75,75	0
57	MG	1A	4086	1/1	0.91	0.18	30,30,30,30	0
57	MG	1N	206	1/1	0.91	0.19	50,50,50,50	0
57	MG	1A	3764	1/1	0.91	0.13	23,23,23,23	0
57	MG	2A	3545	1/1	0.91	0.12	53,53,53,53	0
57	MG	2A	3391	1/1	0.91	0.77	46,46,46,46	0
57	MG	1A	3146	1/1	0.91	0.23	60,60,60,60	0
57	MG	1A	3083	1/1	0.91	0.38	40,40,40,40	0
57	MG	1A	3067	1/1	0.91	0.33	63,63,63,63	0
57	MG	2A	3366	1/1	0.91	0.13	49,49,49,49	0
57	MG	1A	3977	1/1	0.91	0.21	75,75,75,75	0
57	MG	1A	3879	1/1	0.91	0.08	75,75,75,75	0
57	MG	1a	1647	1/1	0.91	0.10	72,72,72,72	0
57	MG	2A	3155	1/1	0.91	0.10	62,62,62,62	0
57	MG	2A	3357	1/1	0.91	0.23	49,49,49,49	0
57	MG	2A	3065	1/1	0.91	0.30	53,53,53,53	0
57	MG	2a	1735	1/1	0.91	0.13	66,66,66,66	0
57	MG	1A	3469	1/1	0.91	0.25	70,70,70,70	0
57	MG	1A	3605	1/1	0.91	0.16	55,55,55,55	0
57	MG	2A	3761	1/1	0.91	0.17	41,41,41,41	0
57	MG	2a	1613	1/1	0.91	0.09	63,63,63,63	0
57	MG	2A	3297	1/1	0.91	0.90	61,61,61,61	0
57	MG	2E	310	1/1	0.91	0.18	43,43,43,43	0
57	MG	2A	3277	1/1	0.91	0.16	67,67,67,67	0
57	MG	2A	3460	1/1	0.91	0.15	55,55,55,55	0
57	MG	16	102	1/1	0.91	0.29	57,57,57,57	0
57	MG	2A	3583	1/1	0.91	0.13	68,68,68,68	0
57	MG	1A	4013	1/1	0.91	0.22	63,63,63,63	0
57	MG	1B	234	1/1	0.91	0.29	84,84,84,84	0
57	MG	1a	1651	1/1	0.91	0.16	76,76,76,76	0
57	MG	1a	1777	1/1	0.91	0.10	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3399	1/1	0.91	0.17	69,69,69,69	0
57	MG	1A	3413	1/1	0.91	0.09	84,84,84,84	0
57	MG	1a	1903	1/1	0.91	0.22	77,77,77,77	0
57	MG	2a	1660	1/1	0.91	0.21	72,72,72,72	0
57	MG	2A	3192	1/1	0.91	0.15	62,62,62,62	0
57	MG	2A	3083	1/1	0.91	0.10	63,63,63,63	0
57	MG	1A	4000	1/1	0.91	0.11	77,77,77,77	0
57	MG	1A	3908	1/1	0.91	0.13	56,56,56,56	0
57	MG	1A	4077	1/1	0.91	0.21	51,51,51,51	0
57	MG	1w	101	1/1	0.91	0.21	65,65,65,65	0
57	MG	1X	3003	1/1	0.91	0.28	51,51,51,51	0
57	MG	1A	3959	1/1	0.91	0.23	61,61,61,61	0
57	MG	1A	3599	1/1	0.91	0.13	61,61,61,61	0
57	MG	2A	3509	1/1	0.91	0.09	64,64,64,64	0
57	MG	1B	230	1/1	0.91	0.14	72,72,72,72	0
57	MG	1A	3600	1/1	0.91	0.09	67,67,67,67	0
57	MG	1a	1836	1/1	0.91	0.22	62,62,62,62	0
57	MG	1A	3720	1/1	0.91	0.14	51,51,51,51	0
57	MG	1A	3534	1/1	0.91	0.12	39,39,39,39	0
57	MG	1A	3580	1/1	0.91	0.17	28,28,28,28	0
57	MG	2a	1732	1/1	0.91	0.17	90,90,90,90	0
57	MG	2A	3655	1/1	0.91	0.11	36,36,36,36	0
57	MG	1A	3177	1/1	0.91	0.46	45,45,45,45	0
57	MG	1A	3811	1/1	0.91	0.15	67,67,67,67	0
57	MG	1A	3294	1/1	0.91	0.43	46,46,46,46	0
57	MG	2A	3013	1/1	0.91	0.15	62,62,62,62	0
57	MG	2A	3336	1/1	0.91	0.23	52,52,52,52	0
57	MG	1A	3937	1/1	0.91	0.14	42,42,42,42	0
57	MG	1A	3060	1/1	0.91	0.35	54,54,54,54	0
57	MG	1A	3903	1/1	0.91	0.13	49,49,49,49	0
57	MG	1A	3620	1/1	0.91	0.20	64,64,64,64	0
57	MG	1A	3350	1/1	0.91	0.32	57,57,57,57	0
57	MG	1B	224	1/1	0.91	0.17	71,71,71,71	0
57	MG	2A	3566	1/1	0.91	0.21	51,51,51,51	0
57	MG	2A	3355	1/1	0.91	0.26	43,43,43,43	0
57	MG	2A	3200	1/1	0.91	0.51	66,66,66,66	0
57	MG	1A	3555	1/1	0.91	0.22	26,26,26,26	0
57	MG	1A	3011	1/1	0.91	0.19	43,43,43,43	0
57	MG	1P	204	1/1	0.91	0.15	62,62,62,62	0
57	MG	2A	3620	1/1	0.91	0.16	34,34,34,34	0
57	MG	2a	1729	1/1	0.91	0.05	71,71,71,71	0
57	MG	2A	3822	1/1	0.91	0.10	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3896	1/1	0.91	0.16	50,50,50,50	0
57	MG	1A	3070	1/1	0.91	0.19	60,60,60,60	0
57	MG	1a	1636	1/1	0.91	0.21	70,70,70,70	0
57	MG	2A	3272	1/1	0.91	0.14	67,67,67,67	0
57	MG	1A	3691	1/1	0.91	0.11	44,44,44,44	0
57	MG	1a	1788	1/1	0.91	0.14	43,43,43,43	0
57	MG	1A	3193	1/1	0.91	0.28	50,50,50,50	0
57	MG	1a	1662	1/1	0.91	0.12	54,54,54,54	0
57	MG	2A	3275	1/1	0.91	0.16	75,75,75,75	0
57	MG	1a	1896	1/1	0.91	0.13	63,63,63,63	0
57	MG	1A	4056	1/1	0.91	0.15	53,53,53,53	0
57	MG	1A	4085	1/1	0.91	0.17	48,48,48,48	0
57	MG	1A	3410	1/1	0.91	0.35	62,62,62,62	0
57	MG	1A	4016	1/1	0.91	0.14	51,51,51,51	0
57	MG	1A	3377	1/1	0.91	0.52	59,59,59,59	0
57	MG	1A	3320	1/1	0.91	0.87	54,54,54,54	0
57	MG	1A	3726	1/1	0.91	0.28	47,47,47,47	0
57	MG	1a	1872	1/1	0.91	0.11	93,93,93,93	0
57	MG	2A	3176	1/1	0.91	0.10	66,66,66,66	0
57	MG	1A	3634	1/1	0.91	0.20	45,45,45,45	0
57	MG	1A	3252	1/1	0.91	0.65	36,36,36,36	0
57	MG	1A	3227	1/1	0.91	0.21	42,42,42,42	0
57	MG	1S	3001	1/1	0.91	0.61	57,57,57,57	0
57	MG	1a	1861	1/1	0.91	0.19	57,57,57,57	0
57	MG	2A	3381	1/1	0.91	0.18	53,53,53,53	0
57	MG	1A	3066	1/1	0.91	0.61	39,39,39,39	0
57	MG	1B	220	1/1	0.91	0.15	63,63,63,63	0
57	MG	1A	4014	1/1	0.91	0.10	57,57,57,57	0
57	MG	1O	3004	1/1	0.91	0.26	73,73,73,73	0
57	MG	1A	3629	1/1	0.91	0.14	17,17,17,17	0
57	MG	2A	3175	1/1	0.91	0.12	64,64,64,64	0
57	MG	1B	228	1/1	0.91	0.19	69,69,69,69	0
57	MG	1B	221	1/1	0.91	0.20	54,54,54,54	0
57	MG	1A	4098	1/1	0.92	0.17	52,52,52,52	0
57	MG	1a	1739	1/1	0.92	0.15	53,53,53,53	0
57	MG	1a	1680	1/1	0.92	0.21	61,61,61,61	0
57	MG	1a	1747	1/1	0.92	0.12	67,67,67,67	0
57	MG	2A	3658	1/1	0.92	0.61	47,47,47,47	0
57	MG	1a	1643	1/1	0.92	0.34	54,54,54,54	0
57	MG	2A	3533	1/1	0.92	0.19	48,48,48,48	0
57	MG	1A	4062	1/1	0.92	0.08	80,80,80,80	0
57	MG	1A	3826	1/1	0.92	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3482	1/1	0.92	0.13	41,41,41,41	0
57	MG	1A	3149	1/1	0.92	0.44	40,40,40,40	0
57	MG	1a	1893	1/1	0.92	0.33	73,73,73,73	0
57	MG	1a	1624	1/1	0.92	0.13	51,51,51,51	0
57	MG	1a	1675	1/1	0.92	0.29	68,68,68,68	0
57	MG	1A	3766	1/1	0.92	0.07	61,61,61,61	0
57	MG	2A	3433	1/1	0.92	0.08	67,67,67,67	0
57	MG	1A	3969	1/1	0.92	0.13	70,70,70,70	0
57	MG	1A	3467	1/1	0.92	0.24	52,52,52,52	0
57	MG	1A	3152	1/1	0.92	0.48	37,37,37,37	0
57	MG	1A	3314	1/1	0.92	0.27	40,40,40,40	0
57	MG	2A	3044	1/1	0.92	0.70	49,49,49,49	0
57	MG	1x	3004	1/1	0.92	0.16	70,70,70,70	0
57	MG	2A	3678	1/1	0.92	0.18	54,54,54,54	0
57	MG	2E	306	1/1	0.92	0.15	40,40,40,40	0
57	MG	2A	3174	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3857	1/1	0.92	0.30	43,43,43,43	0
57	MG	2A	3037	1/1	0.92	0.07	75,75,75,75	0
57	MG	2A	3369	1/1	0.92	0.18	65,65,65,65	0
57	MG	2A	3552	1/1	0.92	0.12	43,43,43,43	0
57	MG	1A	3414	1/1	0.92	0.13	53,53,53,53	0
57	MG	1a	1666	1/1	0.92	0.10	73,73,73,73	0
57	MG	2A	3538	1/1	0.92	0.18	39,39,39,39	0
57	MG	2A	3632	1/1	0.92	0.32	70,70,70,70	0
57	MG	1A	3936	1/1	0.92	0.16	60,60,60,60	0
57	MG	1A	3489	1/1	0.92	0.13	44,44,44,44	0
57	MG	1A	3847	1/1	0.92	0.13	36,36,36,36	0
57	MG	1A	3873	1/1	0.92	0.18	74,74,74,74	0
57	MG	2A	3476	1/1	0.92	0.18	35,35,35,35	0
57	MG	2A	3500	1/1	0.92	0.10	70,70,70,70	0
57	MG	2A	3841	1/1	0.92	0.14	61,61,61,61	0
57	MG	2A	3190	1/1	0.92	0.18	56,56,56,56	0
57	MG	2A	3772	1/1	0.92	0.15	30,30,30,30	0
57	MG	1A	3085	1/1	0.92	0.13	38,38,38,38	0
57	MG	1A	3218	1/1	0.92	0.46	49,49,49,49	0
59	ZN	14	501	1/1	0.92	0.11	99,99,99,99	0
57	MG	1Y	201	1/1	0.92	0.22	52,52,52,52	0
57	MG	2A	3571	1/1	0.92	0.11	77,77,77,77	0
57	MG	1A	4027	1/1	0.92	0.19	55,55,55,55	0
57	MG	1a	1864	1/1	0.92	0.15	48,48,48,48	0
57	MG	2A	3438	1/1	0.92	0.17	36,36,36,36	0
57	MG	2A	3111	1/1	0.92	0.81	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3110	1/1	0.92	0.28	54,54,54,54	0
57	MG	2A	3073	1/1	0.92	0.39	58,58,58,58	0
57	MG	1A	3699	1/1	0.92	0.15	31,31,31,31	0
57	MG	2a	1605	1/1	0.92	0.22	52,52,52,52	0
57	MG	1A	3898	1/1	0.92	0.09	47,47,47,47	0
57	MG	1A	3530	1/1	0.92	0.15	17,17,17,17	0
57	MG	1A	4012	1/1	0.92	0.10	52,52,52,52	0
57	MG	2A	3419	1/1	0.92	0.11	70,70,70,70	0
57	MG	1A	3293	1/1	0.92	0.22	44,44,44,44	0
57	MG	2A	3585	1/1	0.92	0.24	71,71,71,71	0
57	MG	1a	1633	1/1	0.92	0.33	66,66,66,66	0
57	MG	2A	3745	1/1	0.92	0.11	57,57,57,57	0
57	MG	2a	1725	1/1	0.92	0.15	77,77,77,77	0
57	MG	1A	4032	1/1	0.92	0.12	71,71,71,71	0
57	MG	1A	3242	1/1	0.92	0.20	51,51,51,51	0
57	MG	1a	1712	1/1	0.92	0.14	48,48,48,48	0
57	MG	1E	302	1/1	0.92	0.41	36,36,36,36	0
57	MG	2a	1756	1/1	0.92	0.13	72,72,72,72	0
57	MG	1A	3247	1/1	0.92	0.26	49,49,49,49	0
57	MG	1A	3986	1/1	0.92	0.12	68,68,68,68	0
57	MG	1A	3948	1/1	0.92	0.07	76,76,76,76	0
57	MG	2a	1781	1/1	0.92	0.15	76,76,76,76	0
57	MG	2l	202	1/1	0.92	0.18	62,62,62,62	0
57	MG	2a	1670	1/1	0.92	0.23	62,62,62,62	0
57	MG	2a	1801	1/1	0.92	0.16	63,63,63,63	0
57	MG	1A	3755	1/1	0.92	0.15	28,28,28,28	0
57	MG	2A	3852	1/1	0.92	0.50	50,50,50,50	0
57	MG	1A	3183	1/1	0.92	0.69	34,34,34,34	0
57	MG	1a	1787	1/1	0.92	0.08	77,77,77,77	0
57	MG	2a	1669	1/1	0.92	0.19	69,69,69,69	0
57	MG	2A	3491	1/1	0.92	0.18	58,58,58,58	0
57	MG	2A	3348	1/1	0.92	0.25	78,78,78,78	0
57	MG	1A	3284	1/1	0.92	0.14	63,63,63,63	0
57	MG	1a	1768	1/1	0.92	0.11	75,75,75,75	0
57	MG	1A	4049	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3400	1/1	0.92	0.18	61,61,61,61	0
57	MG	1Q	203	1/1	0.92	0.24	73,73,73,73	0
57	MG	1O	3002	1/1	0.92	0.64	56,56,56,56	0
57	MG	1A	3231	1/1	0.92	0.26	70,70,70,70	0
57	MG	2A	3802	1/1	0.92	0.21	68,68,68,68	0
57	MG	1A	3524	1/1	0.92	0.18	32,32,32,32	0
57	MG	2A	3425	1/1	0.92	0.20	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3727	1/1	0.92	0.07	67,67,67,67	0
57	MG	1A	3664	1/1	0.92	0.15	52,52,52,52	0
57	MG	2A	3415	1/1	0.92	0.18	69,69,69,69	0
57	MG	2A	3351	1/1	0.92	0.09	73,73,73,73	0
57	MG	1A	4005	1/1	0.92	0.12	63,63,63,63	0
57	MG	1A	3429	1/1	0.92	0.42	67,67,67,67	0
57	MG	2A	3056	1/1	0.92	0.39	61,61,61,61	0
57	MG	2a	1702	1/1	0.92	0.24	73,73,73,73	0
57	MG	1A	3131	1/1	0.92	0.18	59,59,59,59	0
57	MG	2A	3050	1/1	0.92	0.20	59,59,59,59	0
57	MG	1A	3921	1/1	0.92	0.23	57,57,57,57	0
57	MG	2A	3084	1/1	0.92	0.13	41,41,41,41	0
57	MG	2A	3813	1/1	0.92	0.49	72,72,72,72	0
57	MG	1A	4116	1/1	0.92	0.47	37,37,37,37	0
57	MG	1A	3055	1/1	0.92	0.13	28,28,28,28	0
57	MG	1A	3434	1/1	0.92	0.31	51,51,51,51	0
57	MG	2A	3372	1/1	0.92	0.26	71,71,71,71	0
57	MG	1A	3623	1/1	0.92	0.17	63,63,63,63	0
57	MG	2A	3835	1/1	0.92	0.25	56,56,56,56	0
57	MG	1A	3253	1/1	0.92	0.21	48,48,48,48	0
57	MG	1A	3730	1/1	0.92	0.11	66,66,66,66	0
57	MG	1A	3488	1/1	0.92	0.38	38,38,38,38	0
57	MG	2a	1790	1/1	0.92	0.09	74,74,74,74	0
57	MG	1A	3872	1/1	0.92	0.10	42,42,42,42	0
57	MG	2A	3486	1/1	0.92	0.18	81,81,81,81	0
57	MG	1A	3833	1/1	0.92	0.10	64,64,64,64	0
57	MG	1A	3971	1/1	0.92	0.27	42,42,42,42	0
57	MG	1A	3877	1/1	0.92	0.08	77,77,77,77	0
57	MG	1A	3322	1/1	0.92	0.35	65,65,65,65	0
57	MG	1A	3563	1/1	0.92	0.17	21,21,21,21	0
57	MG	1A	4136	1/1	0.92	0.28	45,45,45,45	0
57	MG	2A	3201	1/1	0.92	0.12	54,54,54,54	0
57	MG	2A	3651	1/1	0.92	0.19	75,75,75,75	0
57	MG	2A	3656	1/1	0.92	0.10	67,67,67,67	0
57	MG	2A	3861	1/1	0.92	0.21	50,50,50,50	0
57	MG	1A	3116	1/1	0.92	0.64	37,37,37,37	0
57	MG	1a	1895	1/1	0.92	0.10	88,88,88,88	0
57	MG	2A	3229	1/1	0.92	1.27	63,63,63,63	0
57	MG	2A	3356	1/1	0.92	0.17	58,58,58,58	0
57	MG	1A	3956	1/1	0.92	0.24	53,53,53,53	0
57	MG	2A	3546	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	4069	1/1	0.92	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1634	1/1	0.92	0.15	62,62,62,62	0
57	MG	1a	1618	1/1	0.92	0.10	46,46,46,46	0
57	MG	1A	3202	1/1	0.92	0.95	50,50,50,50	0
57	MG	1A	3343	1/1	0.92	0.18	57,57,57,57	0
57	MG	2a	1606	1/1	0.92	0.24	65,65,65,65	0
57	MG	2A	3488	1/1	0.92	0.17	42,42,42,42	0
57	MG	2A	3125	1/1	0.92	0.10	54,54,54,54	0
57	MG	1a	1823	1/1	0.92	0.14	72,72,72,72	0
57	MG	2A	3838	1/1	0.92	0.88	79,79,79,79	0
57	MG	1A	3079	1/1	0.92	0.12	28,28,28,28	0
57	MG	2A	3373	1/1	0.92	0.19	63,63,63,63	0
57	MG	2A	3623	1/1	0.92	0.08	71,71,71,71	0
57	MG	2a	1734	1/1	0.92	0.06	76,76,76,76	0
57	MG	1x	3012	1/1	0.92	0.18	69,69,69,69	0
57	MG	1A	4072	1/1	0.92	0.11	47,47,47,47	0
57	MG	1A	3337	1/1	0.92	0.09	64,64,64,64	0
57	MG	2A	3148	1/1	0.92	0.51	62,62,62,62	0
57	MG	1A	3983	1/1	0.92	0.10	63,63,63,63	0
57	MG	2a	1773	1/1	0.92	0.31	88,88,88,88	0
57	MG	1A	3635	1/1	0.92	0.20	56,56,56,56	0
57	MG	1A	3728	1/1	0.92	0.39	56,56,56,56	0
57	MG	1B	222	1/1	0.92	0.12	57,57,57,57	0
57	MG	2A	3246	1/1	0.92	0.22	63,63,63,63	0
57	MG	1A	3397	1/1	0.92	0.22	62,62,62,62	0
57	MG	1A	4087	1/1	0.92	0.33	59,59,59,59	0
57	MG	1A	3851	1/1	0.92	0.19	46,46,46,46	0
57	MG	2A	3006	1/1	0.92	0.11	54,54,54,54	0
57	MG	2A	3564	1/1	0.92	0.16	62,62,62,62	0
57	MG	2a	1646	1/1	0.92	0.10	67,67,67,67	0
57	MG	1A	4033	1/1	0.92	0.14	48,48,48,48	0
57	MG	1A	3124	1/1	0.92	0.44	37,37,37,37	0
57	MG	1A	3348	1/1	0.92	0.37	50,50,50,50	0
57	MG	1A	3569	1/1	0.92	0.06	57,57,57,57	0
57	MG	1A	3694	1/1	0.92	0.12	73,73,73,73	0
57	MG	1A	3964	1/1	0.92	0.37	33,33,33,33	0
57	MG	1A	3034	1/1	0.92	0.13	38,38,38,38	0
57	MG	1A	3288	1/1	0.92	0.13	65,65,65,65	0
57	MG	2A	3439	1/1	0.92	0.12	55,55,55,55	0
57	MG	1A	3145	1/1	0.92	0.13	37,37,37,37	0
57	MG	1A	3978	1/1	0.92	0.22	69,69,69,69	0
57	MG	1A	3188	1/1	0.92	0.60	33,33,33,33	0
57	MG	1A	3531	1/1	0.92	0.14	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1767	1/1	0.92	0.17	78,78,78,78	0
57	MG	2A	3447	1/1	0.92	0.25	62,62,62,62	0
57	MG	1a	1698	1/1	0.92	0.18	66,66,66,66	0
57	MG	1A	3526	1/1	0.92	0.12	55,55,55,55	0
57	MG	2B	3006	1/1	0.92	0.08	84,84,84,84	0
57	MG	1A	3715	1/1	0.92	0.14	53,53,53,53	0
57	MG	1A	3939	1/1	0.92	0.08	65,65,65,65	0
57	MG	1A	3807	1/1	0.92	0.18	63,63,63,63	0
57	MG	1A	3399	1/1	0.92	0.69	44,44,44,44	0
57	MG	2e	3001	1/1	0.93	0.13	81,81,81,81	0
57	MG	1A	4050	1/1	0.93	0.16	34,34,34,34	0
57	MG	1U	206	1/1	0.93	0.43	40,40,40,40	0
57	MG	1A	3592	1/1	0.93	0.09	48,48,48,48	0
57	MG	2A	3368	1/1	0.93	0.28	66,66,66,66	0
57	MG	2A	3306	1/1	0.93	0.27	71,71,71,71	0
57	MG	1A	3272	1/1	0.93	0.21	53,53,53,53	0
57	MG	2W	3002	1/1	0.93	0.35	52,52,52,52	0
57	MG	2A	3740	1/1	0.93	0.13	48,48,48,48	0
57	MG	1a	1847	1/1	0.93	0.14	63,63,63,63	0
57	MG	1A	3947	1/1	0.93	0.07	59,59,59,59	0
57	MG	2A	3461	1/1	0.93	0.14	44,44,44,44	0
57	MG	1A	3835	1/1	0.93	0.08	72,72,72,72	0
57	MG	2A	3434	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3261	1/1	0.93	0.67	59,59,59,59	0
57	MG	1A	3001	1/1	0.93	0.18	50,50,50,50	0
57	MG	1a	1786	1/1	0.93	0.14	62,62,62,62	0
57	MG	1A	3636	1/1	0.93	0.13	40,40,40,40	0
57	MG	1Q	205	1/1	0.93	0.19	51,51,51,51	0
57	MG	1A	4059	1/1	0.93	0.11	60,60,60,60	0
57	MG	1A	3604	1/1	0.93	0.07	58,58,58,58	0
57	MG	2A	3855	1/1	0.93	0.26	72,72,72,72	0
57	MG	1A	3934	1/1	0.93	0.12	57,57,57,57	0
57	MG	2A	3183	1/1	0.93	0.13	63,63,63,63	0
57	MG	2A	3382	1/1	0.93	0.17	49,49,49,49	0
57	MG	1A	3312	1/1	0.93	0.51	35,35,35,35	0
57	MG	1A	3103	1/1	0.93	0.21	41,41,41,41	0
57	MG	2a	1645	1/1	0.93	0.10	61,61,61,61	0
57	MG	1A	3624	1/1	0.93	0.14	54,54,54,54	0
57	MG	2a	1631	1/1	0.93	0.19	75,75,75,75	0
57	MG	1A	3443	1/1	0.93	0.13	47,47,47,47	0
57	MG	1A	3487	1/1	0.93	0.33	47,47,47,47	0
57	MG	1A	3457	1/1	0.93	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1716	1/1	0.93	0.10	60,60,60,60	0
57	MG	1a	1810	1/1	0.93	0.12	72,72,72,72	0
57	MG	2A	3605	1/1	0.93	0.21	66,66,66,66	0
57	MG	1A	3675	1/1	0.93	0.10	60,60,60,60	0
57	MG	1A	3823	1/1	0.93	0.06	65,65,65,65	0
57	MG	1A	3278	1/1	0.93	0.39	35,35,35,35	0
57	MG	1A	3698	1/1	0.93	0.11	29,29,29,29	0
57	MG	1A	3832	1/1	0.93	0.09	59,59,59,59	0
57	MG	1A	3391	1/1	0.93	0.23	49,49,49,49	0
57	MG	1A	3383	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3655	1/1	0.93	0.12	50,50,50,50	0
57	MG	2A	3810	1/1	0.93	0.13	61,61,61,61	0
57	MG	1A	3317	1/1	0.93	0.07	42,42,42,42	0
57	MG	2A	3033	1/1	0.93	0.14	32,32,32,32	0
57	MG	2A	3490	1/1	0.93	0.12	49,49,49,49	0
57	MG	1a	1858	1/1	0.93	0.20	57,57,57,57	0
58	K	1A	3435	1/1	0.93	0.17	57,57,57,57	0
57	MG	2a	1731	1/1	0.93	0.21	77,77,77,77	0
57	MG	2A	3499	1/1	0.93	0.19	61,61,61,61	0
57	MG	2A	3506	1/1	0.93	0.20	63,63,63,63	0
57	MG	1A	3336	1/1	0.93	0.99	54,54,54,54	0
57	MG	2A	3153	1/1	0.93	0.10	53,53,53,53	0
57	MG	2A	3375	1/1	0.93	0.29	62,62,62,62	0
57	MG	1R	202	1/1	0.93	0.76	45,45,45,45	0
57	MG	1A	3442	1/1	0.93	0.18	44,44,44,44	0
57	MG	1a	1720	1/1	0.93	0.14	61,61,61,61	0
57	MG	1G	3001	1/1	0.93	0.15	43,43,43,43	0
57	MG	1A	3482	1/1	0.93	0.24	52,52,52,52	0
57	MG	1a	1609	1/1	0.93	0.10	51,51,51,51	0
57	MG	1a	1766	1/1	0.93	0.11	54,54,54,54	0
57	MG	2a	1629	1/1	0.93	0.08	80,80,80,80	0
57	MG	2A	3717	1/1	0.93	0.21	60,60,60,60	0
57	MG	2A	3076	1/1	0.93	0.38	52,52,52,52	0
57	MG	1A	3423	1/1	0.93	0.29	54,54,54,54	0
57	MG	1A	3102	1/1	0.93	0.58	44,44,44,44	0
57	MG	1A	3900	1/1	0.93	0.23	75,75,75,75	0
57	MG	2A	3048	1/1	0.93	0.22	77,77,77,77	0
57	MG	1A	3992	1/1	0.93	0.25	45,45,45,45	0
57	MG	2A	3763	1/1	0.93	0.10	42,42,42,42	0
57	MG	2A	3141	1/1	0.93	0.42	59,59,59,59	0
57	MG	1A	3153	1/1	0.93	0.38	29,29,29,29	0
57	MG	2A	3859	1/1	0.93	0.41	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3466	1/1	0.93	0.16	39,39,39,39	0
57	MG	1A	4051	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3045	1/1	0.93	0.14	54,54,54,54	0
57	MG	2A	3702	1/1	0.93	0.14	57,57,57,57	0
57	MG	2A	3042	1/1	0.93	0.14	58,58,58,58	0
57	MG	2A	3710	1/1	0.93	0.10	82,82,82,82	0
57	MG	1A	3751	1/1	0.93	0.18	64,64,64,64	0
57	MG	1A	3927	1/1	0.93	0.60	44,44,44,44	0
57	MG	1A	3376	1/1	0.93	0.62	62,62,62,62	0
57	MG	1a	1910	1/1	0.93	0.55	59,59,59,59	0
57	MG	1A	3619	1/1	0.93	0.08	53,53,53,53	0
57	MG	2A	3247	1/1	0.93	0.11	62,62,62,62	0
57	MG	1A	3840	1/1	0.93	0.26	62,62,62,62	0
57	MG	25	102	1/1	0.93	0.12	58,58,58,58	0
57	MG	1a	1790	1/1	0.93	0.14	69,69,69,69	0
57	MG	2a	1763	1/1	0.93	0.13	67,67,67,67	0
57	MG	1l	8002	1/1	0.93	0.17	79,79,79,79	0
57	MG	1A	3902	1/1	0.93	0.18	58,58,58,58	0
57	MG	1A	3938	1/1	0.93	0.46	52,52,52,52	0
57	MG	2A	3808	1/1	0.93	0.07	64,64,64,64	0
57	MG	1A	3894	1/1	0.93	0.25	71,71,71,71	0
57	MG	2a	1633	1/1	0.93	0.11	78,78,78,78	0
57	MG	1A	3863	1/1	0.93	0.20	24,24,24,24	0
57	MG	10	103	1/1	0.93	0.14	63,63,63,63	0
57	MG	2A	3562	1/1	0.93	0.48	52,52,52,52	0
57	MG	2a	1737	1/1	0.93	0.16	61,61,61,61	0
57	MG	2F	303	1/1	0.93	0.10	78,78,78,78	0
57	MG	1A	3951	1/1	0.93	0.15	31,31,31,31	0
57	MG	1A	3105	1/1	0.93	0.41	30,30,30,30	0
57	MG	2U	203	1/1	0.93	1.10	67,67,67,67	0
57	MG	1a	1719	1/1	0.93	0.16	55,55,55,55	0
57	MG	1A	3539	1/1	0.93	0.19	61,61,61,61	0
57	MG	1W	204	1/1	0.93	0.23	34,34,34,34	0
57	MG	2A	3729	1/1	0.93	0.12	76,76,76,76	0
57	MG	1B	236	1/1	0.93	0.15	33,33,33,33	0
57	MG	2x	106	1/1	0.93	0.13	69,69,69,69	0
57	MG	1a	1821	1/1	0.93	0.21	69,69,69,69	0
57	MG	1a	1642	1/1	0.93	0.12	70,70,70,70	0
57	MG	2A	3210	1/1	0.93	0.33	56,56,56,56	0
57	MG	2A	3109	1/1	0.93	0.12	39,39,39,39	0
57	MG	1A	3441	1/1	0.93	0.62	59,59,59,59	0
57	MG	2a	1749	1/1	0.93	0.15	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1E	310	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3334	1/1	0.93	0.22	42,42,42,42	0
57	MG	2a	1748	1/1	0.93	0.12	69,69,69,69	0
57	MG	2a	1794	1/1	0.93	0.16	76,76,76,76	0
57	MG	2A	3092	1/1	0.93	0.11	34,34,34,34	0
57	MG	1a	1913	1/1	0.93	0.12	63,63,63,63	0
57	MG	1A	3513	1/1	0.93	0.11	49,49,49,49	0
57	MG	1A	3437	1/1	0.93	0.59	49,49,49,49	0
57	MG	2A	3054	1/1	0.93	0.13	59,59,59,59	0
57	MG	1A	3641	1/1	0.93	0.18	48,48,48,48	0
57	MG	1A	3536	1/1	0.93	0.09	29,29,29,29	0
57	MG	2A	3582	1/1	0.93	0.21	72,72,72,72	0
57	MG	1A	3514	1/1	0.93	0.27	57,57,57,57	0
57	MG	1A	3838	1/1	0.93	0.14	70,70,70,70	0
57	MG	1A	3162	1/1	0.93	0.14	30,30,30,30	0
57	MG	2A	3072	1/1	0.93	0.25	53,53,53,53	0
57	MG	1A	3330	1/1	0.93	0.39	50,50,50,50	0
57	MG	1A	3617	1/1	0.93	0.11	55,55,55,55	0
57	MG	1A	3621	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	4083	1/1	0.93	0.19	57,57,57,57	0
57	MG	2A	3154	1/1	0.93	0.21	71,71,71,71	0
57	MG	2A	3212	1/1	0.93	0.54	49,49,49,49	0
57	MG	1A	3210	1/1	0.93	0.15	74,74,74,74	0
57	MG	1A	3010	1/1	0.93	0.14	57,57,57,57	0
57	MG	1A	3175	1/1	0.93	0.72	49,49,49,49	0
57	MG	1A	3480	1/1	0.93	0.36	38,38,38,38	0
57	MG	2A	3611	1/1	0.93	0.10	49,49,49,49	0
57	MG	1A	3385	1/1	0.93	0.28	53,53,53,53	0
57	MG	1A	3013	1/1	0.93	0.17	28,28,28,28	0
57	MG	2A	3474	1/1	0.93	0.15	64,64,64,64	0
57	MG	1e	201	1/1	0.93	0.12	75,75,75,75	0
57	MG	2A	3711	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3270	1/1	0.93	0.18	66,66,66,66	0
57	MG	2A	3805	1/1	0.93	0.13	73,73,73,73	0
57	MG	1A	4043	1/1	0.93	0.09	63,63,63,63	0
57	MG	1A	4023	1/1	0.93	0.23	53,53,53,53	0
57	MG	1A	3522	1/1	0.93	0.15	25,25,25,25	0
57	MG	1A	4145	1/1	0.93	0.35	47,47,47,47	0
57	MG	2A	3442	1/1	0.93	0.09	38,38,38,38	0
57	MG	1A	3916	1/1	0.93	0.12	32,32,32,32	0
57	MG	1A	4100	1/1	0.93	0.73	49,49,49,49	0
57	MG	1A	4107	1/1	0.93	0.37	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3443	1/1	0.93	0.48	62,62,62,62	0
57	MG	2A	3736	1/1	0.93	0.10	60,60,60,60	0
57	MG	1A	3405	1/1	0.93	0.23	29,29,29,29	0
57	MG	2B	3011	1/1	0.93	0.11	80,80,80,80	0
57	MG	2A	3826	1/1	0.93	0.30	70,70,70,70	0
57	MG	2a	1619	1/1	0.93	0.29	89,89,89,89	0
57	MG	2A	3597	1/1	0.93	0.11	64,64,64,64	0
57	MG	2A	3470	1/1	0.93	0.14	41,41,41,41	0
57	MG	1A	4039	1/1	0.93	0.26	40,40,40,40	0
57	MG	2A	3096	1/1	0.93	0.38	51,51,51,51	0
57	MG	1A	4088	1/1	0.93	0.15	62,62,62,62	0
57	MG	2A	3563	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3669	1/1	0.93	0.13	38,38,38,38	0
57	MG	2a	1780	1/1	0.93	0.14	65,65,65,65	0
57	MG	1E	307	1/1	0.93	0.15	29,29,29,29	0
57	MG	2A	3483	1/1	0.93	0.16	61,61,61,61	0
57	MG	1A	3107	1/1	0.93	0.13	38,38,38,38	0
57	MG	1A	4092	1/1	0.93	0.60	42,42,42,42	0
57	MG	1A	3996	1/1	0.93	0.12	56,56,56,56	0
57	MG	1A	3143	1/1	0.93	0.20	56,56,56,56	0
57	MG	1A	3606	1/1	0.93	0.11	46,46,46,46	0
57	MG	2A	3685	1/1	0.93	0.11	75,75,75,75	0
57	MG	2A	3503	1/1	0.93	0.16	63,63,63,63	0
57	MG	1A	3679	1/1	0.93	0.22	29,29,29,29	0
57	MG	2A	3798	1/1	0.93	0.26	59,59,59,59	0
57	MG	2A	3787	1/1	0.93	0.20	63,63,63,63	0
57	MG	1N	205	1/1	0.93	0.23	43,43,43,43	0
57	MG	2a	1770	1/1	0.93	0.18	74,74,74,74	0
57	MG	2A	3390	1/1	0.93	0.18	64,64,64,64	0
57	MG	1a	1909	1/1	0.94	0.22	68,68,68,68	0
57	MG	1A	4147	1/1	0.94	0.20	34,34,34,34	0
57	MG	2A	3055	1/1	0.94	0.11	46,46,46,46	0
57	MG	1A	3987	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3511	1/1	0.94	0.14	63,63,63,63	0
57	MG	1A	3122	1/1	0.94	0.42	34,34,34,34	0
57	MG	1A	3588	1/1	0.94	0.10	62,62,62,62	0
57	MG	2A	3631	1/1	0.94	0.20	61,61,61,61	0
57	MG	1A	3052	1/1	0.94	0.29	34,34,34,34	0
57	MG	2A	3676	1/1	0.94	0.16	74,74,74,74	0
57	MG	2a	1706	1/1	0.94	0.08	73,73,73,73	0
57	MG	1A	3233	1/1	0.94	0.17	34,34,34,34	0
57	MG	2A	3548	1/1	0.94	0.24	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4081	1/1	0.94	0.13	46,46,46,46	0
57	MG	1A	3603	1/1	0.94	0.21	45,45,45,45	0
57	MG	1x	3001	1/1	0.94	0.20	74,74,74,74	0
57	MG	2A	3345	1/1	0.94	0.15	64,64,64,64	0
57	MG	1A	4114	1/1	0.94	0.61	46,46,46,46	0
57	MG	1a	1621	1/1	0.94	0.20	52,52,52,52	0
57	MG	2A	3430	1/1	0.94	0.09	56,56,56,56	0
57	MG	1A	3821	1/1	0.94	0.14	36,36,36,36	0
57	MG	1A	3295	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3028	1/1	0.94	0.70	36,36,36,36	0
57	MG	1A	3139	1/1	0.94	0.17	22,22,22,22	0
57	MG	2A	3269	1/1	0.94	0.08	77,77,77,77	0
57	MG	1F	302	1/1	0.94	0.26	28,28,28,28	0
57	MG	1A	3378	1/1	0.94	0.17	37,37,37,37	0
57	MG	1A	4112	1/1	0.94	0.51	37,37,37,37	0
57	MG	2A	3537	1/1	0.94	0.12	41,41,41,41	0
57	MG	1A	3283	1/1	0.94	0.18	39,39,39,39	0
57	MG	1a	1796	1/1	0.94	0.09	69,69,69,69	0
57	MG	1A	4010	1/1	0.94	0.18	60,60,60,60	0
57	MG	1A	3450	1/1	0.94	0.10	59,59,59,59	0
57	MG	1a	1715	1/1	0.94	0.16	63,63,63,63	0
57	MG	2a	1657	1/1	0.94	0.29	64,64,64,64	0
57	MG	1B	213	1/1	0.94	0.13	46,46,46,46	0
57	MG	1A	3585	1/1	0.94	0.16	26,26,26,26	0
57	MG	1a	1744	1/1	0.94	0.14	54,54,54,54	0
57	MG	2A	3232	1/1	0.94	0.08	66,66,66,66	0
57	MG	1a	1696	1/1	0.94	0.54	72,72,72,72	0
57	MG	1a	1914	1/1	0.94	0.05	74,74,74,74	0
57	MG	1A	4111	1/1	0.94	0.38	38,38,38,38	0
57	MG	2A	3543	1/1	0.94	0.20	68,68,68,68	0
57	MG	2A	3762	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3744	1/1	0.94	0.17	37,37,37,37	0
57	MG	2a	1634	1/1	0.94	0.13	92,92,92,92	0
57	MG	1A	4084	1/1	0.94	0.26	35,35,35,35	0
57	MG	1a	1737	1/1	0.94	0.07	81,81,81,81	0
57	MG	2A	3603	1/1	0.94	0.10	69,69,69,69	0
57	MG	1A	3255	1/1	0.94	0.15	40,40,40,40	0
57	MG	2A	3844	1/1	0.94	0.21	65,65,65,65	0
57	MG	2B	3021	1/1	0.94	0.10	79,79,79,79	0
57	MG	2a	1639	1/1	0.94	0.10	55,55,55,55	0
57	MG	1A	3550	1/1	0.94	0.18	21,21,21,21	0
57	MG	1a	1677	1/1	0.94	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
57	MG	2a	1603	1/1	0.94	0.10	64,64,64,64	0
57	MG	1A	3104	1/1	0.94	0.12	44,44,44,44	0
57	MG	1A	4106	1/1	0.94	0.31	67,67,67,67	0
57	MG	2B	3007	1/1	0.94	0.13	70,70,70,70	0
57	MG	1A	3394	1/1	0.94	0.26	36,36,36,36	0
57	MG	1A	4118	1/1	0.94	0.14	36,36,36,36	0
57	MG	1A	3082	1/1	0.94	0.10	40,40,40,40	0
57	MG	1A	3520	1/1	0.94	0.14	19,19,19,19	0
57	MG	1A	3706	1/1	0.94	0.15	47,47,47,47	0
57	MG	2A	3629	1/1	0.94	0.23	64,64,64,64	0
57	MG	1A	4052	1/1	0.94	0.07	59,59,59,59	0
57	MG	1a	1850	1/1	0.94	0.07	76,76,76,76	0
57	MG	1a	1704	1/1	0.94	0.14	83,83,83,83	0
57	MG	1A	3704	1/1	0.94	0.16	62,62,62,62	0
57	MG	2A	3821	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	4140	1/1	0.94	0.49	38,38,38,38	0
57	MG	1w	105	1/1	0.94	0.13	69,69,69,69	0
57	MG	1T	201	1/1	0.94	0.21	51,51,51,51	0
57	MG	2A	3039	1/1	0.94	0.10	68,68,68,68	0
57	MG	1A	3812	1/1	0.94	0.47	60,60,60,60	0
57	MG	1A	3151	1/1	0.94	0.14	51,51,51,51	0
57	MG	2A	3432	1/1	0.94	0.13	62,62,62,62	0
57	MG	2a	1697	1/1	0.94	0.10	70,70,70,70	0
57	MG	2A	3492	1/1	0.94	0.11	51,51,51,51	0
57	MG	1a	1831	1/1	0.94	0.20	82,82,82,82	0
57	MG	1A	4018	1/1	0.94	0.30	48,48,48,48	0
57	MG	2A	3839	1/1	0.94	0.48	66,66,66,66	0
57	MG	1A	3644	1/1	0.94	0.18	45,45,45,45	0
57	MG	2A	3518	1/1	0.94	0.23	63,63,63,63	0
57	MG	2A	3743	1/1	0.94	0.14	44,44,44,44	0
57	MG	2n	502	1/1	0.94	0.11	84,84,84,84	0
57	MG	2A	3738	1/1	0.94	0.09	45,45,45,45	0
57	MG	12	3002	1/1	0.94	0.36	42,42,42,42	0
57	MG	1A	3742	1/1	0.94	0.10	25,25,25,25	0
57	MG	1A	3021	1/1	0.94	0.34	34,34,34,34	0
57	MG	1D	3002	1/1	0.94	0.43	45,45,45,45	0
57	MG	2A	3827	1/1	0.94	0.16	58,58,58,58	0
57	MG	1A	3689	1/1	0.94	0.10	75,75,75,75	0
57	MG	1a	1617	1/1	0.94	0.40	59,59,59,59	0
57	MG	1A	3708	1/1	0.94	0.14	59,59,59,59	0
57	MG	1A	3808	1/1	0.94	0.07	45,45,45,45	0
57	MG	1A	3243	1/1	0.94	0.15	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1706	1/1	0.94	0.56	69,69,69,69	0
57	MG	2a	1707	1/1	0.94	0.08	82,82,82,82	0
57	MG	1a	1789	1/1	0.94	0.80	67,67,67,67	0
57	MG	2A	3014	1/1	0.94	0.17	36,36,36,36	0
57	MG	2a	1618	1/1	0.94	0.17	70,70,70,70	0
57	MG	2A	3730	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	4047	1/1	0.94	0.06	62,62,62,62	0
57	MG	2A	3315	1/1	0.94	0.15	62,62,62,62	0
57	MG	1A	4048	1/1	0.94	0.15	51,51,51,51	0
57	MG	2A	3124	1/1	0.94	0.32	45,45,45,45	0
57	MG	1a	1781	1/1	0.94	0.07	55,55,55,55	0
57	MG	2A	3477	1/1	0.94	0.14	61,61,61,61	0
57	MG	1A	3972	1/1	0.94	0.15	62,62,62,62	0
57	MG	1a	1746	1/1	0.94	0.12	61,61,61,61	0
57	MG	2A	3456	1/1	0.94	0.15	50,50,50,50	0
57	MG	1A	3827	1/1	0.94	0.11	45,45,45,45	0
57	MG	1A	3717	1/1	0.94	0.22	58,58,58,58	0
57	MG	1a	1626	1/1	0.94	0.24	71,71,71,71	0
57	MG	1x	3013	1/1	0.94	0.09	77,77,77,77	0
57	MG	1a	1782	1/1	0.94	0.09	77,77,77,77	0
57	MG	1A	3389	1/1	0.94	0.39	42,42,42,42	0
57	MG	1A	3904	1/1	0.94	0.23	66,66,66,66	0
57	MG	1A	3714	1/1	0.94	0.25	61,61,61,61	0
57	MG	1A	3479	1/1	0.94	0.23	49,49,49,49	0
57	MG	1A	3738	1/1	0.94	0.14	59,59,59,59	0
57	MG	2A	3030	1/1	0.94	0.15	44,44,44,44	0
57	MG	1A	4148	1/1	0.94	0.32	37,37,37,37	0
57	MG	2A	3335	1/1	0.94	0.15	56,56,56,56	0
57	MG	1a	1619	1/1	0.94	0.11	70,70,70,70	0
57	MG	2B	3016	1/1	0.94	0.10	74,74,74,74	0
57	MG	1A	3198	1/1	0.94	0.47	41,41,41,41	0
57	MG	1W	201	1/1	0.94	0.29	44,44,44,44	0
57	MG	1A	3794	1/1	0.94	0.14	42,42,42,42	0
57	MG	2a	1684	1/1	0.94	0.21	76,76,76,76	0
57	MG	1A	3791	1/1	0.94	0.16	64,64,64,64	0
57	MG	1a	1674	1/1	0.94	0.14	69,69,69,69	0
57	MG	1a	1663	1/1	0.94	0.29	50,50,50,50	0
57	MG	1A	3843	1/1	0.94	0.13	29,29,29,29	0
57	MG	2A	3133	1/1	0.94	0.17	49,49,49,49	0
57	MG	1A	3874	1/1	0.94	0.05	56,56,56,56	0
57	MG	1A	3981	1/1	0.94	0.16	60,60,60,60	0
57	MG	1A	3112	1/1	0.94	0.36	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3061	1/1	0.94	0.38	45,45,45,45	0
57	MG	2A	3577	1/1	0.94	0.09	60,60,60,60	0
57	MG	2A	3024	1/1	0.94	0.18	63,63,63,63	0
57	MG	1a	1620	1/1	0.94	0.07	60,60,60,60	0
57	MG	2A	3164	1/1	0.94	0.17	41,41,41,41	0
57	MG	1a	1615	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3213	1/1	0.94	0.28	45,45,45,45	0
57	MG	1A	3692	1/1	0.94	0.21	46,46,46,46	0
57	MG	1x	3008	1/1	0.94	0.17	81,81,81,81	0
57	MG	2a	1723	1/1	0.94	0.12	52,52,52,52	0
57	MG	2A	3152	1/1	0.94	0.12	59,59,59,59	0
57	MG	2a	1651	1/1	0.94	0.19	61,61,61,61	0
57	MG	2A	3596	1/1	0.94	0.08	68,68,68,68	0
57	MG	1B	216	1/1	0.94	0.19	51,51,51,51	0
57	MG	1A	4067	1/1	0.94	0.12	60,60,60,60	0
57	MG	2a	1690	1/1	0.94	0.16	65,65,65,65	0
57	MG	2a	1622	1/1	0.94	0.27	63,63,63,63	0
57	MG	2A	3404	1/1	0.94	0.37	48,48,48,48	0
57	MG	2A	3167	1/1	0.94	0.26	66,66,66,66	0
57	MG	1A	3370	1/1	0.94	0.49	51,51,51,51	0
57	MG	2A	3295	1/1	0.94	0.34	53,53,53,53	0
57	MG	2A	3450	1/1	0.94	0.17	49,49,49,49	0
57	MG	2A	3682	1/1	0.94	0.12	41,41,41,41	0
57	MG	2A	3679	1/1	0.94	0.12	66,66,66,66	0
57	MG	2A	3590	1/1	0.94	0.10	70,70,70,70	0
57	MG	2l	201	1/1	0.94	0.24	72,72,72,72	0
57	MG	1a	1640	1/1	0.94	0.16	50,50,50,50	0
57	MG	2A	3085	1/1	0.94	0.14	70,70,70,70	0
57	MG	1A	3886	1/1	0.94	0.10	52,52,52,52	0
57	MG	1A	3693	1/1	0.94	0.18	64,64,64,64	0
57	MG	1A	3432	1/1	0.94	0.53	43,43,43,43	0
57	MG	2a	1650	1/1	0.94	0.11	76,76,76,76	0
57	MG	1A	3078	1/1	0.94	0.35	40,40,40,40	0
57	MG	1a	1667	1/1	0.94	0.17	66,66,66,66	0
57	MG	1W	205	1/1	0.94	0.21	32,32,32,32	0
57	MG	2A	3440	1/1	0.94	0.20	46,46,46,46	0
57	MG	1A	3214	1/1	0.94	0.36	46,46,46,46	0
57	MG	1A	3187	1/1	0.94	0.15	54,54,54,54	0
57	MG	2A	3572	1/1	0.94	0.41	79,79,79,79	0
57	MG	2a	1681	1/1	0.94	0.14	85,85,85,85	0
57	MG	2A	3035	1/1	0.94	0.62	56,56,56,56	0
57	MG	1A	3825	1/1	0.94	0.42	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1707	1/1	0.94	0.14	67,67,67,67	0
57	MG	1A	4074	1/1	0.94	0.44	67,67,67,67	0
57	MG	1A	4135	1/1	0.94	0.43	44,44,44,44	0
57	MG	1a	1877	1/1	0.94	0.31	81,81,81,81	0
57	MG	2O	8001	1/1	0.94	0.09	62,62,62,62	0
57	MG	2a	1692	1/1	0.94	0.21	51,51,51,51	0
57	MG	2A	3321	1/1	0.94	0.16	64,64,64,64	0
57	MG	2a	1682	1/1	0.94	0.11	63,63,63,63	0
57	MG	2A	3683	1/1	0.94	0.17	38,38,38,38	0
57	MG	1A	3409	1/1	0.94	0.16	57,57,57,57	0
57	MG	1A	3866	1/1	0.94	0.16	28,28,28,28	0
57	MG	1A	3640	1/1	0.94	0.20	64,64,64,64	0
57	MG	1E	303	1/1	0.94	0.27	29,29,29,29	0
57	MG	1y	101	1/1	0.94	0.38	48,48,48,48	0
57	MG	2a	1621	1/1	0.94	0.14	64,64,64,64	0
57	MG	2a	1726	1/1	0.94	0.07	79,79,79,79	0
57	MG	2A	3671	1/1	0.94	0.08	65,65,65,65	0
57	MG	1A	3622	1/1	0.94	0.17	54,54,54,54	0
57	MG	2A	3785	1/1	0.94	0.33	69,69,69,69	0
57	MG	1A	3876	1/1	0.94	0.16	66,66,66,66	0
57	MG	1A	3130	1/1	0.94	0.37	43,43,43,43	0
57	MG	2A	3803	1/1	0.94	0.23	71,71,71,71	0
57	MG	2a	1741	1/1	0.94	0.06	70,70,70,70	0
57	MG	2A	3512	1/1	0.94	0.25	71,71,71,71	0
57	MG	1A	3700	1/1	0.94	0.28	43,43,43,43	0
57	MG	1A	3858	1/1	0.94	0.20	18,18,18,18	0
57	MG	1A	3537	1/1	0.94	0.11	32,32,32,32	0
57	MG	1A	3419	1/1	0.94	0.20	49,49,49,49	0
57	MG	1A	3518	1/1	0.94	0.15	33,33,33,33	0
57	MG	1A	3007	1/1	0.94	0.34	34,34,34,34	0
57	MG	1a	1851	1/1	0.94	0.19	73,73,73,73	0
57	MG	2A	3760	1/1	0.94	0.15	51,51,51,51	0
57	MG	1A	3123	1/1	0.94	0.22	41,41,41,41	0
57	MG	1A	3696	1/1	0.94	0.10	39,39,39,39	0
57	MG	1A	4142	1/1	0.94	0.64	52,52,52,52	0
57	MG	1A	3712	1/1	0.94	0.10	48,48,48,48	0
57	MG	1a	1745	1/1	0.94	0.12	66,66,66,66	0
57	MG	1A	3492	1/1	0.94	0.21	26,26,26,26	0
57	MG	1A	3509	1/1	0.94	0.06	57,57,57,57	0
57	MG	2A	3640	1/1	0.94	0.15	45,45,45,45	0
57	MG	1A	4006	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3441	1/1	0.94	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1884	1/1	0.94	0.25	72,72,72,72	0
57	MG	2A	3102	1/1	0.94	0.20	69,69,69,69	0
57	MG	1A	3056	1/1	0.94	0.09	41,41,41,41	0
57	MG	1A	4080	1/1	0.94	0.20	57,57,57,57	0
57	MG	1A	3502	1/1	0.94	0.15	54,54,54,54	0
57	MG	2A	3555	1/1	0.94	0.41	48,48,48,48	0
57	MG	2A	3635	1/1	0.94	0.07	82,82,82,82	0
57	MG	2A	3626	1/1	0.95	0.20	45,45,45,45	0
57	MG	2A	3800	1/1	0.95	0.07	68,68,68,68	0
57	MG	1A	3806	1/1	0.95	0.16	41,41,41,41	0
57	MG	1P	201	1/1	0.95	0.28	34,34,34,34	0
57	MG	2a	1658	1/1	0.95	0.11	82,82,82,82	0
57	MG	2E	301	1/1	0.95	0.61	59,59,59,59	0
57	MG	2A	3831	1/1	0.95	0.20	47,47,47,47	0
57	MG	2A	3558	1/1	0.95	0.18	39,39,39,39	0
57	MG	1A	3684	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3044	1/1	0.95	0.11	65,65,65,65	0
57	MG	2A	3156	1/1	0.95	0.16	45,45,45,45	0
57	MG	1A	3814	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3776	1/1	0.95	0.11	55,55,55,55	0
57	MG	1A	3219	1/1	0.95	0.46	40,40,40,40	0
57	MG	2A	3593	1/1	0.95	0.10	65,65,65,65	0
57	MG	1A	3201	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3899	1/1	0.95	0.22	22,22,22,22	0
57	MG	1Q	201	1/1	0.95	0.21	34,34,34,34	0
57	MG	1A	3919	1/1	0.95	0.13	27,27,27,27	0
57	MG	1A	3029	1/1	0.95	0.17	61,61,61,61	0
57	MG	1A	3922	1/1	0.95	0.07	62,62,62,62	0
57	MG	2y	3002	1/1	0.95	0.27	86,86,86,86	0
57	MG	1A	3306	1/1	0.95	0.18	49,49,49,49	0
57	MG	1A	3737	1/1	0.95	0.09	41,41,41,41	0
57	MG	1A	3677	1/1	0.95	0.16	19,19,19,19	0
57	MG	1d	502	1/1	0.95	0.13	81,81,81,81	0
57	MG	2A	3862	1/1	0.95	0.17	68,68,68,68	0
57	MG	1A	3478	1/1	0.95	0.26	32,32,32,32	0
57	MG	1A	3009	1/1	0.95	0.28	38,38,38,38	0
57	MG	2A	3837	1/1	0.95	0.10	58,58,58,58	0
57	MG	2A	3361	1/1	0.95	0.27	44,44,44,44	0
57	MG	1a	1650	1/1	0.95	0.10	69,69,69,69	0
57	MG	1A	3341	1/1	0.95	0.40	38,38,38,38	0
57	MG	1a	1904	1/1	0.95	0.13	67,67,67,67	0
57	MG	2A	3149	1/1	0.95	0.80	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3653	1/1	0.95	0.15	58,58,58,58	0
57	MG	2A	3687	1/1	0.95	0.13	67,67,67,67	0
57	MG	2A	3333	1/1	0.95	0.12	41,41,41,41	0
57	MG	2a	1643	1/1	0.95	0.13	54,54,54,54	0
57	MG	1A	3490	1/1	0.95	0.16	61,61,61,61	0
57	MG	1A	3192	1/1	0.95	0.56	39,39,39,39	0
57	MG	1a	1718	1/1	0.95	0.10	55,55,55,55	0
57	MG	2A	3060	1/1	0.95	0.11	53,53,53,53	0
57	MG	1a	1721	1/1	0.95	0.14	31,31,31,31	0
57	MG	1D	3007	1/1	0.95	0.51	47,47,47,47	0
57	MG	2a	1758	1/1	0.95	0.17	55,55,55,55	0
57	MG	2A	3530	1/1	0.95	0.22	57,57,57,57	0
57	MG	1A	3545	1/1	0.95	0.12	46,46,46,46	0
57	MG	1A	3579	1/1	0.95	0.17	17,17,17,17	0
57	MG	2A	3095	1/1	0.95	0.13	55,55,55,55	0
57	MG	1A	3406	1/1	0.95	0.47	37,37,37,37	0
57	MG	1A	3230	1/1	0.95	0.40	48,48,48,48	0
57	MG	1A	4105	1/1	0.95	0.14	61,61,61,61	0
57	MG	1A	3932	1/1	0.95	0.08	56,56,56,56	0
57	MG	1A	4089	1/1	0.95	0.62	38,38,38,38	0
57	MG	1a	1828	1/1	0.95	0.19	69,69,69,69	0
57	MG	2A	3610	1/1	0.95	0.10	58,58,58,58	0
57	MG	1A	3081	1/1	0.95	0.23	28,28,28,28	0
57	MG	1a	1752	1/1	0.95	0.12	55,55,55,55	0
57	MG	1A	3338	1/1	0.95	0.13	44,44,44,44	0
57	MG	1a	1902	1/1	0.95	0.15	56,56,56,56	0
57	MG	2A	3814	1/1	0.95	0.06	66,66,66,66	0
57	MG	1A	3427	1/1	0.95	0.13	61,61,61,61	0
57	MG	1A	4120	1/1	0.95	0.22	30,30,30,30	0
57	MG	1A	3880	1/1	0.95	0.23	59,59,59,59	0
57	MG	2A	3208	1/1	0.95	0.72	41,41,41,41	0
57	MG	1a	1730	1/1	0.95	0.15	35,35,35,35	0
57	MG	2T	3004	1/1	0.95	0.19	67,67,67,67	0
57	MG	2A	3436	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3701	1/1	0.95	0.17	33,33,33,33	0
57	MG	1A	3707	1/1	0.95	0.16	61,61,61,61	0
57	MG	1A	4144	1/1	0.95	0.33	39,39,39,39	0
57	MG	2A	3169	1/1	0.95	0.17	54,54,54,54	0
57	MG	1a	1891	1/1	0.95	0.07	69,69,69,69	0
57	MG	1A	4019	1/1	0.95	0.13	73,73,73,73	0
57	MG	2A	3750	1/1	0.95	0.11	48,48,48,48	0
57	MG	2A	3624	1/1	0.95	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2N	8001	1/1	0.95	0.12	63,63,63,63	0
57	MG	1A	3722	1/1	0.95	0.09	52,52,52,52	0
57	MG	1A	3705	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	4149	1/1	0.95	0.53	48,48,48,48	0
57	MG	2A	3143	1/1	0.95	0.19	64,64,64,64	0
57	MG	1A	3910	1/1	0.95	0.19	62,62,62,62	0
57	MG	1a	1604	1/1	0.95	0.10	67,67,67,67	0
57	MG	1A	3917	1/1	0.95	0.39	67,67,67,67	0
57	MG	1A	3308	1/1	0.95	0.56	31,31,31,31	0
57	MG	1A	3533	1/1	0.95	0.11	68,68,68,68	0
57	MG	1A	4101	1/1	0.95	0.73	32,32,32,32	0
57	MG	2A	3659	1/1	0.95	0.18	74,74,74,74	0
57	MG	2A	3012	1/1	0.95	0.22	48,48,48,48	0
57	MG	1Q	202	1/1	0.95	0.19	49,49,49,49	0
57	MG	2A	3186	1/1	0.95	0.24	55,55,55,55	0
57	MG	1A	3676	1/1	0.95	0.20	60,60,60,60	0
57	MG	1A	3119	1/1	0.95	0.11	38,38,38,38	0
57	MG	2A	3508	1/1	0.95	0.10	46,46,46,46	0
57	MG	2q	202	1/1	0.95	0.13	77,77,77,77	0
57	MG	2A	3858	1/1	0.95	0.20	55,55,55,55	0
57	MG	2A	3264	1/1	0.95	0.16	60,60,60,60	0
57	MG	2A	3549	1/1	0.95	0.11	52,52,52,52	0
57	MG	2A	3043	1/1	0.95	0.15	34,34,34,34	0
57	MG	1A	3608	1/1	0.95	0.08	70,70,70,70	0
57	MG	1A	3830	1/1	0.95	0.25	64,64,64,64	0
57	MG	1A	3864	1/1	0.95	0.09	31,31,31,31	0
57	MG	2A	3132	1/1	0.95	0.17	45,45,45,45	0
57	MG	1b	3001	1/1	0.95	0.48	87,87,87,87	0
57	MG	1A	3090	1/1	0.95	0.31	39,39,39,39	0
57	MG	1A	3274	1/1	0.95	0.11	60,60,60,60	0
57	MG	1A	3525	1/1	0.95	0.14	25,25,25,25	0
57	MG	1A	3220	1/1	0.95	0.27	56,56,56,56	0
57	MG	2A	3097	1/1	0.95	0.15	51,51,51,51	0
57	MG	1A	3697	1/1	0.95	0.10	29,29,29,29	0
57	MG	1A	3229	1/1	0.95	0.13	50,50,50,50	0
57	MG	1A	3158	1/1	0.95	0.19	30,30,30,30	0
57	MG	2a	1740	1/1	0.95	0.15	52,52,52,52	0
57	MG	2A	3028	1/1	0.95	0.14	55,55,55,55	0
57	MG	1A	3784	1/1	0.95	0.20	45,45,45,45	0
57	MG	1A	3889	1/1	0.95	0.14	29,29,29,29	0
57	MG	1X	3006	1/1	0.95	0.13	35,35,35,35	0
57	MG	2A	3244	1/1	0.95	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3595	1/1	0.95	0.13	44,44,44,44	0
57	MG	1A	3549	1/1	0.95	0.21	24,24,24,24	0
57	MG	2A	3842	1/1	0.95	0.55	67,67,67,67	0
57	MG	1A	3658	1/1	0.95	0.11	40,40,40,40	0
57	MG	1A	3352	1/1	0.95	0.63	39,39,39,39	0
57	MG	2a	1694	1/1	0.95	0.28	90,90,90,90	0
57	MG	1A	3015	1/1	0.95	0.12	18,18,18,18	0
57	MG	1A	3271	1/1	0.95	0.43	35,35,35,35	0
57	MG	2a	1700	1/1	0.95	0.14	71,71,71,71	0
57	MG	2A	3779	1/1	0.95	0.10	73,73,73,73	0
57	MG	1A	3048	1/1	0.95	0.15	54,54,54,54	0
57	MG	1A	3005	1/1	0.95	0.15	42,42,42,42	0
57	MG	1A	3425	1/1	0.95	0.11	48,48,48,48	0
57	MG	1A	3859	1/1	0.95	0.09	34,34,34,34	0
57	MG	1E	309	1/1	0.95	0.58	45,45,45,45	0
57	MG	1A	3095	1/1	0.95	0.44	39,39,39,39	0
57	MG	2A	3613	1/1	0.95	0.08	76,76,76,76	0
57	MG	2a	1636	1/1	0.95	0.27	86,86,86,86	0
57	MG	1A	3663	1/1	0.95	0.13	46,46,46,46	0
57	MG	1A	3012	1/1	0.95	0.15	48,48,48,48	0
57	MG	1A	3496	1/1	0.95	0.15	43,43,43,43	0
57	MG	1A	3915	1/1	0.95	0.31	33,33,33,33	0
57	MG	1A	3222	1/1	0.95	0.44	42,42,42,42	0
57	MG	1a	1757	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3837	1/1	0.95	0.15	62,62,62,62	0
57	MG	1A	4078	1/1	0.95	0.22	44,44,44,44	0
57	MG	2A	3523	1/1	0.95	0.12	49,49,49,49	0
57	MG	2A	3206	1/1	0.95	0.21	72,72,72,72	0
57	MG	2A	3680	1/1	0.95	0.16	69,69,69,69	0
57	MG	2A	3783	1/1	0.95	0.14	73,73,73,73	0
57	MG	1A	3976	1/1	0.95	0.23	65,65,65,65	0
57	MG	2A	3081	1/1	0.95	0.39	45,45,45,45	0
57	MG	2A	3217	1/1	0.95	0.45	37,37,37,37	0
57	MG	1A	3108	1/1	0.95	0.32	46,46,46,46	0
57	MG	2A	3223	1/1	0.95	0.27	36,36,36,36	0
57	MG	1A	3654	1/1	0.95	0.21	23,23,23,23	0
57	MG	1a	1907	1/1	0.95	0.17	46,46,46,46	0
57	MG	1A	3402	1/1	0.95	0.47	44,44,44,44	0
57	MG	2A	3392	1/1	0.95	0.19	73,73,73,73	0
57	MG	2A	3262	1/1	0.95	0.69	68,68,68,68	0
57	MG	2B	3003	1/1	0.95	0.29	73,73,73,73	0
57	MG	2A	3428	1/1	0.95	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3824	1/1	0.95	0.35	93,93,93,93	0
57	MG	1a	1700	1/1	0.95	0.12	67,67,67,67	0
57	MG	1A	3065	1/1	0.95	0.28	39,39,39,39	0
57	MG	2A	3365	1/1	0.95	0.18	37,37,37,37	0
57	MG	2A	3422	1/1	0.95	0.20	56,56,56,56	0
57	MG	1A	3633	1/1	0.95	0.21	34,34,34,34	0
57	MG	2A	3532	1/1	0.95	0.14	41,41,41,41	0
57	MG	2A	3791	1/1	0.95	0.15	62,62,62,62	0
57	MG	1A	3672	1/1	0.95	0.15	39,39,39,39	0
57	MG	2A	3374	1/1	0.95	0.21	64,64,64,64	0
57	MG	1G	3002	1/1	0.95	0.19	62,62,62,62	0
57	MG	1a	1732	1/1	0.95	0.22	64,64,64,64	0
57	MG	2V	201	1/1	0.95	0.36	52,52,52,52	0
57	MG	1A	3989	1/1	0.95	0.23	58,58,58,58	0
57	MG	2A	3358	1/1	0.95	0.28	50,50,50,50	0
57	MG	2A	3424	1/1	0.95	0.16	31,31,31,31	0
57	MG	1A	3523	1/1	0.95	0.20	60,60,60,60	0
57	MG	1a	1637	1/1	0.95	0.19	64,64,64,64	0
57	MG	1a	1623	1/1	0.95	0.24	64,64,64,64	0
57	MG	2A	3527	1/1	0.95	0.17	35,35,35,35	0
57	MG	1A	3069	1/1	0.95	0.15	59,59,59,59	0
57	MG	1w	107	1/1	0.95	0.41	49,49,49,49	0
59	ZN	2Y	501	1/1	0.95	0.13	94,94,94,94	0
57	MG	1A	3094	1/1	0.95	0.62	41,41,41,41	0
57	MG	1a	1894	1/1	0.95	0.20	64,64,64,64	0
57	MG	1A	3680	1/1	0.95	0.20	19,19,19,19	0
57	MG	2D	301	1/1	0.96	0.68	53,53,53,53	0
57	MG	2A	3367	1/1	0.96	0.33	53,53,53,53	0
57	MG	2a	1656	1/1	0.96	0.15	66,66,66,66	0
57	MG	2A	3560	1/1	0.96	0.11	63,63,63,63	0
57	MG	1D	3006	1/1	0.96	0.20	34,34,34,34	0
57	MG	1A	3854	1/1	0.96	0.18	52,52,52,52	0
57	MG	2a	1738	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	3792	1/1	0.96	0.13	66,66,66,66	0
57	MG	2U	204	1/1	0.96	0.48	56,56,56,56	0
57	MG	1a	1835	1/1	0.96	0.06	66,66,66,66	0
57	MG	2a	1654	1/1	0.96	0.13	71,71,71,71	0
57	MG	1A	3613	1/1	0.96	0.08	47,47,47,47	0
57	MG	1a	1775	1/1	0.96	0.06	72,72,72,72	0
57	MG	1a	1878	1/1	0.96	0.30	95,95,95,95	0
57	MG	2A	3496	1/1	0.96	0.17	72,72,72,72	0
57	MG	2A	3768	1/1	0.96	0.16	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3494	1/1	0.96	0.23	35,35,35,35	0
57	MG	2a	1715	1/1	0.96	0.19	60,60,60,60	0
57	MG	1A	3761	1/1	0.96	0.10	23,23,23,23	0
57	MG	1A	3022	1/1	0.96	0.37	32,32,32,32	0
57	MG	1A	3125	1/1	0.96	0.22	29,29,29,29	0
57	MG	2A	3142	1/1	0.96	0.18	65,65,65,65	0
57	MG	2A	3581	1/1	0.96	0.13	55,55,55,55	0
57	MG	1a	1798	1/1	0.96	0.15	63,63,63,63	0
57	MG	2a	1797	1/1	0.96	0.11	67,67,67,67	0
57	MG	1A	3251	1/1	0.96	0.41	40,40,40,40	0
57	MG	1A	3030	1/1	0.96	0.12	34,34,34,34	0
57	MG	2A	3445	1/1	0.96	0.16	29,29,29,29	0
57	MG	2A	3463	1/1	0.96	0.15	44,44,44,44	0
57	MG	2a	1745	1/1	0.96	0.14	64,64,64,64	0
57	MG	18	103	1/1	0.96	0.54	50,50,50,50	0
57	MG	1a	1819	1/1	0.96	0.10	62,62,62,62	0
57	MG	1A	3527	1/1	0.96	0.08	56,56,56,56	0
57	MG	1A	3687	1/1	0.96	0.09	39,39,39,39	0
57	MG	1A	3820	1/1	0.96	0.36	63,63,63,63	0
57	MG	20	8001	1/1	0.96	0.18	59,59,59,59	0
57	MG	2a	1720	1/1	0.96	0.14	75,75,75,75	0
57	MG	1A	3926	1/1	0.96	0.13	43,43,43,43	0
57	MG	2A	3748	1/1	0.96	0.14	38,38,38,38	0
57	MG	1A	3418	1/1	0.96	0.27	42,42,42,42	0
57	MG	2F	302	1/1	0.96	0.12	59,59,59,59	0
57	MG	1A	3049	1/1	0.96	0.12	31,31,31,31	0
57	MG	1A	3881	1/1	0.96	0.09	52,52,52,52	0
57	MG	2B	3010	1/1	0.96	0.10	70,70,70,70	0
57	MG	1A	4004	1/1	0.96	0.22	50,50,50,50	0
57	MG	2A	3127	1/1	0.96	0.63	50,50,50,50	0
57	MG	1A	4131	1/1	0.96	0.43	36,36,36,36	0
57	MG	1A	3190	1/1	0.96	0.27	35,35,35,35	0
57	MG	1A	4026	1/1	0.96	0.07	46,46,46,46	0
57	MG	2A	3584	1/1	0.96	0.31	43,43,43,43	0
57	MG	1B	209	1/1	0.96	0.57	65,65,65,65	0
57	MG	1A	3662	1/1	0.96	0.19	22,22,22,22	0
57	MG	2A	3741	1/1	0.96	0.16	43,43,43,43	0
57	MG	1A	3475	1/1	0.96	0.69	39,39,39,39	0
57	MG	1A	3155	1/1	0.96	0.15	39,39,39,39	0
57	MG	1A	3439	1/1	0.96	0.42	31,31,31,31	0
57	MG	2A	3712	1/1	0.96	0.14	94,94,94,94	0
57	MG	1A	3258	1/1	0.96	0.42	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1906	1/1	0.96	0.12	48,48,48,48	0
57	MG	1a	1610	1/1	0.96	0.18	24,24,24,24	0
57	MG	1B	219	1/1	0.96	0.10	60,60,60,60	0
57	MG	1A	4103	1/1	0.96	0.19	38,38,38,38	0
57	MG	1A	3510	1/1	0.96	0.16	30,30,30,30	0
57	MG	1A	3072	1/1	0.96	0.08	36,36,36,36	0
57	MG	1A	3856	1/1	0.96	0.13	13,13,13,13	0
57	MG	1A	3071	1/1	0.96	0.22	39,39,39,39	0
57	MG	2A	3113	1/1	0.96	0.15	69,69,69,69	0
57	MG	1A	3543	1/1	0.96	0.21	34,34,34,34	0
57	MG	1A	3150	1/1	0.96	0.56	42,42,42,42	0
57	MG	1A	3861	1/1	0.96	0.09	58,58,58,58	0
57	MG	1A	3189	1/1	0.96	0.41	34,34,34,34	0
57	MG	2A	3465	1/1	0.96	0.20	37,37,37,37	0
57	MG	1A	3731	1/1	0.96	0.15	20,20,20,20	0
57	MG	1A	3762	1/1	0.96	0.19	25,25,25,25	0
57	MG	2A	3608	1/1	0.96	0.16	37,37,37,37	0
57	MG	2A	3697	1/1	0.96	0.10	53,53,53,53	0
57	MG	1A	3431	1/1	0.96	0.57	37,37,37,37	0
57	MG	1A	4094	1/1	0.96	0.10	43,43,43,43	0
57	MG	2A	3330	1/1	0.96	0.21	48,48,48,48	0
57	MG	2A	3510	1/1	0.96	0.14	55,55,55,55	0
57	MG	2A	3435	1/1	0.96	0.08	59,59,59,59	0
57	MG	2a	1604	1/1	0.96	0.13	75,75,75,75	0
57	MG	1A	3665	1/1	0.96	0.36	57,57,57,57	0
57	MG	1a	1800	1/1	0.96	0.14	67,67,67,67	0
57	MG	1A	3771	1/1	0.96	0.20	41,41,41,41	0
57	MG	1A	3631	1/1	0.96	0.14	55,55,55,55	0
57	MG	1A	3575	1/1	0.96	0.17	27,27,27,27	0
57	MG	2A	3150	1/1	0.96	0.25	42,42,42,42	0
57	MG	2A	3526	1/1	0.96	0.14	69,69,69,69	0
57	MG	20	8002	1/1	0.96	0.24	75,75,75,75	0
57	MG	2A	3820	1/1	0.96	0.15	54,54,54,54	0
57	MG	1a	1639	1/1	0.96	0.11	56,56,56,56	0
57	MG	2A	3529	1/1	0.96	0.13	53,53,53,53	0
57	MG	1a	1722	1/1	0.96	0.12	36,36,36,36	0
57	MG	1A	3846	1/1	0.96	0.18	25,25,25,25	0
57	MG	1A	3075	1/1	0.96	0.17	55,55,55,55	0
57	MG	2A	3016	1/1	0.96	0.14	37,37,37,37	0
57	MG	2A	3681	1/1	0.96	0.21	59,59,59,59	0
57	MG	1A	3732	1/1	0.96	0.16	27,27,27,27	0
57	MG	1A	3511	1/1	0.96	0.15	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4129	1/1	0.96	0.33	35,35,35,35	0
57	MG	2A	3764	1/1	0.96	0.11	35,35,35,35	0
57	MG	1A	3630	1/1	0.96	0.12	67,67,67,67	0
57	MG	2a	1721	1/1	0.96	0.09	63,63,63,63	0
57	MG	1A	3584	1/1	0.96	0.10	33,33,33,33	0
57	MG	2y	3004	1/1	0.96	0.08	64,64,64,64	0
57	MG	1A	3914	1/1	0.96	0.25	33,33,33,33	0
57	MG	1A	3120	1/1	0.96	0.28	42,42,42,42	0
57	MG	1A	3110	1/1	0.96	0.22	16,16,16,16	0
57	MG	2A	3475	1/1	0.96	0.08	62,62,62,62	0
57	MG	1A	3660	1/1	0.96	0.09	43,43,43,43	0
57	MG	2A	3525	1/1	0.96	0.17	65,65,65,65	0
57	MG	1A	3824	1/1	0.96	0.14	23,23,23,23	0
57	MG	1Z	301	1/1	0.96	0.35	43,43,43,43	0
57	MG	1A	3302	1/1	0.96	0.18	26,26,26,26	0
57	MG	1a	1881	1/1	0.96	0.41	70,70,70,70	0
57	MG	1A	3026	1/1	0.96	0.19	37,37,37,37	0
57	MG	1A	3780	1/1	0.96	0.19	30,30,30,30	0
57	MG	1A	3753	1/1	0.96	0.11	40,40,40,40	0
57	MG	1A	3008	1/1	0.96	0.23	33,33,33,33	0
57	MG	2a	1668	1/1	0.96	0.22	63,63,63,63	0
57	MG	2a	1698	1/1	0.96	0.07	68,68,68,68	0
57	MG	1a	1743	1/1	0.96	0.11	41,41,41,41	0
57	MG	1A	3074	1/1	0.96	0.47	47,47,47,47	0
57	MG	2A	3811	1/1	0.96	0.11	76,76,76,76	0
57	MG	1a	1740	1/1	0.96	0.18	55,55,55,55	0
57	MG	1A	3895	1/1	0.96	0.12	32,32,32,32	0
57	MG	1A	3778	1/1	0.96	0.40	43,43,43,43	0
57	MG	1A	4041	1/1	0.96	0.15	56,56,56,56	0
57	MG	1a	1661	1/1	0.96	0.24	61,61,61,61	0
57	MG	1A	3140	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3767	1/1	0.96	0.08	33,33,33,33	0
57	MG	1A	3711	1/1	0.96	0.14	37,37,37,37	0
57	MG	2A	3170	1/1	0.96	0.14	44,44,44,44	0
57	MG	1a	1820	1/1	0.96	0.14	70,70,70,70	0
57	MG	2a	1768	1/1	0.96	0.16	63,63,63,63	0
57	MG	2A	3029	1/1	0.96	0.26	53,53,53,53	0
57	MG	1a	1622	1/1	0.96	0.23	57,57,57,57	0
57	MG	2a	1718	1/1	0.96	0.07	74,74,74,74	0
57	MG	2a	1765	1/1	0.96	0.19	75,75,75,75	0
57	MG	1A	4137	1/1	0.96	0.74	40,40,40,40	0
57	MG	1a	1711	1/1	0.96	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3954	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	4138	1/1	0.96	0.77	42,42,42,42	0
57	MG	1a	1750	1/1	0.96	0.09	63,63,63,63	0
57	MG	1A	4125	1/1	0.96	0.24	33,33,33,33	0
57	MG	1A	3342	1/1	0.96	0.48	49,49,49,49	0
57	MG	2A	3771	1/1	0.96	0.15	52,52,52,52	0
59	ZN	29	102	1/1	0.96	0.17	70,70,70,70	0
57	MG	1A	3504	1/1	0.96	0.20	17,17,17,17	0
57	MG	1A	3800	1/1	0.96	0.23	60,60,60,60	0
57	MG	2A	3804	1/1	0.96	0.13	75,75,75,75	0
57	MG	2A	3288	1/1	0.96	0.28	70,70,70,70	0
57	MG	1a	1717	1/1	0.96	0.13	65,65,65,65	0
57	MG	2a	1750	1/1	0.96	0.11	83,83,83,83	0
57	MG	2A	3007	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	3024	1/1	0.96	0.36	33,33,33,33	0
57	MG	1A	3587	1/1	0.96	0.19	35,35,35,35	0
57	MG	1A	3461	1/1	0.96	0.28	34,34,34,34	0
57	MG	2A	3650	1/1	0.96	0.14	46,46,46,46	0
57	MG	2A	3023	1/1	0.96	1.06	56,56,56,56	0
57	MG	2A	3068	1/1	0.96	0.13	45,45,45,45	0
57	MG	2A	3589	1/1	0.96	0.19	40,40,40,40	0
57	MG	1A	3033	1/1	0.96	0.12	32,32,32,32	0
57	MG	2A	3108	1/1	0.96	0.10	71,71,71,71	0
57	MG	2A	3619	1/1	0.96	0.15	58,58,58,58	0
57	MG	2l	203	1/1	0.96	0.17	69,69,69,69	0
57	MG	1t	3001	1/1	0.96	0.10	67,67,67,67	0
57	MG	1A	3424	1/1	0.96	0.27	59,59,59,59	0
57	MG	1A	3688	1/1	0.96	0.13	30,30,30,30	0
57	MG	1a	1630	1/1	0.96	0.14	62,62,62,62	0
57	MG	2A	3004	1/1	0.96	0.16	46,46,46,46	0
57	MG	1B	218	1/1	0.96	0.20	62,62,62,62	0
57	MG	1a	1738	1/1	0.96	0.18	44,44,44,44	0
57	MG	1A	3573	1/1	0.96	0.10	43,43,43,43	0
57	MG	1a	1649	1/1	0.96	0.21	75,75,75,75	0
57	MG	2Q	3001	1/1	0.96	0.09	66,66,66,66	0
57	MG	13	102	1/1	0.96	0.30	45,45,45,45	0
57	MG	1A	3064	1/1	0.96	0.27	32,32,32,32	0
57	MG	1A	3016	1/1	0.96	0.24	38,38,38,38	0
57	MG	2A	3400	1/1	0.96	0.19	57,57,57,57	0
57	MG	1a	1807	1/1	0.96	0.17	71,71,71,71	0
57	MG	1A	3023	1/1	0.96	0.41	32,32,32,32	0
57	MG	2a	1787	1/1	0.96	0.18	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1753	1/1	0.96	0.18	64,64,64,64	0
57	MG	1A	3035	1/1	0.96	0.15	38,38,38,38	0
57	MG	2a	1777	1/1	0.96	0.10	82,82,82,82	0
57	MG	1A	3088	1/1	0.96	0.39	30,30,30,30	0
57	MG	1A	4096	1/1	0.96	0.32	36,36,36,36	0
57	MG	2e	3002	1/1	0.97	0.07	76,76,76,76	0
57	MG	1A	3516	1/1	0.97	0.18	17,17,17,17	0
57	MG	1A	3810	1/1	0.97	0.17	40,40,40,40	0
57	MG	1A	3002	1/1	0.97	0.16	19,19,19,19	0
57	MG	2A	3531	1/1	0.97	0.15	42,42,42,42	0
57	MG	1A	3943	1/1	0.97	0.19	68,68,68,68	0
57	MG	1A	3436	1/1	0.97	0.12	55,55,55,55	0
57	MG	2A	3017	1/1	0.97	0.14	46,46,46,46	0
57	MG	1A	3602	1/1	0.97	0.16	15,15,15,15	0
57	MG	1A	4128	1/1	0.97	0.39	31,31,31,31	0
57	MG	2A	3795	1/1	0.97	0.27	78,78,78,78	0
57	MG	2A	3780	1/1	0.97	0.14	57,57,57,57	0
57	MG	1a	1742	1/1	0.97	0.13	57,57,57,57	0
57	MG	1A	3493	1/1	0.97	0.12	34,34,34,34	0
57	MG	1A	4117	1/1	0.97	0.48	39,39,39,39	0
57	MG	17	101	1/1	0.97	0.15	45,45,45,45	0
57	MG	2A	3161	1/1	0.97	0.09	48,48,48,48	0
57	MG	1A	4058	1/1	0.97	0.22	31,31,31,31	0
57	MG	1A	3591	1/1	0.97	0.10	10,10,10,10	0
57	MG	2A	3452	1/1	0.97	0.21	62,62,62,62	0
57	MG	1A	3126	1/1	0.97	0.34	32,32,32,32	0
57	MG	1A	3138	1/1	0.97	0.34	36,36,36,36	0
57	MG	1A	3032	1/1	0.97	0.38	32,32,32,32	0
57	MG	1A	3661	1/1	0.97	0.10	29,29,29,29	0
57	MG	1A	3562	1/1	0.97	0.17	27,27,27,27	0
57	MG	1D	3009	1/1	0.97	0.43	28,28,28,28	0
57	MG	1A	3168	1/1	0.97	0.55	35,35,35,35	0
57	MG	2D	302	1/1	0.97	0.16	33,33,33,33	0
57	MG	1A	3828	1/1	0.97	0.20	47,47,47,47	0
57	MG	2A	3020	1/1	0.97	0.57	56,56,56,56	0
57	MG	1A	3888	1/1	0.97	0.06	50,50,50,50	0
57	MG	1a	1887	1/1	0.97	0.15	76,76,76,76	0
57	MG	1a	1862	1/1	0.97	0.16	34,34,34,34	0
57	MG	1A	3031	1/1	0.97	0.43	34,34,34,34	0
57	MG	1A	3627	1/1	0.97	0.22	29,29,29,29	0
57	MG	2A	3714	1/1	0.97	0.11	69,69,69,69	0
57	MG	2a	1759	1/1	0.97	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1612	1/1	0.97	0.07	71,71,71,71	0
57	MG	2A	3289	1/1	0.97	0.35	81,81,81,81	0
57	MG	2A	3467	1/1	0.97	0.19	58,58,58,58	0
57	MG	1a	1885	1/1	0.97	0.29	71,71,71,71	0
57	MG	2A	3221	1/1	0.97	0.05	76,76,76,76	0
57	MG	1a	1888	1/1	0.97	0.13	66,66,66,66	0
57	MG	2A	3015	1/1	0.97	0.13	58,58,58,58	0
57	MG	2x	105	1/1	0.97	0.14	78,78,78,78	0
57	MG	1A	3096	1/1	0.97	0.37	40,40,40,40	0
57	MG	1A	4007	1/1	0.97	0.10	43,43,43,43	0
57	MG	1N	203	1/1	0.97	0.20	44,44,44,44	0
57	MG	2A	3379	1/1	0.97	0.19	58,58,58,58	0
57	MG	1A	3993	1/1	0.97	0.14	42,42,42,42	0
57	MG	2A	3634	1/1	0.97	0.07	52,52,52,52	0
57	MG	1a	1664	1/1	0.97	0.25	54,54,54,54	0
57	MG	1A	3733	1/1	0.97	0.14	40,40,40,40	0
57	MG	2A	3137	1/1	0.97	0.17	39,39,39,39	0
57	MG	1A	3678	1/1	0.97	0.21	24,24,24,24	0
57	MG	1A	3133	1/1	0.97	0.42	42,42,42,42	0
57	MG	1A	3109	1/1	0.97	0.30	34,34,34,34	0
57	MG	2A	3429	1/1	0.97	0.15	42,42,42,42	0
57	MG	1D	3003	1/1	0.97	0.16	18,18,18,18	0
57	MG	2A	3840	1/1	0.97	0.14	64,64,64,64	0
57	MG	2A	3567	1/1	0.97	0.07	68,68,68,68	0
57	MG	1A	3485	1/1	0.97	0.58	36,36,36,36	0
57	MG	2A	3625	1/1	0.97	0.16	30,30,30,30	0
57	MG	1a	1701	1/1	0.97	0.49	73,73,73,73	0
57	MG	1a	1729	1/1	0.97	0.14	39,39,39,39	0
57	MG	1A	3685	1/1	0.97	0.17	23,23,23,23	0
57	MG	1A	3262	1/1	0.97	0.18	54,54,54,54	0
57	MG	2A	3495	1/1	0.97	0.17	26,26,26,26	0
57	MG	1A	4121	1/1	0.97	0.32	31,31,31,31	0
57	MG	1a	1733	1/1	0.97	0.17	70,70,70,70	0
57	MG	1x	3011	1/1	0.97	0.08	68,68,68,68	0
57	MG	1A	3099	1/1	0.97	0.11	68,68,68,68	0
57	MG	1U	203	1/1	0.97	0.49	37,37,37,37	0
57	MG	2A	3478	1/1	0.97	0.13	34,34,34,34	0
57	MG	1A	3541	1/1	0.97	0.07	42,42,42,42	0
57	MG	2A	3431	1/1	0.97	0.10	57,57,57,57	0
57	MG	1a	1723	1/1	0.97	0.11	62,62,62,62	0
57	MG	1E	305	1/1	0.97	0.14	33,33,33,33	0
57	MG	2a	1704	1/1	0.97	0.16	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4099	1/1	0.97	0.26	34,34,34,34	0
57	MG	1A	3014	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3505	1/1	0.97	0.15	41,41,41,41	0
57	MG	1A	4115	1/1	0.97	0.32	31,31,31,31	0
57	MG	1a	1912	1/1	0.97	0.11	66,66,66,66	0
57	MG	1A	3610	1/1	0.97	0.25	59,59,59,59	0
57	MG	2A	3757	1/1	0.97	0.05	68,68,68,68	0
57	MG	1A	3366	1/1	0.97	0.25	34,34,34,34	0
57	MG	1A	3567	1/1	0.97	0.18	25,25,25,25	0
57	MG	1A	3367	1/1	0.97	0.46	39,39,39,39	0
57	MG	1A	3913	1/1	0.97	0.38	57,57,57,57	0
57	MG	2A	3788	1/1	0.97	0.14	63,63,63,63	0
57	MG	1A	3027	1/1	0.97	0.16	20,20,20,20	0
57	MG	2A	3069	1/1	0.97	0.21	27,27,27,27	0
57	MG	2A	3754	1/1	0.97	0.11	43,43,43,43	0
57	MG	1A	3611	1/1	0.97	0.11	44,44,44,44	0
57	MG	1a	1702	1/1	0.97	0.32	66,66,66,66	0
57	MG	1a	1874	1/1	0.97	0.08	72,72,72,72	0
57	MG	2A	3755	1/1	0.97	0.19	55,55,55,55	0
57	MG	1A	3589	1/1	0.97	0.22	23,23,23,23	0
57	MG	1A	3718	1/1	0.97	0.15	49,49,49,49	0
57	MG	2f	3001	1/1	0.97	0.14	58,58,58,58	0
57	MG	2a	1696	1/1	0.97	0.19	69,69,69,69	0
57	MG	1A	3815	1/1	0.97	0.12	58,58,58,58	0
57	MG	1A	3057	1/1	0.97	0.22	45,45,45,45	0
57	MG	1A	3554	1/1	0.97	0.17	41,41,41,41	0
57	MG	1A	3593	1/1	0.97	0.18	25,25,25,25	0
57	MG	1A	3089	1/1	0.97	0.27	39,39,39,39	0
57	MG	2a	1663	1/1	0.97	0.17	47,47,47,47	0
57	MG	2A	3448	1/1	0.97	0.18	55,55,55,55	0
57	MG	2A	3066	1/1	0.97	0.52	51,51,51,51	0
57	MG	1A	3566	1/1	0.97	0.14	28,28,28,28	0
57	MG	1A	4102	1/1	0.97	0.51	39,39,39,39	0
57	MG	1A	4132	1/1	0.97	0.80	37,37,37,37	0
57	MG	1A	4141	1/1	0.97	0.70	30,30,30,30	0
57	MG	1A	3483	1/1	0.97	0.46	37,37,37,37	0
57	MG	1A	3004	1/1	0.97	0.11	24,24,24,24	0
57	MG	1A	3905	1/1	0.97	0.21	41,41,41,41	0
57	MG	1X	3004	1/1	0.97	0.48	41,41,41,41	0
57	MG	1A	3507	1/1	0.97	0.19	34,34,34,34	0
57	MG	1A	3752	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	4134	1/1	0.97	0.26	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3041	1/1	0.97	0.19	24,24,24,24	0
59	ZN	1Y	202	1/1	0.97	0.20	63,63,63,63	0
57	MG	1A	3968	1/1	0.97	0.11	72,72,72,72	0
57	MG	1A	3157	1/1	0.97	0.24	24,24,24,24	0
57	MG	1A	3161	1/1	0.97	0.17	24,24,24,24	0
57	MG	2A	3517	1/1	0.97	0.16	63,63,63,63	0
57	MG	1A	3203	1/1	0.97	0.31	33,33,33,33	0
57	MG	2a	1789	1/1	0.97	0.08	77,77,77,77	0
57	MG	1A	3651	1/1	0.97	0.15	47,47,47,47	0
57	MG	1a	1676	1/1	0.97	0.11	76,76,76,76	0
57	MG	2a	1677	1/1	0.97	0.10	69,69,69,69	0
57	MG	1A	3878	1/1	0.97	0.17	51,51,51,51	0
57	MG	1a	1705	1/1	0.97	0.40	62,62,62,62	0
57	MG	2A	3021	1/1	0.97	0.74	50,50,50,50	0
57	MG	1A	3607	1/1	0.97	0.15	25,25,25,25	0
57	MG	1A	3535	1/1	0.97	0.17	32,32,32,32	0
57	MG	1a	1628	1/1	0.97	0.13	54,54,54,54	0
57	MG	2A	3578	1/1	0.97	0.18	36,36,36,36	0
57	MG	2a	1743	1/1	0.97	0.16	72,72,72,72	0
57	MG	2A	3002	1/1	0.97	0.14	57,57,57,57	0
57	MG	1F	307	1/1	0.97	0.14	52,52,52,52	0
57	MG	1A	3576	1/1	0.97	0.14	25,25,25,25	0
57	MG	1A	3182	1/1	0.97	0.48	34,34,34,34	0
57	MG	1A	3844	1/1	0.97	0.17	30,30,30,30	0
57	MG	1A	4126	1/1	0.97	0.33	38,38,38,38	0
57	MG	1A	3115	1/1	0.97	0.16	56,56,56,56	0
57	MG	1I	101	1/1	0.97	0.17	45,45,45,45	0
57	MG	1A	3612	1/1	0.97	0.12	47,47,47,47	0
57	MG	2A	3639	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3051	1/1	0.97	0.14	18,18,18,18	0
57	MG	1A	3582	1/1	0.97	0.20	20,20,20,20	0
57	MG	2a	1602	1/1	0.97	0.49	72,72,72,72	0
57	MG	2A	3129	1/1	0.97	0.19	40,40,40,40	0
57	MG	1A	3901	1/1	0.97	0.20	19,19,19,19	0
57	MG	1A	3087	1/1	0.97	0.41	39,39,39,39	0
57	MG	1A	4124	1/1	0.97	0.19	37,37,37,37	0
57	MG	1A	3561	1/1	0.97	0.17	18,18,18,18	0
57	MG	1A	3777	1/1	0.97	0.24	48,48,48,48	0
57	MG	2A	3130	1/1	0.97	0.22	63,63,63,63	0
57	MG	1A	3883	1/1	0.98	0.17	17,17,17,17	0
57	MG	2A	3145	1/1	0.98	0.20	38,38,38,38	0
57	MG	1A	3058	1/1	0.98	0.22	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3815	1/1	0.98	0.09	72,72,72,72	0
57	MG	1A	4066	1/1	0.98	0.11	54,54,54,54	0
57	MG	2A	3857	1/1	0.98	0.73	48,48,48,48	0
57	MG	1A	3036	1/1	0.98	0.21	34,34,34,34	0
57	MG	1U	205	1/1	0.98	0.39	30,30,30,30	0
60	SF4	1d	501	8/8	0.98	0.19	63,72,78,81	0
57	MG	1A	3892	1/1	0.98	0.20	28,28,28,28	0
57	MG	1A	3756	1/1	0.98	0.18	27,27,27,27	0
57	MG	1B	201	1/1	0.98	0.26	56,56,56,56	0
60	SF4	2d	501	8/8	0.98	0.19	66,75,87,95	0
57	MG	1X	3001	1/1	0.98	0.13	54,54,54,54	0
57	MG	1a	1726	1/1	0.98	0.11	60,60,60,60	0
57	MG	1A	3238	1/1	0.98	0.14	37,37,37,37	0
57	MG	2A	3453	1/1	0.98	0.12	52,52,52,52	0
57	MG	2A	3551	1/1	0.98	0.24	45,45,45,45	0
57	MG	1A	4143	1/1	0.98	0.45	37,37,37,37	0
57	MG	1A	3508	1/1	0.98	0.17	39,39,39,39	0
57	MG	2A	3058	1/1	0.98	0.20	57,57,57,57	0
57	MG	2A	3618	1/1	0.98	0.06	70,70,70,70	0
57	MG	2A	3359	1/1	0.98	0.31	55,55,55,55	0
57	MG	1A	3019	1/1	0.98	0.24	31,31,31,31	0
57	MG	1B	205	1/1	0.98	0.13	45,45,45,45	0
57	MG	1A	3006	1/1	0.98	0.14	24,24,24,24	0
57	MG	1A	3506	1/1	0.98	0.15	12,12,12,12	0
57	MG	2a	1754	1/1	0.98	0.19	70,70,70,70	0
57	MG	2A	3645	1/1	0.98	0.11	63,63,63,63	0
57	MG	1D	3005	1/1	0.98	0.29	33,33,33,33	0
57	MG	2A	3756	1/1	0.98	0.12	46,46,46,46	0
57	MG	1A	3775	1/1	0.98	0.17	41,41,41,41	0
59	ZN	26	501	1/1	0.98	0.21	67,67,67,67	0
57	MG	1A	3909	1/1	0.98	0.08	38,38,38,38	0
57	MG	1B	225	1/1	0.98	0.15	33,33,33,33	0
57	MG	1A	4146	1/1	0.98	0.13	29,29,29,29	0
57	MG	1A	3547	1/1	0.98	0.14	38,38,38,38	0
57	MG	1A	3225	1/1	0.98	0.72	35,35,35,35	0
57	MG	1A	4123	1/1	0.98	0.69	33,33,33,33	0
57	MG	1A	3960	1/1	0.98	0.24	47,47,47,47	0
57	MG	1A	3982	1/1	0.98	0.04	59,59,59,59	0
57	MG	1A	3073	1/1	0.98	0.17	21,21,21,21	0
57	MG	1A	3136	1/1	0.98	0.43	40,40,40,40	0
57	MG	1A	3666	1/1	0.98	0.20	19,19,19,19	0
57	MG	1A	3572	1/1	0.98	0.22	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3360	1/1	0.98	0.28	47,47,47,47	0
57	MG	2A	3293	1/1	0.98	0.18	58,58,58,58	0
57	MG	1A	3750	1/1	0.98	0.40	39,39,39,39	0
57	MG	2A	3378	1/1	0.98	0.24	52,52,52,52	0
57	MG	2A	3131	1/1	0.98	0.14	55,55,55,55	0
57	MG	1A	3147	1/1	0.98	0.44	43,43,43,43	0
57	MG	1A	4130	1/1	0.98	0.55	31,31,31,31	0
57	MG	1A	3639	1/1	0.98	0.08	44,44,44,44	0
57	MG	1A	3836	1/1	0.98	0.22	71,71,71,71	0
57	MG	1a	1769	1/1	0.98	0.09	54,54,54,54	0
57	MG	2A	3362	1/1	0.98	0.23	55,55,55,55	0
57	MG	1A	4133	1/1	0.98	0.17	39,39,39,39	0
57	MG	1A	4139	1/1	0.98	0.12	37,37,37,37	0
57	MG	1B	235	1/1	0.98	0.10	40,40,40,40	0
57	MG	1A	3668	1/1	0.98	0.14	44,44,44,44	0
57	MG	1a	1783	1/1	0.98	0.12	58,58,58,58	0
57	MG	1A	3438	1/1	0.98	0.38	31,31,31,31	0
57	MG	1A	3614	1/1	0.98	0.18	21,21,21,21	0
57	MG	1D	3001	1/1	0.98	0.36	43,43,43,43	0
57	MG	2A	3454	1/1	0.98	0.18	64,64,64,64	0
57	MG	1A	3481	1/1	0.98	0.46	34,34,34,34	0
57	MG	1A	3867	1/1	0.98	0.10	27,27,27,27	0
57	MG	1A	3540	1/1	0.98	0.13	29,29,29,29	0
57	MG	1A	3159	1/1	0.98	0.12	31,31,31,31	0
57	MG	1A	3239	1/1	0.98	0.17	36,36,36,36	0
57	MG	1A	3137	1/1	0.98	0.48	32,32,32,32	0
57	MG	1A	3551	1/1	0.98	0.18	23,23,23,23	0
57	MG	1A	4150	1/1	0.98	0.41	45,45,45,45	0
57	MG	1F	303	1/1	0.98	0.45	31,31,31,31	0
57	MG	1A	3462	1/1	0.98	0.49	39,39,39,39	0
57	MG	2A	3501	1/1	0.98	0.11	37,37,37,37	0
57	MG	1A	3495	1/1	0.98	0.13	42,42,42,42	0
57	MG	2A	3418	1/1	0.98	0.22	58,58,58,58	0
57	MG	1A	3181	1/1	0.98	0.27	37,37,37,37	0
57	MG	1A	3710	1/1	0.98	0.13	63,63,63,63	0
57	MG	1A	3228	1/1	0.98	0.22	48,48,48,48	0
57	MG	2A	3411	1/1	0.98	0.62	55,55,55,55	0
57	MG	2A	3752	1/1	0.98	0.18	36,36,36,36	0
57	MG	1A	3113	1/1	0.98	0.47	31,31,31,31	0
57	MG	1A	3059	1/1	0.98	0.14	31,31,31,31	0
57	MG	1A	3191	1/1	0.98	0.43	37,37,37,37	0
57	MG	1B	215	1/1	0.98	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1Y	204	1/1	0.98	0.25	46,46,46,46	0
57	MG	10	106	1/1	0.98	0.10	54,54,54,54	0
57	MG	1a	1708	1/1	0.98	0.26	50,50,50,50	0
57	MG	1a	1679	1/1	0.98	0.15	65,65,65,65	0
57	MG	2A	3238	1/1	0.98	0.50	69,69,69,69	0
57	MG	1A	3517	1/1	0.98	0.09	51,51,51,51	0
57	MG	1A	3466	1/1	0.98	0.35	41,41,41,41	0
57	MG	1A	3686	1/1	0.98	0.20	25,25,25,25	0
57	MG	2A	3485	1/1	0.98	0.15	38,38,38,38	0
57	MG	2A	3600	1/1	0.98	0.11	74,74,74,74	0
57	MG	2A	3759	1/1	0.98	0.18	42,42,42,42	0
57	MG	1G	3004	1/1	0.98	0.14	46,46,46,46	0
57	MG	1A	3047	1/1	0.98	0.16	39,39,39,39	0
57	MG	1a	1856	1/1	0.98	0.15	68,68,68,68	0
57	MG	1A	3224	1/1	0.98	0.56	29,29,29,29	0
59	ZN	25	101	1/1	0.98	0.24	59,59,59,59	0
57	MG	1A	3470	1/1	0.98	0.26	33,33,33,33	0
57	MG	1A	3080	1/1	0.98	0.28	35,35,35,35	0
57	MG	1A	3798	1/1	0.98	0.12	57,57,57,57	0
57	MG	1A	3223	1/1	0.98	0.08	44,44,44,44	0
57	MG	2a	1659	1/1	0.98	0.14	65,65,65,65	0
57	MG	1a	1837	1/1	0.98	0.27	70,70,70,70	0
57	MG	2A	3695	1/1	0.99	0.07	60,60,60,60	0
57	MG	1w	108	1/1	0.99	0.18	68,68,68,68	0
57	MG	1A	3557	1/1	0.99	0.17	19,19,19,19	0
57	MG	1A	3638	1/1	0.99	0.15	24,24,24,24	0
57	MG	1A	3560	1/1	0.99	0.13	34,34,34,34	0
57	MG	1A	3615	1/1	0.99	0.19	24,24,24,24	0
57	MG	1G	3005	1/1	0.99	0.16	64,64,64,64	0
59	ZN	15	101	1/1	0.99	0.24	43,43,43,43	0
59	ZN	16	101	1/1	0.99	0.26	45,45,45,45	0
57	MG	1A	3773	1/1	0.99	0.10	61,61,61,61	0
57	MG	1A	3548	1/1	0.99	0.17	25,25,25,25	0
57	MG	1A	3802	1/1	0.99	0.14	24,24,24,24	0
57	MG	1A	3484	1/1	0.99	0.32	37,37,37,37	0
57	MG	2a	1782	1/1	0.99	0.11	84,84,84,84	0
57	MG	1a	1764	1/1	0.99	0.09	49,49,49,49	0
57	MG	1W	203	1/1	0.99	0.29	38,38,38,38	0
57	MG	2A	3426	1/1	0.99	0.19	26,26,26,26	0
57	MG	2A	3507	1/1	0.99	0.17	37,37,37,37	0
57	MG	2A	3032	1/1	0.99	0.21	44,44,44,44	0
57	MG	2A	3437	1/1	0.99	0.08	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3471	1/1	0.99	0.30	28,28,28,28	0
59	ZN	1n	501	1/1	0.99	0.17	67,67,67,67	0
57	MG	1A	3512	1/1	0.99	0.20	26,26,26,26	0
57	MG	1A	3958	1/1	0.99	0.21	26,26,26,26	0
57	MG	1A	3884	1/1	0.99	0.12	46,46,46,46	0
57	MG	1A	3870	1/1	0.99	0.18	35,35,35,35	0
57	MG	1A	3565	1/1	0.99	0.15	21,21,21,21	0
57	MG	1A	3673	1/1	0.99	0.18	17,17,17,17	0
57	MG	2A	3405	1/1	0.99	0.18	22,22,22,22	0
57	MG	1A	3333	1/1	0.99	0.16	33,33,33,33	0
57	MG	2A	3008	1/1	0.99	0.12	45,45,45,45	0
58	K	2A	3849	1/1	0.99	0.11	72,72,72,72	0
57	MG	1A	4082	1/1	0.99	0.22	14,14,14,14	0
57	MG	1A	3053	1/1	0.99	0.17	20,20,20,20	0
59	ZN	19	102	1/1	1.00	0.24	47,47,47,47	0
57	MG	1A	3748	1/1	1.00	0.26	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.