



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2020 – 11:47 PM EST

PDB ID : 6XHV
Title : Crystal structure of the A2058-dimethylated *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A- and P-site tRNAs, and deacylated E-site tRNA at 2.40Å resolution
Authors : Svetlov, M.S.; Syroegin, E.A.; Aleksandrova, E.V.; Atkinson, G.C.; Gregory, S.T.; Mankin, A.S.; Polikanov, Y.S.
Deposited on : 2020-06-19
Resolution : 2.40 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	:	2.15.1
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)	:	2.15.1

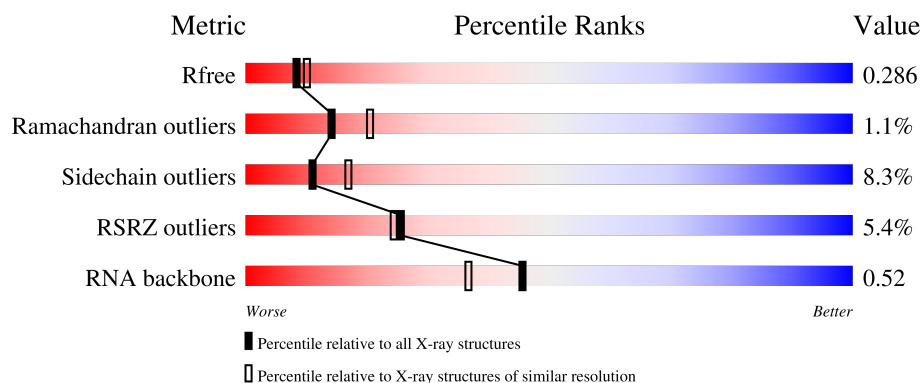
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>3%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
1	2A	2915	<div> <div>4%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>
2	1B	121	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
2	2B	121	<div> <div>74%</div> <div>25%</div> <div>.</div> </div>
3	1D	276	<div> <div>%</div> <div>96%</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	<div> <div></div> <div>94%</div> <div>• •</div> </div>
16	2U	118	<div> <div>4%</div> <div>93%</div> <div>5% •</div> </div>
17	1V	101	<div> <div></div> <div>95%</div> <div>• •</div> </div>
17	2V	101	<div> <div>4%</div> <div>91%</div> <div>9%</div> </div>
18	1W	113	<div> <div></div> <div>93%</div> <div>6% •</div> </div>
18	2W	113	<div> <div>4%</div> <div>96%</div> <div>• •</div> </div>
19	1X	96	<div> <div></div> <div>92%</div> <div>7% •</div> </div>
19	2X	96	<div> <div>11%</div> <div>94%</div> <div>5% •</div> </div>
20	1Y	110	<div> <div></div> <div>88%</div> <div>9% •</div> </div>
20	2Y	110	<div> <div>12%</div> <div>90%</div> <div>6% • •</div> </div>
21	1Z	206	<div> <div>3%</div> <div>68%</div> <div>6% 25%</div> </div>
21	2Z	206	<div> <div>13%</div> <div>67%</div> <div>10% 22%</div> </div>
22	10	85	<div> <div></div> <div>98%</div> <div>•</div> </div>
22	20	85	<div> <div>5%</div> <div>96%</div> <div>• •</div> </div>
23	11	98	<div> <div>2%</div> <div>97%</div> <div>• •</div> </div>
23	21	98	<div> <div>5%</div> <div>95%</div> <div>• •</div> </div>
24	12	72	<div> <div></div> <div>92%</div> <div>6% •</div> </div>
24	22	72	<div> <div>4%</div> <div>96%</div> <div>• •</div> </div>
25	13	60	<div> <div></div> <div>90%</div> <div>8% •</div> </div>
25	23	60	<div> <div>10%</div> <div>87%</div> <div>12% •</div> </div>
26	14	71	<div> <div></div> <div>79%</div> <div>17% • •</div> </div>
26	24	71	<div> <div>14%</div> <div>85%</div> <div>13% •</div> </div>
27	15	60	<div> <div>2%</div> <div>88%</div> <div>10% •</div> </div>
27	25	60	<div> <div>2%</div> <div>93%</div> <div>5% •</div> </div>
28	16	54	<div> <div></div> <div>91%</div> <div>7% •</div> </div>

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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	24	

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Mol	Chain	Length	Quality of chain
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	PSU	2y	32	-	-	-	X
56	MIA	2y	37	-	-	-	X
56	5MU	2y	54	-	-	-	X
57	MG	1A	4082	-	-	-	X
57	MG	1E	307	-	-	-	X
57	MG	2A	3235	-	-	-	X
57	MG	2A	3339	-	-	-	X
57	MG	2A	3495	-	-	-	X
57	MG	2A	3530	-	-	-	X
57	MG	2A	3749	-	-	-	X
57	MG	2A	3773	-	-	-	X
57	MG	2A	3863	-	-	-	X
57	MG	2B	218	-	-	-	X
57	MG	2W	202	-	-	-	X
57	MG	2a	1734	-	-	-	X
57	MG	2a	1744	-	-	-	X
57	MG	2w	106	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300906 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
			61854	27533	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60324	26850	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
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0
			1603	722	287	518	74	2		
54	2w	72	Total	C	N	O	P	S	0	0
			1555	699	280	502	72	2		

- 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
			1635	731	296	530	76	2		
55	2x	76	Total	C	N	O	P	S	0	0
			1635	731	296	530	76	2		

- Molecule 56 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
56	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2E	5	Total	Mg	0	0
			5	5		
57	17	5	Total	Mg	0	0
			5	5		
57	2d	2	Total	Mg	0	0
			2	2		
57	1T	4	Total	Mg	0	0
			4	4		
57	1N	5	Total	Mg	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	20	1	Total 1	Mg 1	0	0
57	18	6	Total 6	Mg 6	0	0
57	2W	2	Total 2	Mg 2	0	0
57	1Y	3	Total 3	Mg 3	0	0
57	13	5	Total 5	Mg 5	0	0
57	1f	2	Total 2	Mg 2	0	0
57	1P	4	Total 4	Mg 4	0	0
57	2B	20	Total 20	Mg 20	0	0
57	2a	238	Total 238	Mg 238	0	0
57	1E	13	Total 13	Mg 13	0	0
57	1b	2	Total 2	Mg 2	0	0
57	2l	3	Total 3	Mg 3	0	0
57	2F	6	Total 6	Mg 6	0	0
57	16	1	Total 1	Mg 1	0	0
57	28	3	Total 3	Mg 3	0	0
57	2e	1	Total 1	Mg 1	0	0
57	1W	6	Total 6	Mg 6	0	0
57	1A	1121	Total 1121	Mg 1121	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1n	1	Total 1	Mg 1	0	0
57	2P	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1X	7	Total 7	Mg 7	0	0
57	2q	3	Total 3	Mg 3	0	0
57	12	2	Total 2	Mg 2	0	0
57	1y	3	Total 3	Mg 3	0	0
57	1S	3	Total 3	Mg 3	0	0
57	25	5	Total 5	Mg 5	0	0
57	2T	3	Total 3	Mg 3	0	0
57	1D	12	Total 12	Mg 12	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	2f	2	Total 2	Mg 2	0	0
57	1V	9	Total 9	Mg 9	0	0
57	2X	3	Total 3	Mg 3	0	0
57	1w	10	Total 10	Mg 10	0	0
57	1a	219	Total 219	Mg 219	0	0
57	2Q	5	Total 5	Mg 5	0	0
57	15	7	Total 7	Mg 7	0	0
57	1x	15	Total 15	Mg 15	0	0
57	2j	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1R	4	Total Mg 4 4	0	0
57	26	1	Total Mg 1 1	0	0
57	1m	2	Total Mg 2 2	0	0
57	2U	2	Total Mg 2 2	0	0
57	1G	5	Total Mg 5 5	0	0
57	2O	2	Total Mg 2 2	0	0
57	11	6	Total Mg 6 6	0	0
57	1d	1	Total Mg 1 1	0	0
57	2r	1	Total Mg 1 1	0	0
57	21	1	Total Mg 1 1	0	0
57	2g	1	Total Mg 1 1	0	0
57	1v	1	Total Mg 1 1	0	0
57	2x	5	Total Mg 5 5	0	0
57	2R	2	Total Mg 2 2	0	0
57	1Z	2	Total Mg 2 2	0	0
57	2D	7	Total Mg 7 7	0	0
57	14	1	Total Mg 1 1	0	0
57	1U	9	Total Mg 9 9	0	0
57	1O	4	Total Mg 4 4	0	0
57	27	1	Total Mg 1 1	0	0
57	19	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1l	2	Total Mg 2 2	0	0
57	2V	3	Total Mg 3 3	0	0
57	1F	11	Total Mg 11 11	0	0
57	10	9	Total Mg 9 9	0	0
57	2t	1	Total Mg 1 1	0	0
57	1Q	7	Total Mg 7 7	0	0
57	2A	890	Total Mg 890 890	0	0
57	23	4	Total Mg 4 4	0	0
57	2Z	1	Total Mg 1 1	0	0
57	1B	34	Total Mg 34 34	0	0
57	2y	6	Total Mg 6 6	0	0
57	2w	9	Total Mg 9 9	0	0
57	2v	4	Total Mg 4 4	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
58	2A	1	Total K 1 1	0	0

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

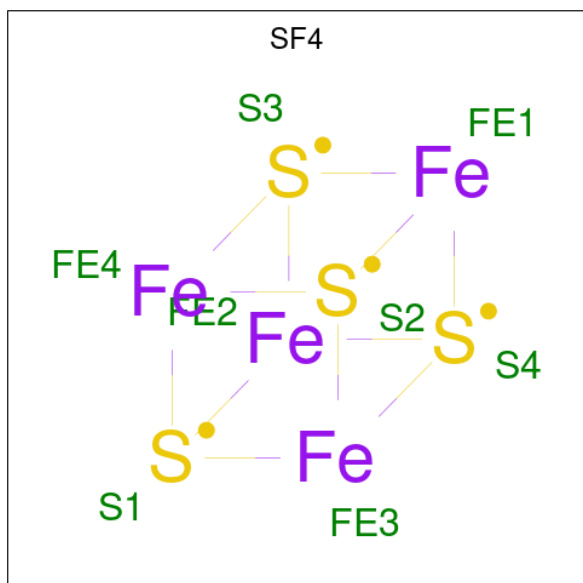
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0
59	14	1	Total Zn 1 1	0	0

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

- 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		

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2266	Total	O	0	0
			2266	2266		
61	1B	69	Total	O	0	0
			69	69		
61	1D	25	Total	O	0	0
			25	25		
61	1E	26	Total	O	0	0
			26	26		
61	1F	19	Total	O	0	0
			19	19		
61	1G	7	Total	O	0	0
			7	7		
61	1H	2	Total	O	0	0
			2	2		
61	1N	7	Total	O	0	0
			7	7		
61	1O	6	Total	O	0	0
			6	6		
61	1P	24	Total	O	0	0
			24	24		
61	1Q	9	Total	O	0	0
			9	9		
61	1R	15	Total	O	0	0
			15	15		
61	1S	6	Total	O	0	0
			6	6		
61	1T	8	Total	O	0	0
			8	8		
61	1U	9	Total	O	0	0
			9	9		
61	1V	8	Total	O	0	0
			8	8		
61	1W	6	Total	O	0	0
			6	6		
61	1X	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1Y	4	Total 4	O 4	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	14	Total 14	O 14	0	0
61	11	11	Total 11	O 11	0	0
61	12	4	Total 4	O 4	0	0
61	13	6	Total 6	O 6	0	0
61	14	1	Total 1	O 1	0	0
61	15	5	Total 5	O 5	0	0
61	16	5	Total 5	O 5	0	0
61	17	7	Total 7	O 7	0	0
61	18	9	Total 9	O 9	0	0
61	19	1	Total 1	O 1	0	0
61	1a	410	Total 410	O 410	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	1	Total 1	O 1	0	0
61	1e	1	Total 1	O 1	0	0
61	1i	1	Total 1	O 1	0	0
61	1l	7	Total 7	O 7	0	0
61	1m	3	Total 3	O 3	0	0
61	1o	2	Total 2	O 2	0	0
61	1p	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1q	2	Total 2	O 2	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	6	Total 6	O 6	0	0
61	1w	21	Total 21	O 21	0	0
61	1x	15	Total 15	O 15	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	1381	Total 1381	O 1381	0	0
61	2B	24	Total 24	O 24	0	0
61	2D	25	Total 25	O 25	0	0
61	2E	16	Total 16	O 16	0	0
61	2F	13	Total 13	O 13	0	0
61	2I	2	Total 2	O 2	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	2	Total 2	O 2	0	0
61	2P	16	Total 16	O 16	0	0
61	2Q	3	Total 3	O 3	0	0
61	2R	3	Total 3	O 3	0	0
61	2T	4	Total 4	O 4	0	0
61	2U	4	Total 4	O 4	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2X	5	Total 5	O 5	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	3	Total 3	O 3	0	0
61	21	12	Total 12	O 12	0	0
61	22	2	Total 2	O 2	0	0
61	23	2	Total 2	O 2	0	0
61	25	6	Total 6	O 6	0	0
61	27	3	Total 3	O 3	0	0
61	28	6	Total 6	O 6	0	0
61	29	1	Total 1	O 1	0	0
61	2a	366	Total 366	O 366	0	0
61	2d	3	Total 3	O 3	0	0
61	2e	3	Total 3	O 3	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	6	Total 6	O 6	0	0
61	2o	2	Total 2	O 2	0	0
61	2p	3	Total 3	O 3	0	0
61	2q	1	Total 1	O 1	0	0

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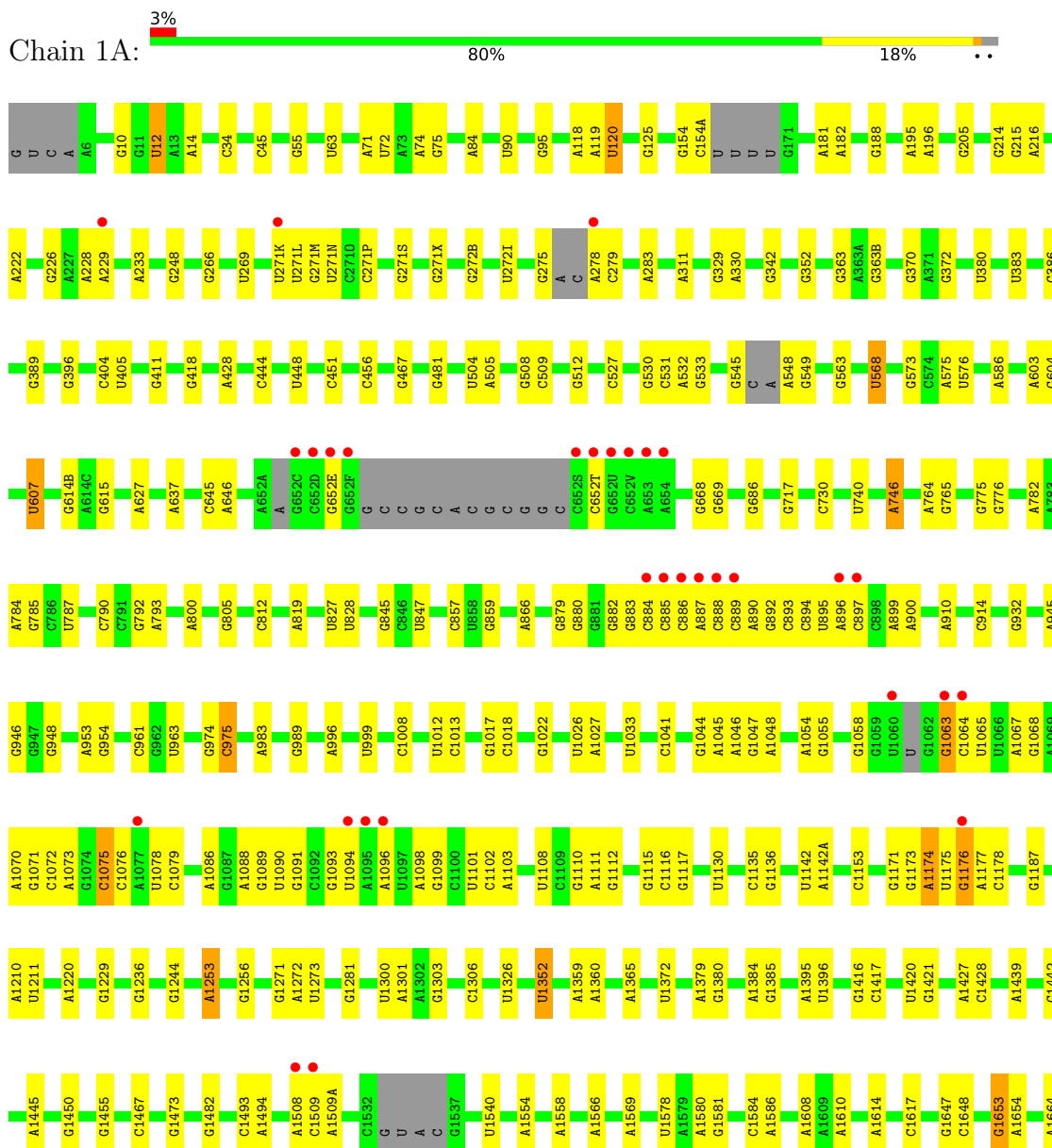
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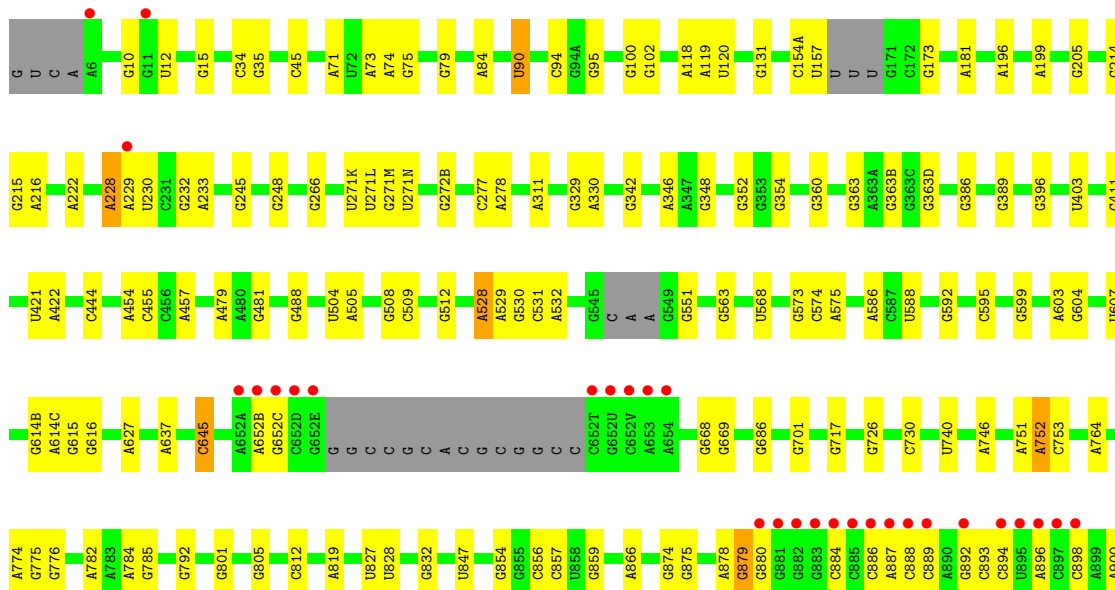
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			1	1		
61	2t	3	Total	O	0	0
			3	3		
61	2v	2	Total	O	0	0
			2	2		
61	2w	1	Total	O	0	0
			1	1		
61	2x	9	Total	O	0	0
			9	9		
61	2y	20	Total	O	0	0
			20	20		

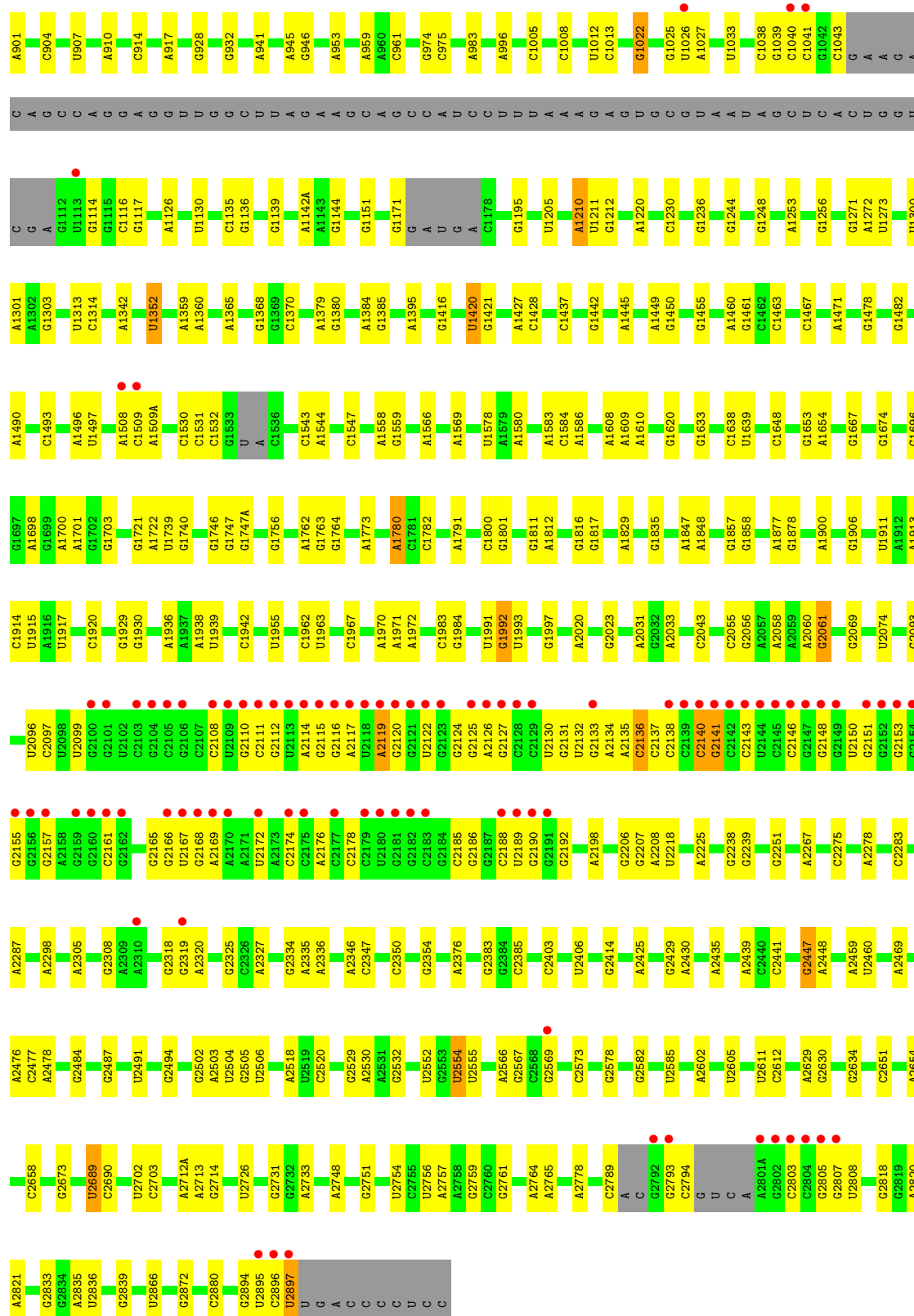
3 Residue-property plots [i](#)

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



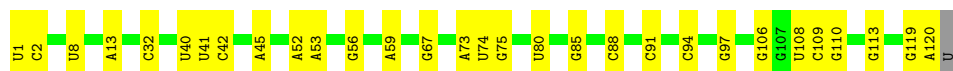






- Molecule 2: 5S Ribosomal RNA

Chain 2B: 74% 25%



- Molecule 3: 50S ribosomal protein L2

Chain 1D: 96%



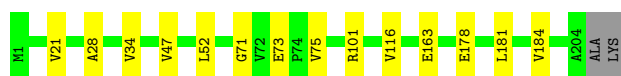
- Molecule 3: 50S ribosomal protein L2

Chain 2D: 95%



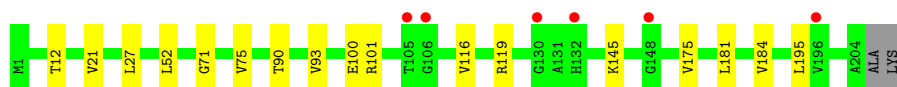
- Molecule 4: 50S ribosomal protein L3

Chain 1E: 92% 7%



- Molecule 4: 50S ribosomal protein L3

Chain 2E: 91% 8%



- Molecule 5: 50S ribosomal protein L4

Chain 1F: 91% 6%

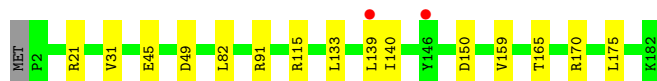
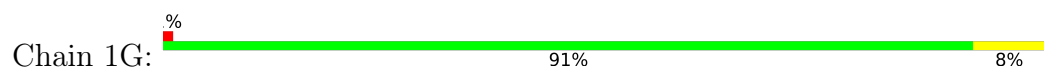


- Molecule 5: 50S ribosomal protein L4

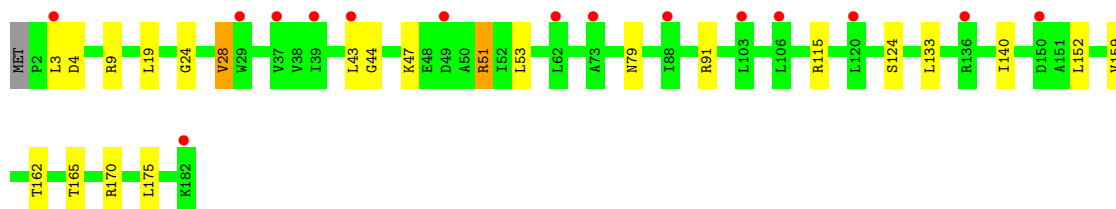
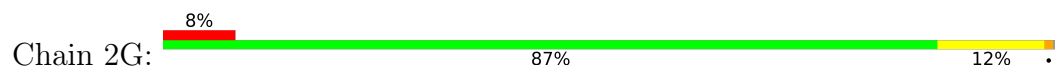
Chain 2F: 88% 9%



- Molecule 6: 50S ribosomal protein L5



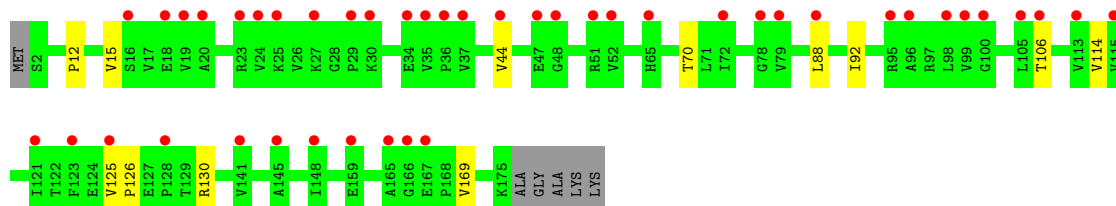
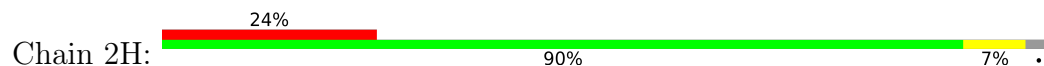
- Molecule 6: 50S ribosomal protein L5



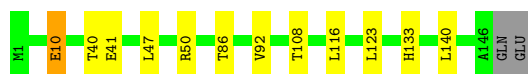
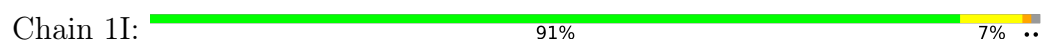
- Molecule 7: 50S ribosomal protein L6



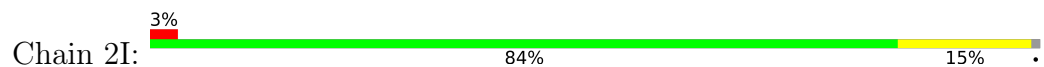
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9





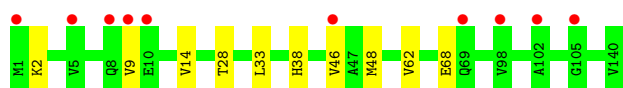
- Molecule 9: 50S ribosomal protein L13

Chain 1N: 93% 7%



- Molecule 9: 50S ribosomal protein L13

Chain 2N: 7% 93% 7%



- Molecule 10: 50S ribosomal protein L14

Chain 1O: 95% 5%



- Molecule 10: 50S ribosomal protein L14

Chain 2O: % 95% 5%



- Molecule 11: 50S ribosomal protein L15

Chain 1P: 90% 9% .



- Molecule 11: 50S ribosomal protein L15

Chain 2P: 6% 91% 8% ..



- Molecule 12: 50S ribosomal protein L16

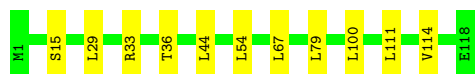
Chain 1Q: % 96% .



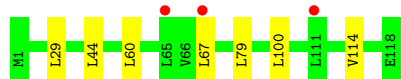
- Molecule 12: 50S ribosomal protein L16



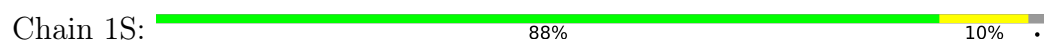
- Molecule 13: 50S ribosomal protein L17



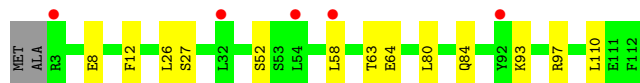
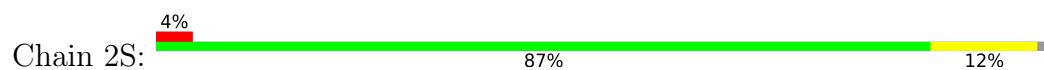
- Molecule 13: 50S ribosomal protein L17



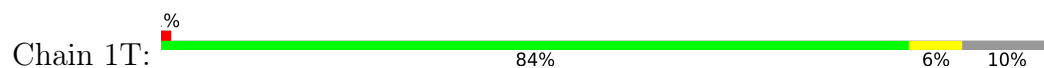
- Molecule 14: 50S ribosomal protein L18



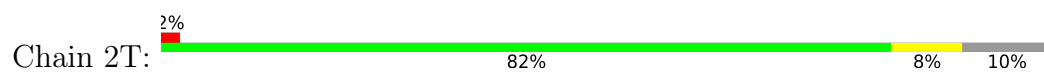
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



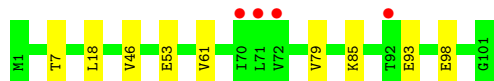
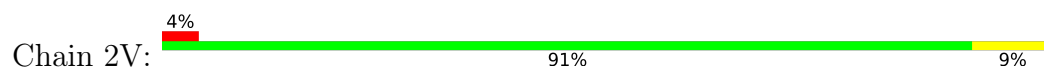
- Molecule 16: 50S ribosomal protein L20



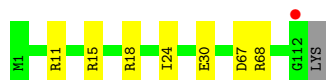
- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



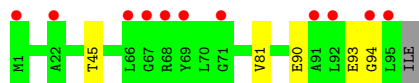
- Molecule 18: 50S ribosomal protein L22




● Molecule 19: 50S ribosomal protein L23

Chain 1X:  92% 7% .

● Molecule 19: 50S ribosomal protein L23

Chain 2X:  11% 94% 5% .

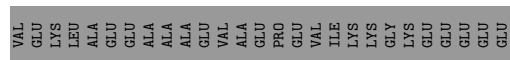
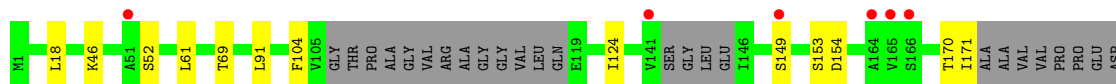
● Molecule 20: 50S ribosomal protein L24

Chain 1Y:  88% 9% .

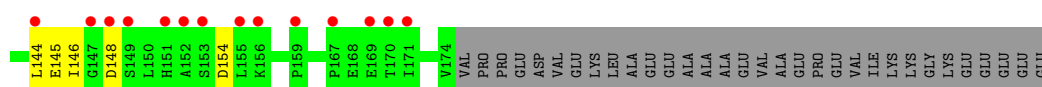
● Molecule 20: 50S ribosomal protein L24

Chain 2Y:  12% 90% 6% . .

● Molecule 21: 50S ribosomal protein L25

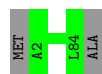
Chain 1Z:  3% 68% 6% 25%

● Molecule 21: 50S ribosomal protein L25

Chain 2Z:  13% 67% 10% 22%

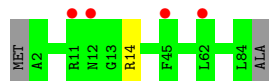
- Molecule 22: 50S ribosomal protein L27

Chain 10:  98% .



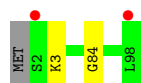
- Molecule 22: 50S ribosomal protein L27

Chain 20:  5% 96% ..



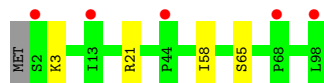
- Molecule 23: 50S ribosomal protein L28

Chain 11:  2% 97% ..



- Molecule 23: 50S ribosomal protein L28

Chain 21:  5% 95% ..



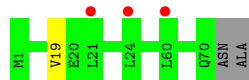
- Molecule 24: 50S ribosomal protein L29

Chain 12:  92% 6% .



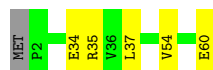
- Molecule 24: 50S ribosomal protein L29

Chain 22:  4% 96% ..

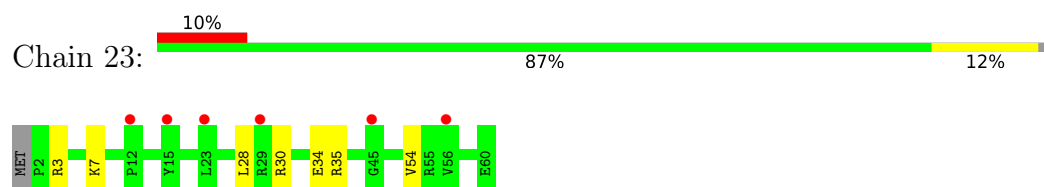


- Molecule 25: 50S ribosomal protein L30

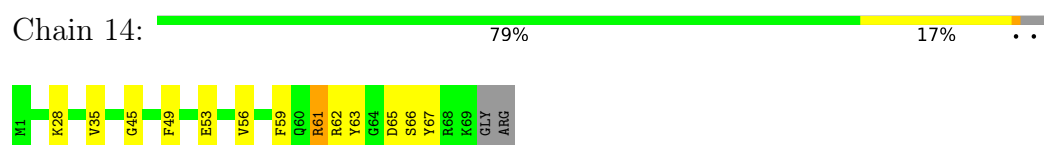
Chain 13:  90% 8% .



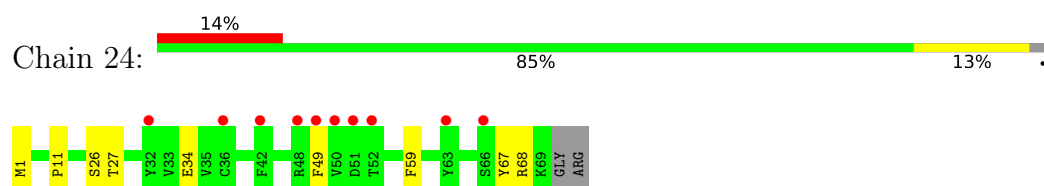
- Molecule 25: 50S ribosomal protein L30



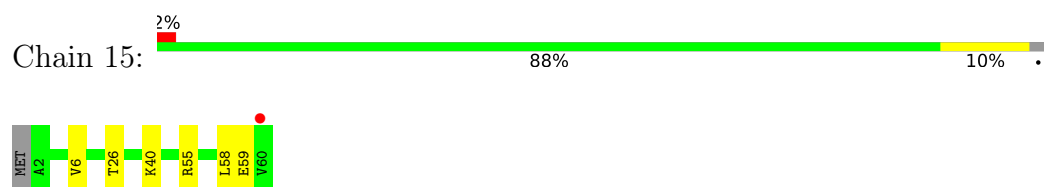
- Molecule 26: 50S ribosomal protein L31



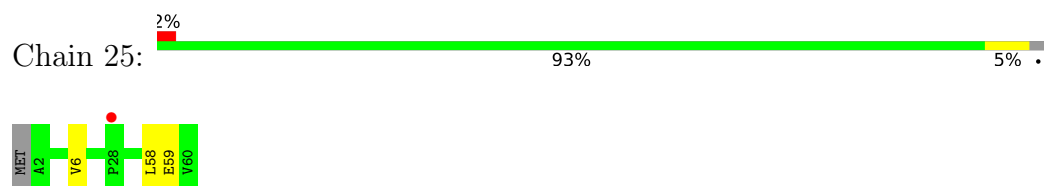
- Molecule 26: 50S ribosomal protein L31



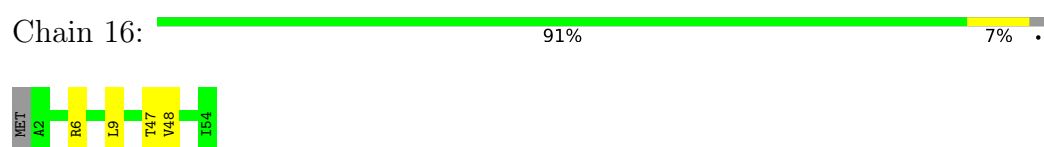
- Molecule 27: 50S ribosomal protein L32



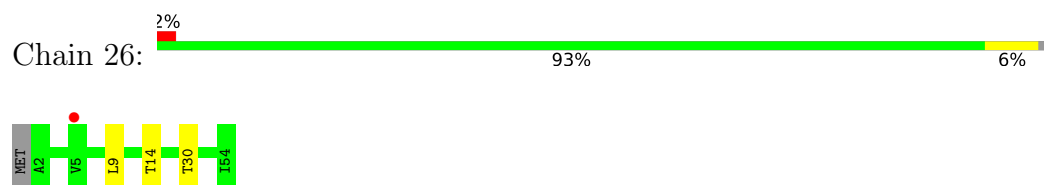
- Molecule 27: 50S ribosomal protein L32



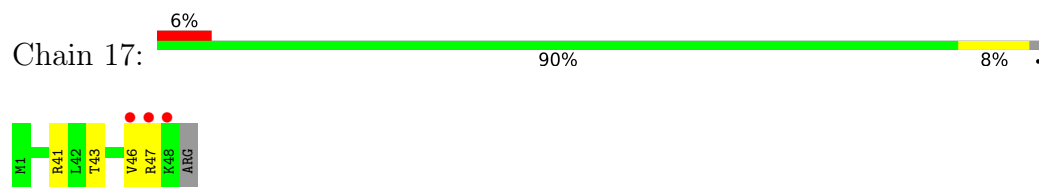
- Molecule 28: 50S ribosomal protein L33



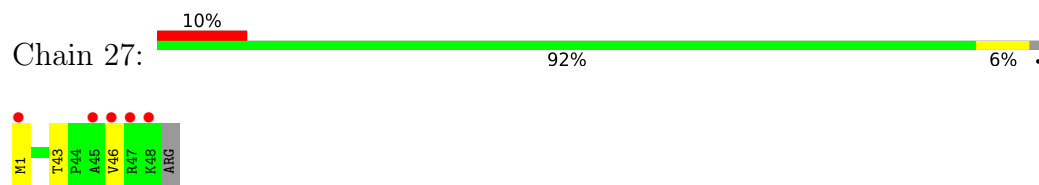
- Molecule 28: 50S ribosomal protein L33



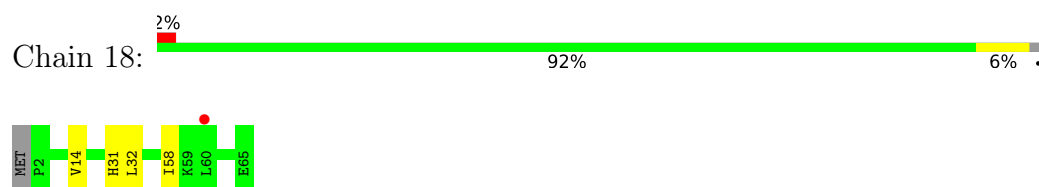
- Molecule 29: 50S ribosomal protein L34



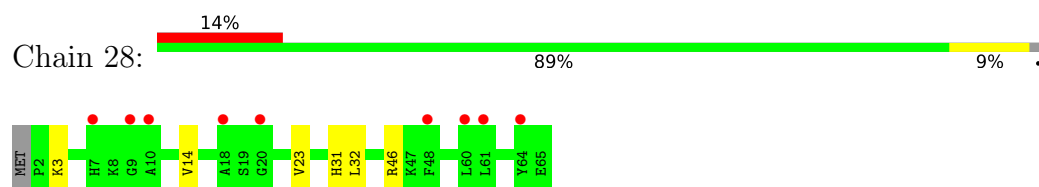
- Molecule 29: 50S ribosomal protein L34



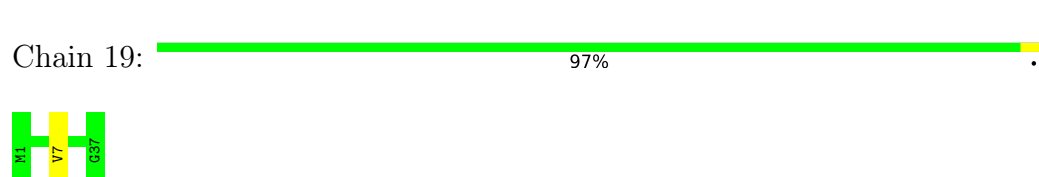
- Molecule 30: 50S ribosomal protein L35



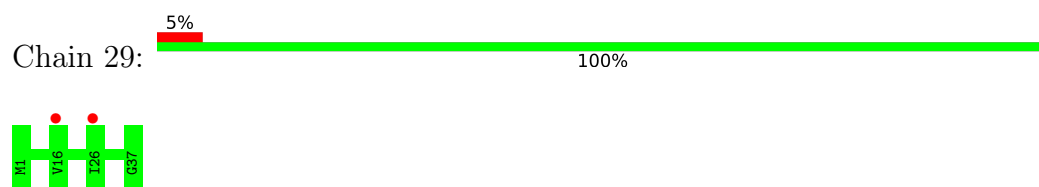
- Molecule 30: 50S ribosomal protein L35



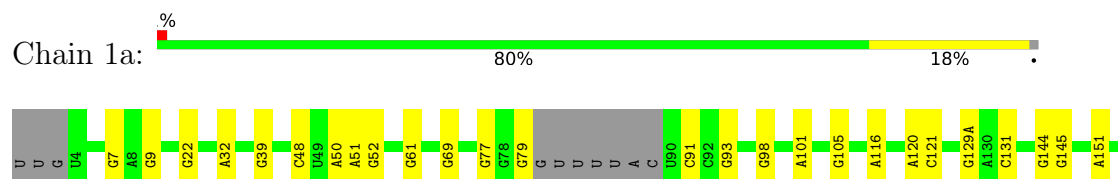
- Molecule 31: 50S ribosomal protein L36

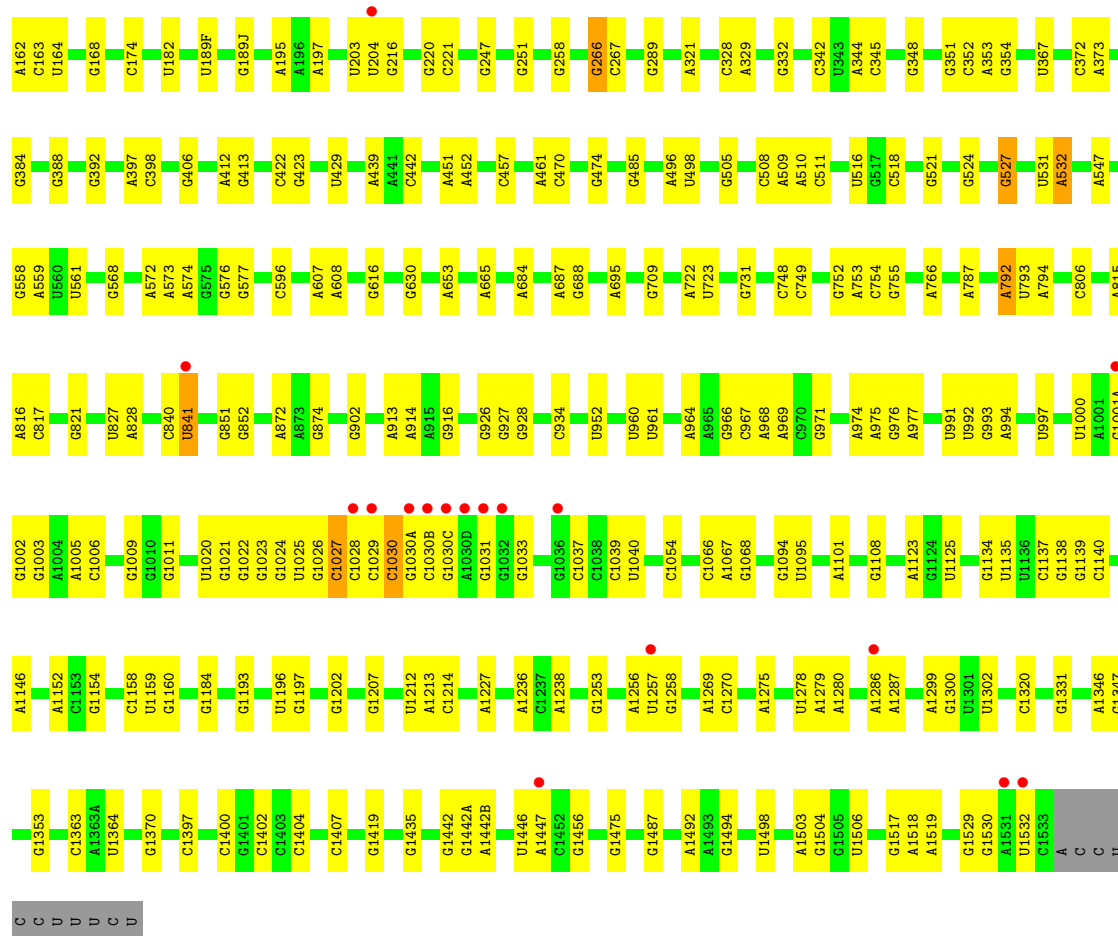


- Molecule 31: 50S ribosomal protein L36

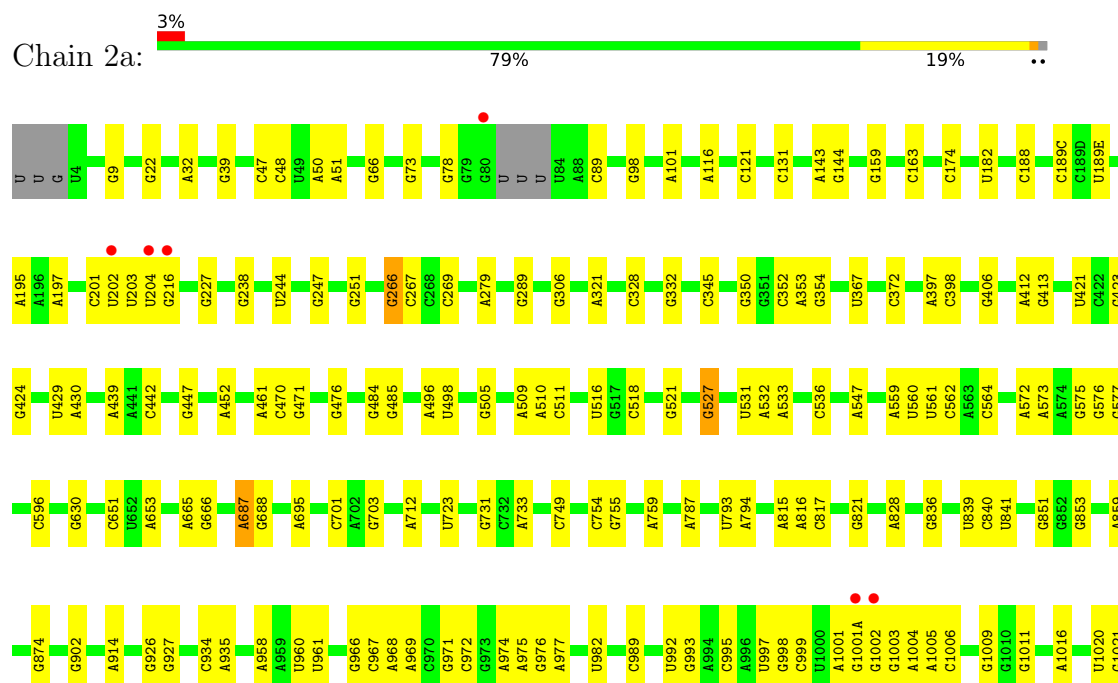


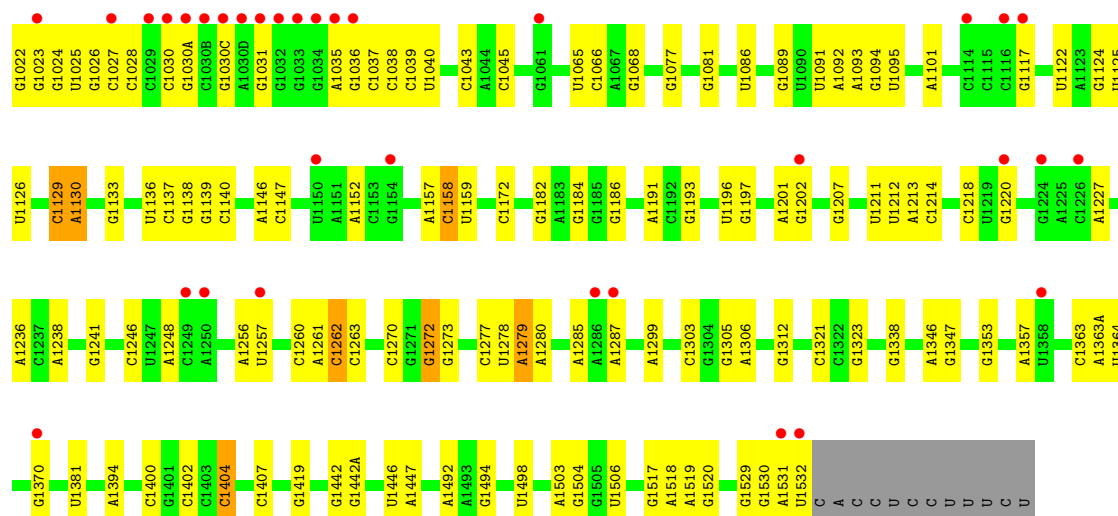
- Molecule 32: 16S Ribosomal RNA



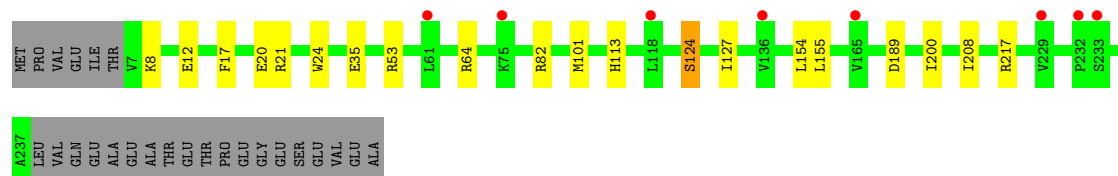
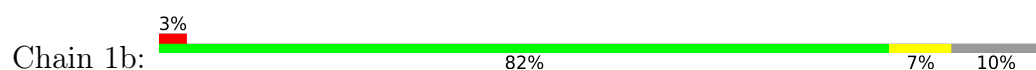


• Molecule 32: 16S Ribosomal RNA

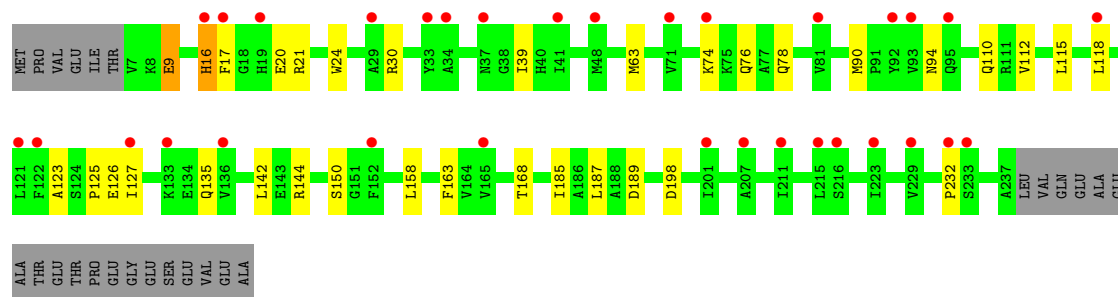
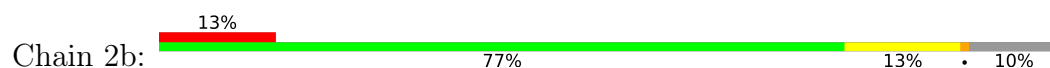




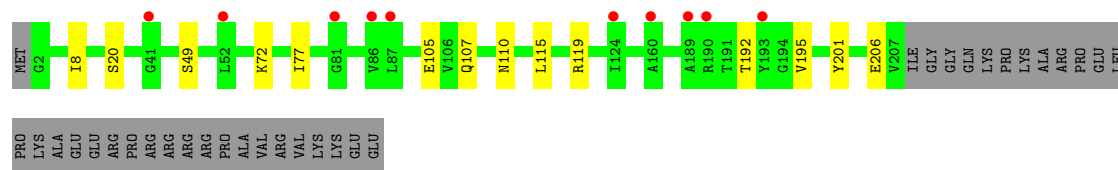
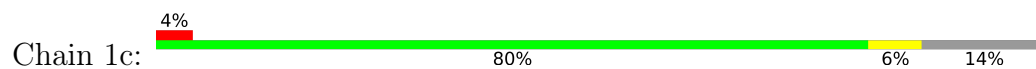
• Molecule 33: 30S ribosomal protein S2



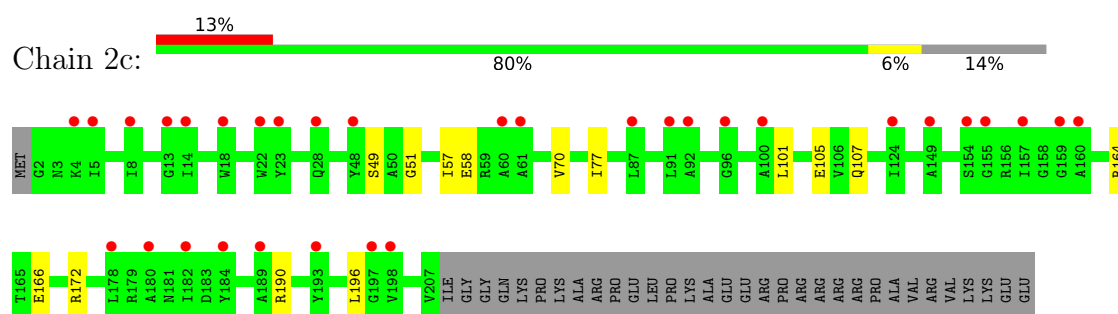
• Molecule 33: 30S ribosomal protein S2



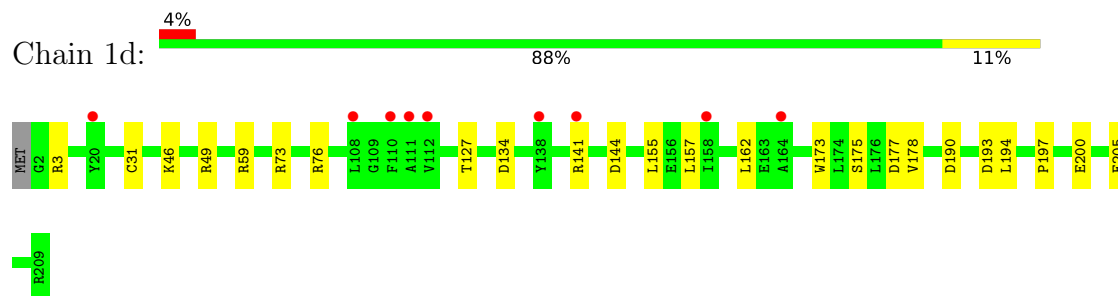
• Molecule 34: 30S ribosomal protein S3



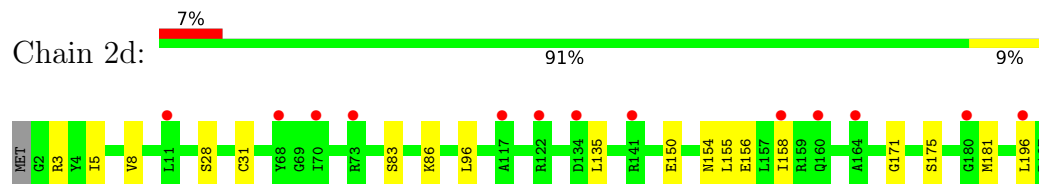
• Molecule 34: 30S ribosomal protein S3



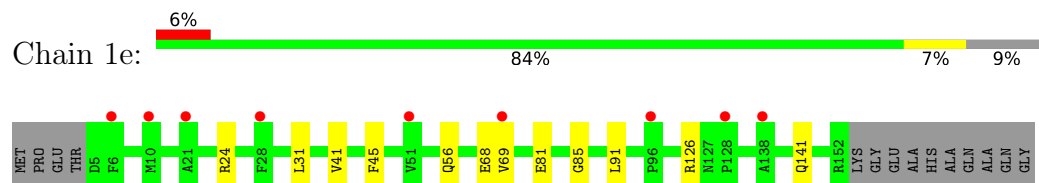
- Molecule 35: 30S ribosomal protein S4



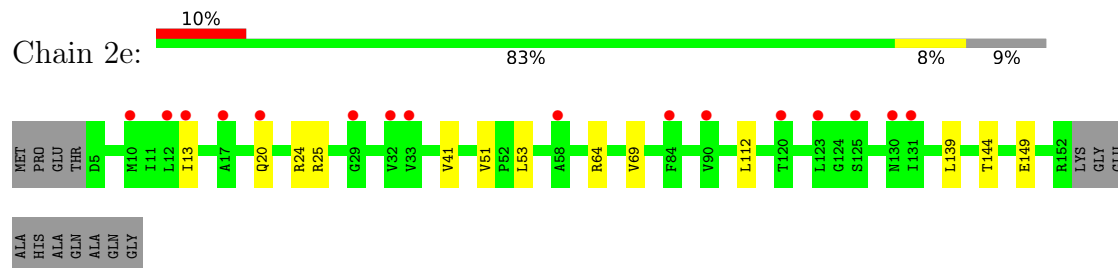
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6





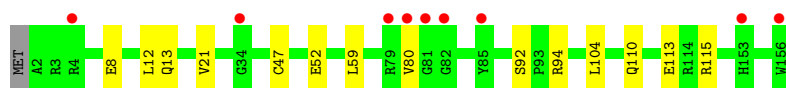
- Molecule 37: 30S ribosomal protein S6

Chain 2f: 94% 5% .



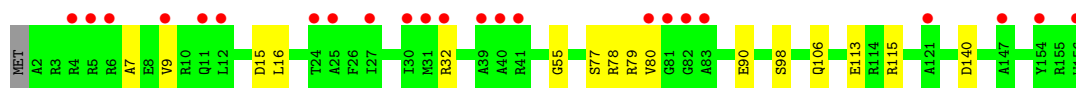
- Molecule 38: 30S ribosomal protein S7

Chain 1g: 6% 90% 9% .



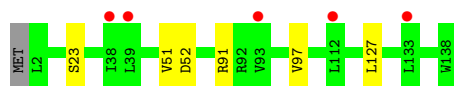
- Molecule 38: 30S ribosomal protein S7

Chain 2g: 15% 89% 10% .



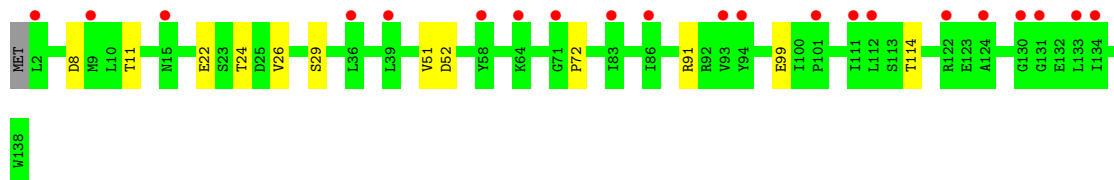
- Molecule 39: 30S ribosomal protein S8

Chain 1h: 4% 95% . .



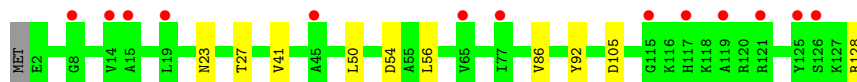
- Molecule 39: 30S ribosomal protein S8

Chain 2h: 15% 91% 9% .

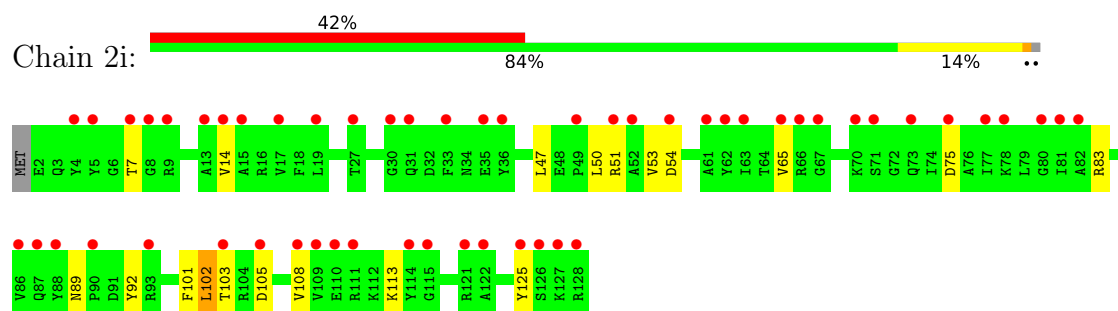


- Molecule 40: 30S ribosomal protein S9

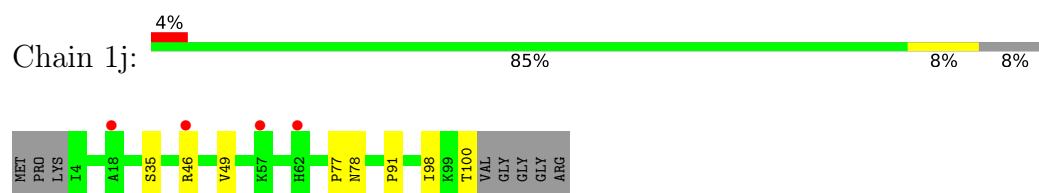
Chain 1i: 10% 91% 8% .



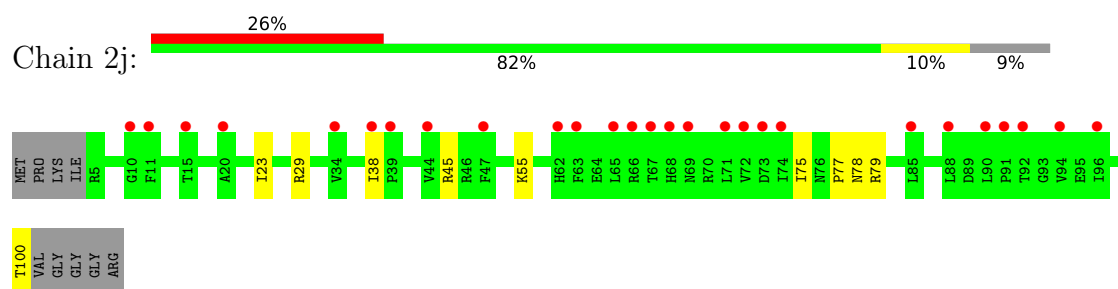
- Molecule 40: 30S ribosomal protein S9



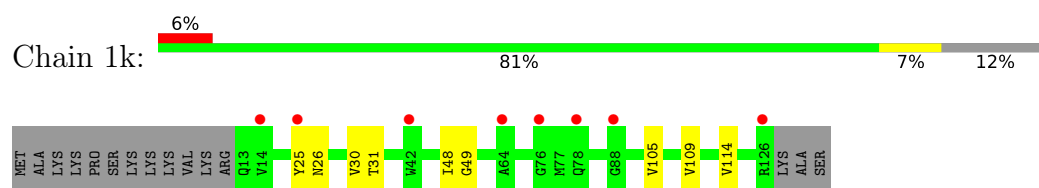
- Molecule 41: 30S ribosomal protein S10



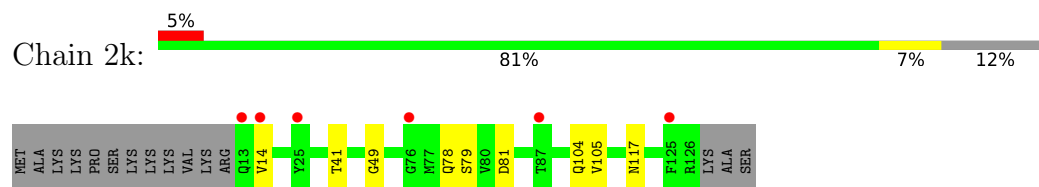
- Molecule 41: 30S ribosomal protein S10



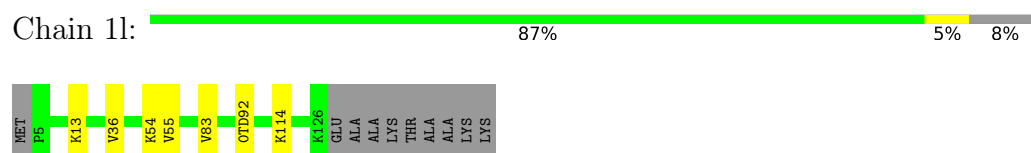
- Molecule 42: 30S ribosomal protein S11



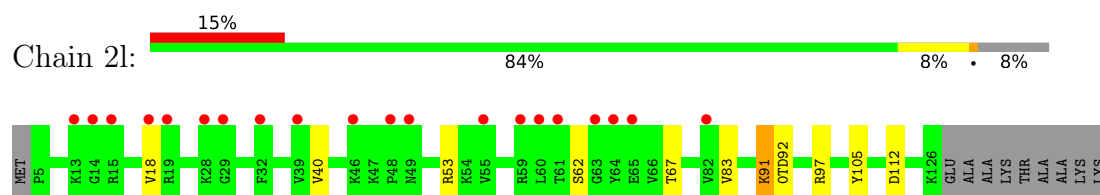
- Molecule 42: 30S ribosomal protein S11



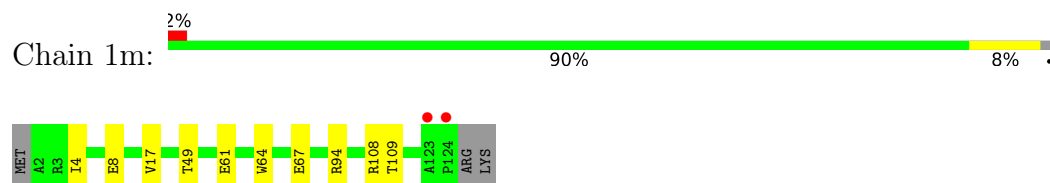
- Molecule 43: 30S ribosomal protein S12



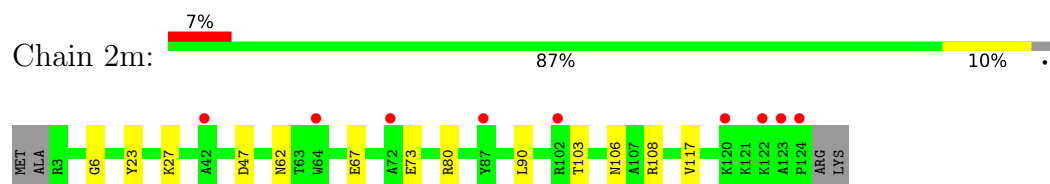
- Molecule 43: 30S ribosomal protein S12



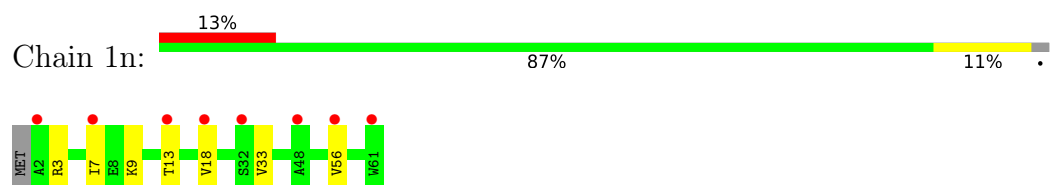
- Molecule 44: 30S ribosomal protein S13



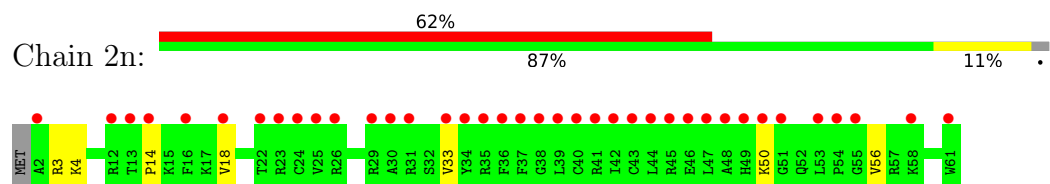
- Molecule 44: 30S ribosomal protein S13



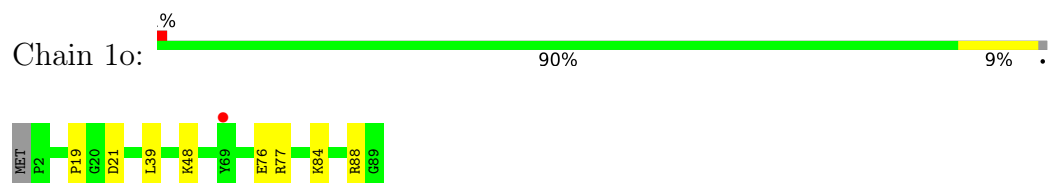
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

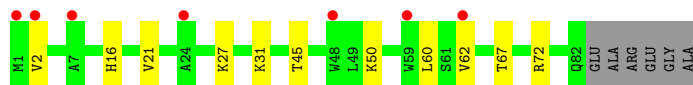
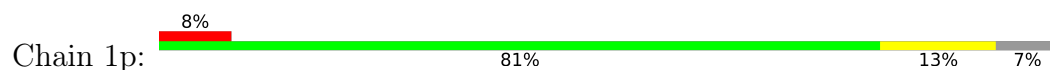


- Molecule 46: 30S ribosomal protein S15

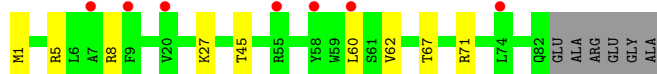
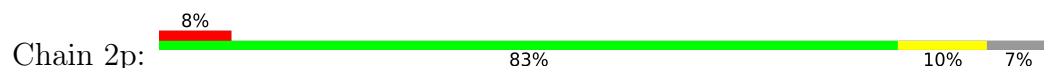




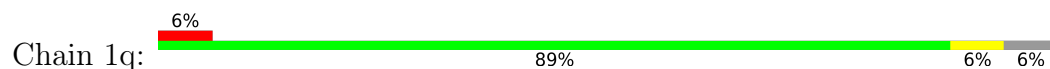
- Molecule 47: 30S ribosomal protein S16



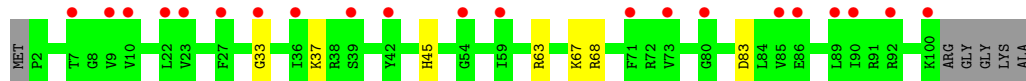
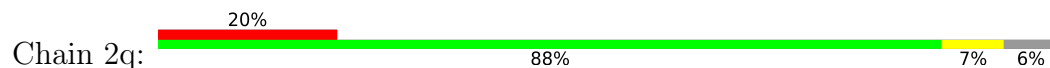
- Molecule 47: 30S ribosomal protein S16



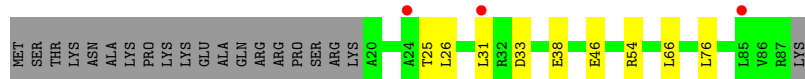
- Molecule 48: 30S ribosomal protein S17



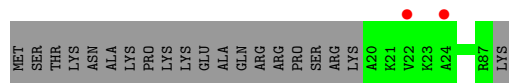
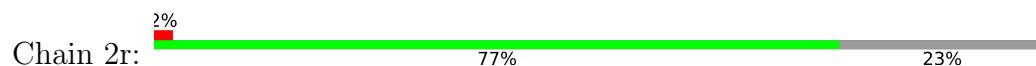
- Molecule 48: 30S ribosomal protein S17




- Molecule 49: 30S ribosomal protein S18

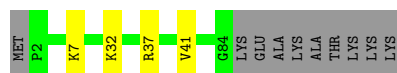


- Molecule 49: 30S ribosomal protein S18




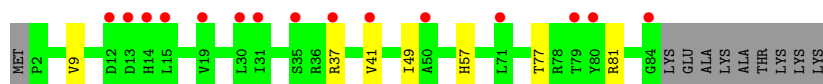
- Molecule 50: 30S ribosomal protein S19

Chain 1s:  85% • 11%




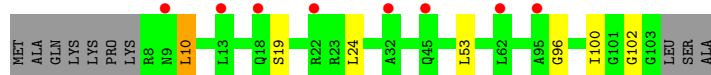
- Molecule 50: 30S ribosomal protein S19

Chain 2s:  16% 82% 8% 11%




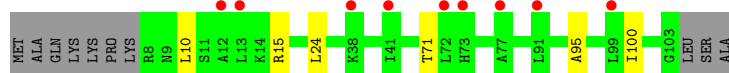
- Molecule 51: 30S ribosomal protein S20

Chain 1t:  8% 84% 6% • 9%




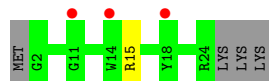
- Molecule 51: 30S ribosomal protein S20

Chain 2t:  8% 85% 6% 9%




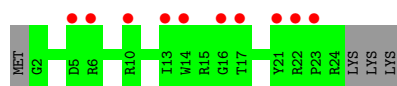
- Molecule 52: 30S ribosomal protein Thx

Chain 1u:  11% 81% • 15%



- Molecule 52: 30S ribosomal protein Thx

Chain 2u:  37% 85% 15%

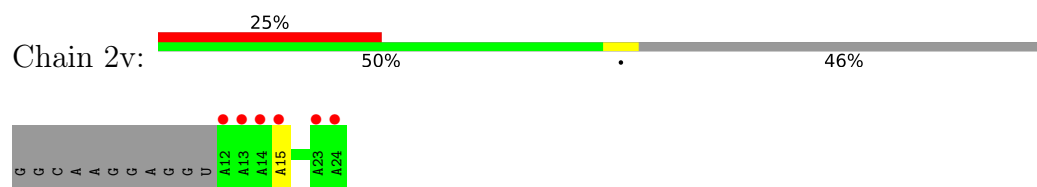


- Molecule 53: mRNA

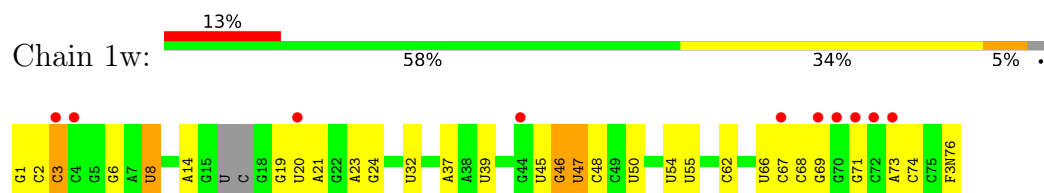
Chain 1v:  13% 50% • 46%



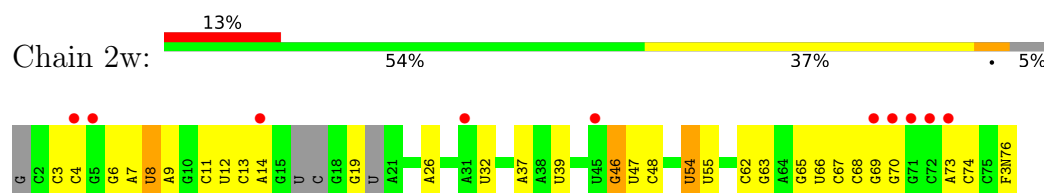
- Molecule 53: mRNA



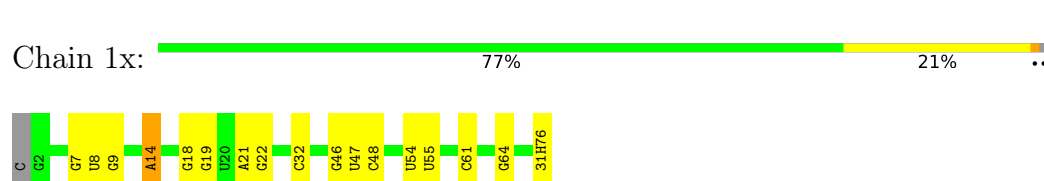
- Molecule 54: A-site tRNA



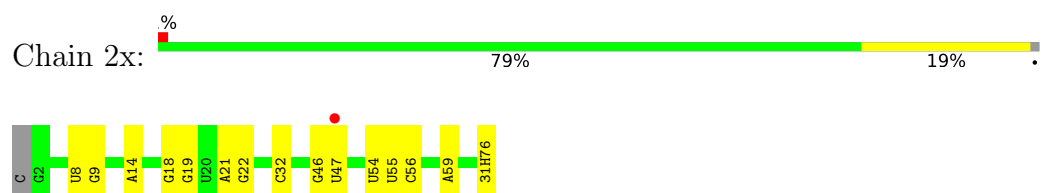
- Molecule 54: A-site tRNA



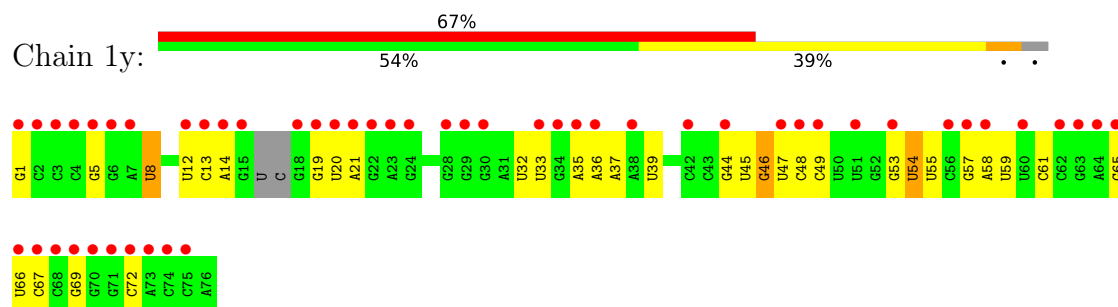
- Molecule 55: P-site tRNA



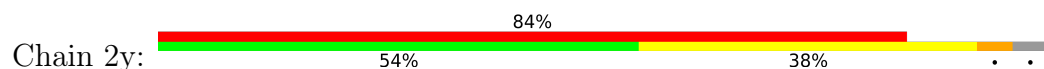
- Molecule 55: P-site tRNA

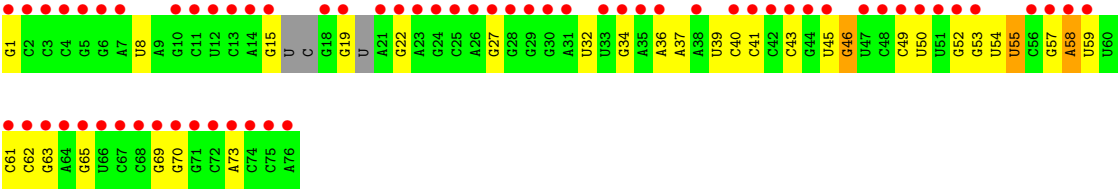


- Molecule 56: E-site tRNA



- Molecule 56: E-site tRNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	207.74Å 444.07Å 613.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	208.79 – 2.40 252.43 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (208.79-2.40) 99.9 (252.43-2.40)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.237 , 0.286 0.237 , 0.286	Depositor DCC
R_{free} test set	108927 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	300906	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: 5MU, ZN, 4SU, OMG, MA6, MIA, 31H, SF4, 0TD, MG, F3N, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, M2G, 7MG, K, PSU

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	0.54	0/68983	1.01	93/107669 (0.1%)
1	2A	0.42	0/67267	0.90	45/104991 (0.0%)
2	1B	0.48	1/2882 (0.0%)	0.92	1/4494 (0.0%)
2	2B	0.41	1/2879 (0.0%)	0.88	2/4487 (0.0%)
3	1D	0.38	0/2186	0.58	0/2944
3	2D	0.33	0/2186	0.52	0/2944
4	1E	0.36	0/1592	0.59	0/2149
4	2E	0.31	0/1592	0.51	0/2149
5	1F	0.34	0/1619	0.54	0/2193
5	2F	0.31	0/1615	0.50	0/2188
6	1G	0.32	0/1448	0.52	0/1957
6	2G	0.29	0/1453	0.49	0/1963
7	1H	0.32	0/1356	0.49	0/1834
7	2H	0.30	0/1356	0.46	0/1834
8	1I	0.29	0/1112	0.51	0/1514
8	2I	0.31	0/1079	0.54	0/1475
9	1N	0.35	0/1144	0.55	1/1543 (0.1%)
9	2N	0.29	0/1144	0.46	0/1543
10	1O	0.37	0/943	0.55	0/1269
10	2O	0.33	0/943	0.51	0/1269
11	1P	0.33	0/1152	0.60	0/1533
11	2P	0.30	0/1152	0.53	0/1533
12	1Q	0.36	0/1143	0.55	0/1527
12	2Q	0.31	0/1143	0.48	0/1527
13	1R	0.33	0/982	0.55	0/1312
13	2R	0.28	0/982	0.51	0/1312
14	1S	0.32	0/883	0.52	0/1176
14	2S	0.30	0/880	0.49	0/1172
15	1T	0.33	0/1105	0.52	0/1477
15	2T	0.30	0/1097	0.49	0/1468
16	1U	0.35	0/977	0.51	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.31	0/977	0.45	0/1301
17	1V	0.35	0/782	0.56	0/1049
17	2V	0.30	0/782	0.53	0/1049
18	1W	0.37	0/897	0.55	0/1205
18	2W	0.31	0/897	0.48	0/1205
19	1X	0.36	0/764	0.57	0/1025
19	2X	0.30	0/764	0.55	0/1025
20	1Y	0.32	0/819	0.54	0/1095
20	2Y	0.32	0/819	0.54	0/1095
21	1Z	0.30	0/1267	0.53	0/1717
21	2Z	0.30	0/1299	0.50	0/1763
22	10	0.37	0/662	0.59	0/881
22	20	0.33	0/662	0.52	0/881
23	11	0.33	0/762	0.52	0/1014
23	21	0.32	0/762	0.49	0/1014
24	12	0.30	0/590	0.45	0/781
24	22	0.27	0/590	0.40	0/781
25	13	0.33	0/474	0.52	0/635
25	23	0.29	0/469	0.52	0/630
26	14	0.31	0/565	0.53	0/761
26	24	0.30	0/545	0.49	0/737
27	15	0.38	0/469	0.59	0/635
27	25	0.34	0/469	0.51	0/635
28	16	0.36	0/460	0.55	0/613
28	26	0.29	0/456	0.50	0/608
29	17	0.34	0/426	0.54	0/561
29	27	0.30	0/426	0.50	0/561
30	18	0.33	0/525	0.54	0/691
30	28	0.30	0/525	0.49	0/691
31	19	0.33	0/310	0.52	0/407
31	29	0.30	0/310	0.50	0/407
32	1a	0.39	0/35795	0.91	28/55864 (0.1%)
32	2a	0.37	3/35886 (0.0%)	0.92	35/56005 (0.1%)
33	1b	0.30	0/1881	0.50	0/2542
33	2b	0.30	0/1860	0.49	0/2518
34	1c	0.30	0/1572	0.48	0/2126
34	2c	0.30	0/1566	0.49	0/2119
35	1d	0.30	0/1685	0.47	0/2262
35	2d	0.28	0/1704	0.46	0/2284
36	1e	0.30	0/1145	0.54	0/1543
36	2e	0.29	0/1149	0.54	0/1548
37	1f	0.29	0/823	0.51	0/1115
37	2f	0.31	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.28	0/1250	0.45	0/1679
38	2g	0.28	0/1254	0.46	0/1683
39	1h	0.30	0/1108	0.47	0/1494
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.29	0/1002	0.50	0/1346
40	2i	0.31	0/997	0.53	1/1343 (0.1%)
41	1j	0.28	0/722	0.51	0/982
41	2j	0.28	0/727	0.51	0/988
42	1k	0.28	0/844	0.50	0/1145
42	2k	0.29	0/848	0.47	0/1149
43	1l	0.33	0/937	0.53	0/1260
43	2l	0.29	0/937	0.49	0/1260
44	1m	0.29	0/969	0.51	0/1302
44	2m	0.29	0/961	0.47	0/1291
45	1n	0.30	0/501	0.49	0/664
45	2n	0.32	0/501	0.48	0/664
46	1o	0.29	0/739	0.44	0/985
46	2o	0.26	0/739	0.43	0/985
47	1p	0.29	0/697	0.49	0/939
47	2p	0.28	0/693	0.50	0/935
48	1q	0.28	0/836	0.50	0/1117
48	2q	0.30	0/836	0.49	0/1117
49	1r	0.28	0/560	0.44	0/746
49	2r	0.29	0/560	0.46	0/746
50	1s	0.29	0/667	0.55	0/900
50	2s	0.28	0/661	0.52	0/893
51	1t	0.28	0/730	0.46	0/965
51	2t	0.28	0/729	0.43	0/965
52	1u	0.29	0/203	0.47	0/266
52	2u	0.27	0/203	0.51	0/266
53	1v	0.47	0/310	0.87	0/480
53	2v	0.43	0/310	0.93	0/480
54	1w	0.51	1/1581 (0.1%)	1.12	5/2458 (0.2%)
54	2w	0.42	0/1531	1.07	1/2379 (0.0%)
55	1x	0.59	4/1700 (0.2%)	1.18	22/2650 (0.8%)
55	2x	0.50	1/1700 (0.1%)	1.08	15/2650 (0.6%)
56	1y	0.56	1/1606 (0.1%)	1.13	5/2497 (0.2%)
56	2y	0.56	1/1583 (0.1%)	1.15	3/2459 (0.1%)
All	All	0.42	13/316534 (0.0%)	0.86	257/473871 (0.1%)

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
11	1P	0	2
11	2P	0	1
44	2m	0	1
All	All	0	4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2B	1	U	OP3-P	-10.45	1.48	1.61
2	1B	1	U	OP3-P	-10.30	1.48	1.61
54	1w	1	G	OP3-P	-10.19	1.49	1.61
56	1y	1	G	OP3-P	-10.18	1.49	1.61
56	2y	1	G	OP3-P	-10.13	1.49	1.61
32	2a	1272	G	N1-C2	-8.62	1.30	1.37
32	2a	1272	G	C6-N1	-7.62	1.34	1.39
55	1x	22	G	N7-C5	7.01	1.43	1.39
55	1x	46	G	C6-N1	5.96	1.43	1.39
55	1x	14	A	C8-N7	-5.44	1.27	1.31
32	2a	1263	C	N3-C4	-5.19	1.30	1.33
55	1x	22	G	C8-N7	5.13	1.34	1.30
55	2x	22	G	N7-C5	5.03	1.42	1.39

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	23.24	132.84	118.90
32	2a	1272	G	N3-C2-N2	20.48	134.24	119.90
32	2a	1272	G	C5-C6-O6	17.98	139.39	128.60
32	2a	1272	G	N1-C2-N2	-17.51	100.44	116.20
32	2a	1263	C	C2-N3-C4	14.39	127.10	119.90
55	1x	46	G	C6-N1-C2	-13.10	117.24	125.10
32	2a	1263	C	N3-C2-O2	-12.43	113.20	121.90
32	2a	1272	G	C6-N1-C2	11.83	132.20	125.10
32	2a	1263	C	C5-C6-N1	11.58	126.79	121.00
32	2a	1272	G	C5-C6-N1	-10.74	106.13	111.50
1	1A	1063	G	C5-C6-O6	10.74	135.04	128.60
1	1A	1075	C	N1-C2-O2	10.49	125.19	118.90
55	2x	46	G	C6-N1-C2	-10.40	118.86	125.10
55	1x	22	G	C5-N7-C8	-10.09	99.26	104.30
1	1A	512	G	O4'-C1'-N9	9.83	116.06	108.20
1	1A	576	U	O5'-P-OP1	-9.45	97.19	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	787	U	O5'-P-OP1	-9.41	97.23	105.70
1	2A	801	G	O5'-P-OP2	-9.41	97.23	105.70
1	2A	2136	C	N1-C2-O2	9.28	124.47	118.90
1	1A	1086	A	N1-C6-N6	-9.16	113.11	118.60
55	2x	14	A	C5-N7-C8	9.11	108.46	103.90
32	2a	1272	G	N1-C6-O6	-9.07	114.46	119.90
1	1A	1075	C	C2-N3-C4	9.02	124.41	119.90
32	1a	1030(B)	C	C2-N1-C1'	9.00	128.70	118.80
55	1x	22	G	C4-C5-C6	-8.95	113.43	118.80
32	2a	1263	C	C2-N1-C1'	8.84	128.53	118.80
55	1x	14	A	C4-C5-C6	8.76	121.38	117.00
2	2B	80	U	O4'-C1'-N1	8.66	115.13	108.20
32	1a	1030	C	N1-C2-O2	8.61	124.06	118.90
55	2x	14	A	C4-C5-C6	8.57	121.29	117.00
55	1x	14	A	C5-N7-C8	8.48	108.14	103.90
1	1A	1063	G	N3-C2-N2	8.43	125.80	119.90
1	1A	2167	U	C2-N1-C1'	8.42	127.81	117.70
54	1w	47	U	C2-N1-C1'	8.40	127.78	117.70
32	2a	1263	C	C4-C5-C6	-8.39	113.20	117.40
55	1x	22	G	N1-C6-O6	-8.38	114.87	119.90
1	1A	1352	U	O5'-P-OP1	-8.36	98.17	105.70
32	2a	1043	C	N1-C2-O2	8.19	123.81	118.90
32	1a	1030(B)	C	N1-C2-O2	8.10	123.76	118.90
32	2a	1272	G	C2-N3-C4	-7.80	108.00	111.90
1	1A	975	C	N1-C2-O2	-7.79	114.22	118.90
32	2a	1263	C	C6-N1-C2	-7.78	117.19	120.30
55	2x	22	G	C5-N7-C8	-7.63	100.48	104.30
1	1A	2577	A	O5'-P-OP1	-7.61	98.86	105.70
32	1a	754	C	C2-N1-C1'	7.61	127.17	118.80
32	2a	1263	C	N1-C2-N3	-7.54	113.92	119.20
32	1a	1030(B)	C	C6-N1-C2	-7.51	117.30	120.30
54	1w	47	U	N1-C2-O2	7.39	127.97	122.80
55	1x	46	G	C5-C6-O6	-7.37	124.18	128.60
1	2A	2155	G	C6-N1-C2	7.34	129.50	125.10
55	1x	46	G	N1-C2-N3	7.33	128.30	123.90
32	2a	1272	G	C8-N9-C1'	-7.33	117.47	127.00
55	1x	22	G	N3-C4-N9	-7.32	121.61	126.00
32	2a	1272	G	C4-N9-C1'	7.29	135.98	126.50
1	1A	2711	A	O5'-P-OP2	-7.28	99.15	105.70
1	1A	800	A	O5'-P-OP1	-7.25	99.17	105.70
1	2A	1698	A	O4'-C1'-N9	7.24	113.99	108.20
56	1y	33	U	C2-N1-C1'	7.21	126.35	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2061	G	O5'-P-OP2	-7.18	99.23	105.70
55	1x	46	G	C5-C6-N1	7.13	115.06	111.50
32	1a	841	U	C5-C6-N1	7.12	126.26	122.70
32	1a	754	C	N1-C2-O2	7.07	123.14	118.90
1	2A	2155	G	C5-C6-O6	7.03	132.82	128.60
32	1a	1027	C	N3-C4-C5	-7.01	119.10	121.90
1	1A	2167	U	N1-C2-O2	7.01	127.70	122.80
1	1A	1063	G	C6-N1-C2	6.99	129.30	125.10
32	1a	558	G	O5'-P-OP1	-6.99	99.41	105.70
1	1A	1992	G	P-O3'-C3'	6.96	128.06	119.70
9	1N	77	GLY	C-N-CA	6.96	139.09	121.70
32	2a	754	C	C2-N1-C1'	6.92	126.42	118.80
55	2x	46	G	N3-C2-N2	-6.92	115.05	119.90
1	2A	2140	C	N1-C2-O2	6.84	123.01	118.90
32	1a	1030(B)	C	N3-C2-O2	-6.83	117.11	121.90
55	1x	14	A	C5-C6-N1	-6.83	114.28	117.70
55	1x	46	G	N3-C2-N2	-6.83	115.12	119.90
1	2A	2136	C	N3-C2-O2	-6.82	117.13	121.90
1	2A	2155	G	N3-C2-N2	6.76	124.64	119.90
55	2x	22	G	C4-C5-C6	-6.76	114.75	118.80
1	1A	607	U	O5'-P-OP1	-6.74	99.64	105.70
55	1x	22	G	N7-C8-N9	6.71	116.45	113.10
1	1A	975	C	C2-N1-C1'	-6.70	111.43	118.80
1	1A	2593	U	N3-C4-O4	-6.68	114.72	119.40
1	1A	2167	U	N3-C2-O2	-6.68	117.52	122.20
1	1A	1075	C	C5-C4-N4	6.59	124.81	120.20
1	1A	568	U	C5-C4-O4	-6.58	121.95	125.90
54	1w	47	U	N3-C2-O2	-6.58	117.59	122.20
1	1A	1614	A	O5'-P-OP1	-6.57	99.78	105.70
1	1A	1063	G	N1-C6-O6	-6.57	115.96	119.90
1	1A	975	C	C5-C6-N1	-6.53	117.73	121.00
1	1A	999	U	O5'-P-OP2	-6.53	99.82	105.70
32	2a	754	C	N1-C2-O2	6.52	122.81	118.90
1	1A	740	U	O5'-P-OP2	-6.52	99.83	105.70
32	1a	266	G	P-O3'-C3'	6.52	127.52	119.70
1	2A	2141	G	C5-C6-O6	-6.50	124.70	128.60
1	1A	1075	C	N3-C2-O2	-6.49	117.35	121.90
56	1y	33	U	N1-C2-O2	6.45	127.31	122.80
32	2a	1263	C	C5-C4-N4	6.44	124.71	120.20
1	1A	948	G	O5'-P-OP1	-6.44	99.91	105.70
1	1A	2689	U	P-O3'-C3'	6.44	127.42	119.70
55	1x	46	G	N9-C4-C5	6.41	107.96	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	14	A	C5-C6-N1	-6.33	114.54	117.70
1	1A	2575	C	O5'-P-OP2	-6.28	100.05	105.70
32	2a	1262	C	N1-C2-O2	6.28	122.67	118.90
32	2a	1158	C	C2-N1-C1'	6.27	125.70	118.80
1	1A	847	U	C2-N1-C1'	6.27	125.22	117.70
1	1A	2454	G	C8-N9-C4	6.26	108.90	106.40
32	1a	1027	C	C6-N1-C1'	6.24	128.29	120.80
1	2A	2689	U	P-O3'-C3'	6.23	127.18	119.70
32	2a	1263	C	N3-C4-N4	-6.22	113.65	118.00
1	2A	2554	U	O5'-P-OP1	-6.22	100.11	105.70
1	1A	2848	G	O4'-C1'-N9	6.19	113.15	108.20
1	1A	527	C	N1-C2-O2	-6.17	115.20	118.90
1	1A	1063	G	N1-C2-N2	-6.17	110.65	116.20
32	2a	266	G	P-O3'-C3'	6.15	127.08	119.70
1	1A	793	A	O5'-P-OP2	-6.15	100.17	105.70
1	1A	1176	G	OP1-P-O3'	6.15	118.72	105.20
54	1w	3	C	C2-N1-C1'	6.13	125.55	118.80
55	2x	22	G	N3-C4-N9	-6.12	122.33	126.00
55	1x	22	G	N3-C4-C5	6.11	131.66	128.60
1	2A	512	G	O4'-C1'-N9	6.11	113.09	108.20
1	1A	2629	A	P-O3'-C3'	6.06	126.97	119.70
1	1A	1153	C	O5'-P-OP2	-6.02	100.29	105.70
1	1A	1439	A	O5'-P-OP1	-6.00	100.30	105.70
54	2w	47	U	C2-N1-C1'	5.99	124.89	117.70
1	2A	1780	A	O5'-P-OP1	-5.99	100.31	105.70
1	1A	1653	G	C8-N9-C4	-5.98	104.01	106.40
1	1A	746	A	O4'-C1'-N9	5.97	112.98	108.20
1	1A	2015	A	OP2-P-O3'	5.95	118.30	105.20
1	1A	226	G	O4'-C1'-N9	5.94	112.95	108.20
1	2A	1313	U	C2-N1-C1'	5.94	124.83	117.70
55	1x	22	G	C6-C5-N7	5.94	133.96	130.40
55	1x	22	G	C5-C6-N1	5.90	114.45	111.50
1	1A	1992	G	C8-N9-C4	-5.90	104.04	106.40
2	2B	1	U	C2-N1-C1'	5.89	124.77	117.70
55	1x	46	G	N3-C4-C5	-5.89	125.66	128.60
55	2x	46	G	C5-C6-N1	5.88	114.44	111.50
1	1A	2041	U	N3-C2-O2	-5.84	118.11	122.20
1	2A	847	U	C2-N1-C1'	5.84	124.70	117.70
56	1y	33	U	N3-C2-O2	-5.82	118.12	122.20
1	1A	845	G	O4'-C1'-N9	5.80	112.84	108.20
1	1A	2506	U	O5'-P-OP1	-5.78	100.50	105.70
1	2A	1352	U	O5'-P-OP1	-5.77	100.51	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2028	U	N3-C4-O4	-5.76	115.37	119.40
55	1x	46	G	C4-C5-N7	-5.75	108.50	110.80
32	2a	1279	A	OP1-P-O3'	5.75	117.85	105.20
56	2y	58	A	OP1-P-O3'	5.75	117.85	105.20
1	1A	963	U	O5'-P-OP2	-5.74	100.54	105.70
32	2a	1129	C	OP1-P-O3'	5.74	117.83	105.20
32	1a	1030(B)	C	C6-N1-C1'	-5.74	113.92	120.80
1	1A	1064	C	C6-N1-C2	-5.72	118.01	120.30
32	1a	1027	C	C2-N1-C1'	-5.71	112.52	118.80
32	1a	841	U	C6-N1-C2	-5.70	117.58	121.00
1	2A	2143	C	C5-C6-N1	5.69	123.84	121.00
55	1x	22	G	C8-N9-C1'	5.67	134.38	127.00
32	1a	1067	A	P-O3'-C3'	5.66	126.49	119.70
32	1a	754	C	N3-C2-O2	-5.65	117.95	121.90
55	2x	22	G	C8-N9-C1'	5.64	134.34	127.00
32	2a	1043	C	C2-N3-C4	5.63	122.72	119.90
1	1A	1187	G	N1-C6-O6	-5.61	116.54	119.90
1	2A	752	A	P-O3'-C3'	5.60	126.42	119.70
55	1x	14	A	C8-N9-C1'	-5.59	117.64	127.70
1	2A	2447	G	C8-N9-C4	5.59	108.64	106.40
1	1A	1617	C	N1-C2-O2	-5.58	115.55	118.90
1	1A	2791	C	C6-N1-C2	-5.58	118.07	120.30
32	1a	1030(B)	C	C5-C6-N1	5.58	123.79	121.00
1	1A	1174	A	OP1-P-O3'	5.57	117.46	105.20
1	1A	1253	A	O4'-C1'-N9	-5.57	103.74	108.20
1	1A	2794	C	N1-C2-O2	5.57	122.24	118.90
1	1A	2682	U	O5'-P-OP2	-5.56	100.70	105.70
54	1w	47	U	C6-N1-C1'	-5.54	113.45	121.20
32	2a	1130	A	O5'-P-OP1	-5.53	100.72	105.70
1	2A	90	U	C2-N1-C1'	5.50	124.30	117.70
32	2a	1263	C	C6-N1-C1'	-5.49	114.21	120.80
1	2A	2318	G	C4-N9-C1'	5.48	133.62	126.50
1	1A	2789	C	N1-C2-O2	-5.47	115.61	118.90
1	1A	1008	C	N1-C2-O2	-5.47	115.62	118.90
55	1x	14	A	C4-N9-C1'	5.47	136.14	126.30
1	1A	2430	A	C2-N3-C4	5.46	113.33	110.60
1	2A	1022	G	N3-C4-N9	-5.46	122.73	126.00
32	1a	754	C	C6-N1-C1'	-5.45	114.26	120.80
1	2A	879	G	N3-C4-N9	5.41	129.25	126.00
32	1a	1030	C	N3-C2-O2	-5.41	118.11	121.90
32	2a	754	C	N3-C2-O2	-5.41	118.11	121.90
1	2A	228	A	P-O3'-C3'	5.39	126.17	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2492	U	O5'-P-OP1	-5.38	100.85	105.70
55	2x	46	G	C4-C5-N7	-5.38	108.65	110.80
55	2x	14	A	C4-C5-N7	-5.38	108.01	110.70
32	1a	532	A	O4'-C1'-N9	5.37	112.50	108.20
55	2x	46	G	N1-C2-N3	5.36	127.11	123.90
1	1A	2500	U	O4'-C1'-N1	5.35	112.48	108.20
32	2a	1043	C	C2-N1-C1'	5.34	124.67	118.80
1	2A	528	A	OP1-P-O3'	5.33	116.93	105.20
1	1A	2554	U	O5'-P-OP1	-5.33	100.90	105.70
1	1A	12	U	C2-N1-C1'	5.33	124.10	117.70
40	2i	102	LEU	CA-CB-CG	5.33	127.55	115.30
1	1A	2167	U	C5-C6-N1	5.33	125.36	122.70
1	1A	2182	G	N9-C4-C5	5.31	107.53	105.40
1	1A	1174	A	P-O3'-C3'	5.31	126.07	119.70
1	1A	2182	G	C4-C5-N7	-5.31	108.68	110.80
1	2A	1638	C	OP2-P-O3'	5.29	116.84	105.20
1	2A	90	U	O4'-C1'-N1	5.29	112.43	108.20
1	1A	2036	C	O5'-P-OP1	-5.28	100.95	105.70
1	2A	528	A	P-O3'-C3'	5.27	126.02	119.70
1	2A	1313	U	N3-C2-O2	-5.26	118.52	122.20
1	2A	2866	U	C2-N1-C1'	5.26	124.01	117.70
1	1A	1075	C	C6-N1-C2	-5.25	118.20	120.30
1	2A	1210	A	P-O3'-C3'	5.25	126.00	119.70
56	1y	58	A	OP1-P-O3'	5.25	116.75	105.20
1	1A	2073	C	C6-N1-C2	5.25	122.40	120.30
1	2A	645	C	N1-C2-O2	5.24	122.05	118.90
56	2y	22	G	N3-C4-N9	5.24	129.14	126.00
1	1A	2167	U	C6-N1-C1'	-5.24	113.87	121.20
1	2A	746	A	O4'-C1'-N9	5.23	112.38	108.20
1	1A	2825	C	C6-N1-C2	-5.22	118.21	120.30
1	1A	2454	G	N7-C8-N9	-5.21	110.50	113.10
1	2A	1698	A	C6-C5-N7	-5.21	128.66	132.30
1	1A	1993	U	O5'-P-OP1	-5.20	101.02	105.70
1	2A	2143	C	C2-N3-C4	5.20	122.50	119.90
56	1y	58	A	P-O3'-C3'	5.19	125.93	119.70
32	1a	1158	C	C2-N1-C1'	5.19	124.51	118.80
1	1A	2447	G	C4-N9-C1'	-5.19	119.76	126.50
1	1A	954	G	O5'-P-OP1	-5.18	101.03	105.70
56	2y	58	A	P-O3'-C3'	5.18	125.92	119.70
32	1a	792	A	O4'-C1'-N9	5.17	112.33	108.20
1	2A	228	A	OP1-P-O3'	5.17	116.56	105.20
32	2a	1158	C	N1-C2-O2	5.16	122.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1331	G	O4'-C1'-N9	5.15	112.32	108.20
32	1a	266	G	OP2-P-O3'	5.14	116.52	105.20
55	2x	14	A	C8-N9-C1'	-5.14	118.44	127.70
1	2A	2155	G	N1-C6-O6	-5.14	116.81	119.90
1	1A	1176	G	P-O3'-C3'	5.13	125.86	119.70
1	1A	1326	U	OP1-P-O3'	5.13	116.48	105.20
1	1A	2032	G	C5-N7-C8	5.13	106.86	104.30
1	1A	1064	C	C5-C6-N1	5.12	123.56	121.00
1	1A	2598	A	O5'-P-OP1	-5.12	101.09	105.70
1	1A	847	U	N1-C2-O2	5.12	126.38	122.80
2	1B	41	U	C5-C6-N1	-5.12	120.14	122.70
32	2a	1129	C	P-O3'-C3'	5.10	125.83	119.70
1	2A	2897	U	C2-N1-C1'	5.10	123.82	117.70
32	1a	928	G	N3-C4-N9	-5.10	122.94	126.00
32	2a	687	A	P-O3'-C3'	5.08	125.80	119.70
1	2A	2155	G	N1-C2-N3	-5.08	120.85	123.90
1	1A	2096	U	N1-C2-O2	5.08	126.36	122.80
32	1a	952	U	C5-C4-O4	5.07	128.94	125.90
1	2A	898	C	C6-N1-C2	-5.06	118.28	120.30
32	1a	1002	G	C4-N9-C1'	5.05	133.07	126.50
1	1A	1008	C	N3-C2-O2	5.05	125.44	121.90
1	2A	1992	G	P-O3'-C3'	5.05	125.76	119.70
1	2A	2119	A	OP1-P-O3'	5.05	116.31	105.20
1	1A	2391	G	N3-C4-C5	5.03	131.12	128.60
1	1A	1063	G	C5-C6-N1	-5.03	108.99	111.50
1	1A	2727	G	O5'-P-OP2	-5.03	101.18	105.70
1	2A	1420	U	P-O3'-C3'	5.02	125.73	119.70
1	1A	120	U	O5'-P-OP1	-5.02	101.18	105.70
1	2A	847	U	N1-C2-O2	5.02	126.31	122.80
1	1A	383	U	C2-N1-C1'	-5.01	111.69	117.70
55	2x	46	G	N3-C4-C5	-5.01	126.10	128.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
11	1P	37	GLY	Peptide
11	2P	35	HIS	Peptide
44	2m	106	ASN	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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%)	261 (96%)	12 (4%)	0	100	100
3	2D	273/276 (99%)	254 (93%)	18 (7%)	1 (0%)	34	48
4	1E	202/206 (98%)	191 (95%)	8 (4%)	3 (2%)	10	14
4	2E	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	15	23
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	29	41
5	2F	201/210 (96%)	179 (89%)	20 (10%)	2 (1%)	15	23
6	1G	179/182 (98%)	165 (92%)	14 (8%)	0	100	100
6	2G	179/182 (98%)	158 (88%)	15 (8%)	6 (3%)	3	3
7	1H	172/180 (96%)	164 (95%)	7 (4%)	1 (1%)	25	36
7	2H	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	6	7
8	1I	144/148 (97%)	123 (85%)	20 (14%)	1 (1%)	22	32
8	2I	144/148 (97%)	121 (84%)	22 (15%)	1 (1%)	22	32
9	1N	138/140 (99%)	136 (99%)	1 (1%)	1 (1%)	22	32
9	2N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	32
10	1O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	29
10	2O	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
11	1P	147/150 (98%)	133 (90%)	14 (10%)	0	100	100
11	2P	147/150 (98%)	130 (88%)	14 (10%)	3 (2%)	7	9
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	119 (86%)	19 (14%)	1 (1%)	22	32
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	2R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	17	25
15	1T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	19	29
15	2T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	19	29
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	23
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	23
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14	20
19	2X	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	14	20
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	15	23
20	2Y	105/110 (96%)	94 (90%)	9 (9%)	2 (2%)	8	10
21	1Z	148/206 (72%)	125 (84%)	22 (15%)	1 (1%)	22	32
21	2Z	156/206 (76%)	133 (85%)	20 (13%)	3 (2%)	8	10
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	90 (95%)	3 (3%)	2 (2%)	7	8
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	20
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%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	50 (75%)	12 (18%)	5 (8%)	1	0
26	24	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	14
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	17	46/49 (94%)	44 (96%)	2 (4%)	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%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	187 (82%)	38 (17%)	4 (2%)	9	11
33	2b	229/256 (90%)	187 (82%)	31 (14%)	11 (5%)	2	1
34	1c	204/239 (85%)	191 (94%)	12 (6%)	1 (0%)	29	41
34	2c	204/239 (85%)	176 (86%)	26 (13%)	2 (1%)	15	23
35	1d	206/209 (99%)	190 (92%)	14 (7%)	2 (1%)	15	23
35	2d	206/209 (99%)	188 (91%)	15 (7%)	3 (2%)	10	14
36	1e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	11	15
36	2e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	11	15
37	1f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	15	23
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	137 (90%)	14 (9%)	2 (1%)	12	17
38	2g	153/156 (98%)	133 (87%)	17 (11%)	3 (2%)	7	9
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	22	32
40	1i	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	19	29
40	2i	125/128 (98%)	98 (78%)	25 (20%)	2 (2%)	9	13
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	4	3
41	2j	94/105 (90%)	80 (85%)	9 (10%)	5 (5%)	2	1
42	1k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8	10
42	2k	112/129 (87%)	98 (88%)	10 (9%)	4 (4%)	3	3
43	1l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
43	2l	119/132 (90%)	107 (90%)	10 (8%)	2 (2%)	9	11
44	1m	121/126 (96%)	109 (90%)	11 (9%)	1 (1%)	19	29
44	2m	120/126 (95%)	100 (83%)	17 (14%)	3 (2%)	5	6
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	2n	58/61 (95%)	47 (81%)	10 (17%)	1 (2%)	9	11
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	19
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13	19
47	1p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
47	2p	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	4 (4%)	2 (2%)	7	8
48	2q	97/105 (92%)	86 (89%)	8 (8%)	3 (3%)	4	3
49	1r	66/88 (75%)	59 (89%)	5 (8%)	2 (3%)	4	3
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	62 (76%)	18 (22%)	1 (1%)	13	19
51	1t	94/106 (89%)	84 (89%)	6 (6%)	4 (4%)	2	2
51	2t	94/106 (89%)	82 (87%)	9 (10%)	3 (3%)	4	3
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	11370/12128 (94%)	10382 (91%)	861 (8%)	127 (1%)	14	20

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	71	GLY
5	1F	130	ALA
7	1H	126	PRO
26	14	62	ARG
33	1b	17	PHE
40	1i	54	ASP
42	1k	49	GLY
44	1m	67	GLU
5	2F	130	ALA
8	2I	10	GLU
11	2P	45	LEU
21	2Z	93	ASP
33	2b	17	PHE
38	2g	7	ALA
40	2i	101	PHE
42	2k	49	GLY
44	2m	67	GLU

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Mol	Chain	Res	Type
48	2q	68	ARG
8	1I	10	GLU
21	1Z	52	SER
23	11	3	LYS
26	14	45	GLY
37	1f	38	GLU
48	1q	68	ARG
49	1r	33	ASP
51	1t	96	GLY
51	1t	100	ILE
4	2E	71	GLY
6	2G	44	GLY
6	2G	47	LYS
6	2G	51	ARG
7	2H	92	ILE
23	21	3	LYS
33	2b	123	ALA
35	2d	3	ARG
35	2d	171	GLY
41	2j	75	ILE
41	2j	79	ARG
42	2k	117	ASN
43	2l	91	LYS
50	2s	81	ARG
4	1E	28	ALA
20	1Y	54	LYS
23	11	84	GLY
26	14	53	GLU
33	1b	124	SER
33	1b	155	LEU
36	1e	85	GLY
41	1j	77	PRO
42	1k	105	VAL
46	1o	19	PRO
51	1t	10	LEU
5	2F	21	ALA
7	2H	126	PRO
9	2N	2	LYS
21	2Z	52	SER
38	2g	55	GLY
39	2h	72	PRO
41	2j	78	ASN

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Mol	Chain	Res	Type
44	2m	6	GLY
51	2t	10	LEU
4	1E	52	LEU
10	1O	25	LEU
15	1T	55	ASN
19	1X	94	GLY
34	1c	107	GLN
35	1d	173	TRP
41	1j	78	ASN
41	1j	91	PRO
49	1r	25	THR
4	2E	52	LEU
6	2G	43	LEU
11	2P	29	LYS
14	2S	84	GLN
21	2Z	146	ILE
33	2b	9	GLU
33	2b	20	GLU
33	2b	74	LYS
33	2b	150	SER
34	2c	51	GLY
34	2c	107	GLN
36	2e	112	LEU
40	2i	54	ASP
41	2j	29	ARG
42	2k	104	GLN
43	2l	105	TYR
44	2m	23	TYR
51	2t	95	ALA
17	1V	79	VAL
26	14	61	ARG
26	14	66	SER
33	1b	20	GLU
38	1g	52	GLU
48	1q	33	GLY
51	1t	102	GLY
7	2H	12	PRO
12	2Q	16	ARG
15	2T	37	GLY
19	2X	94	GLY
26	24	11	PRO
33	2b	16	HIS

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Mol	Chain	Res	Type
33	2b	21	ARG
33	2b	63	MET
35	2d	154	ASN
48	2q	33	GLY
48	2q	67	LYS
51	2t	100	ILE
9	1N	2	LYS
3	2D	125	ILE
6	2G	24	GLY
17	2V	79	VAL
20	2Y	54	LYS
33	2b	125	PRO
36	2e	69	VAL
36	1e	69	VAL
38	1g	80	VAL
6	2G	28	VAL
11	2P	44	GLY
20	2Y	55	TYR
38	2g	80	VAL
42	2k	105	VAL
7	2H	169	VAL
35	1d	197	PRO
33	2b	232	PRO
41	2j	77	PRO
45	2n	14	PRO
46	2o	19	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	206 (96%)	9 (4%)	30	47
3	2D	215/218 (99%)	204 (95%)	11 (5%)	24	39
4	1E	164/166 (99%)	153 (93%)	11 (7%)	16	26
4	2E	164/166 (99%)	149 (91%)	15 (9%)	9	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	1F	160/166 (96%)	149 (93%)	11 (7%)	15	25
5	2F	159/166 (96%)	143 (90%)	16 (10%)	7	11
6	1G	143/156 (92%)	128 (90%)	15 (10%)	7	9
6	2G	143/156 (92%)	124 (87%)	19 (13%)	4	4
7	1H	144/148 (97%)	140 (97%)	4 (3%)	43	63
7	2H	144/148 (97%)	136 (94%)	8 (6%)	21	34
8	1I	113/124 (91%)	101 (89%)	12 (11%)	6	9
8	2I	105/124 (85%)	84 (80%)	21 (20%)	1	1
9	1N	118/119 (99%)	110 (93%)	8 (7%)	16	25
9	2N	118/119 (99%)	109 (92%)	9 (8%)	13	20
10	1O	100/100 (100%)	95 (95%)	5 (5%)	24	40
10	2O	100/100 (100%)	94 (94%)	6 (6%)	19	31
11	1P	115/116 (99%)	103 (90%)	12 (10%)	7	10
11	2P	115/116 (99%)	105 (91%)	10 (9%)	10	15
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	22	36
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	35	54
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	8
13	2R	101/101 (100%)	94 (93%)	7 (7%)	15	25
14	1S	86/88 (98%)	75 (87%)	11 (13%)	4	5
14	2S	85/88 (97%)	73 (86%)	12 (14%)	3	4
15	1T	115/127 (91%)	107 (93%)	8 (7%)	15	24
15	2T	113/127 (89%)	103 (91%)	10 (9%)	10	15
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22	36
16	2U	93/94 (99%)	87 (94%)	6 (6%)	17	27
17	1V	80/82 (98%)	75 (94%)	5 (6%)	18	28
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	11
18	1W	90/92 (98%)	83 (92%)	7 (8%)	12	19
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	45
19	1X	77/78 (99%)	71 (92%)	6 (8%)	12	19
19	2X	77/78 (99%)	73 (95%)	4 (5%)	23	38
20	1Y	85/91 (93%)	76 (89%)	9 (11%)	6	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	11	17
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9	14
21	2Z	137/179 (76%)	119 (87%)	18 (13%)	4	4
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	64 (98%)	1 (2%)	65	80
23	11	80/83 (96%)	80 (100%)	0	100	100
23	21	80/83 (96%)	77 (96%)	3 (4%)	33	51
24	12	65/67 (97%)	61 (94%)	4 (6%)	18	29
24	22	65/67 (97%)	64 (98%)	1 (2%)	65	80
25	13	51/52 (98%)	46 (90%)	5 (10%)	8	11
25	23	50/52 (96%)	43 (86%)	7 (14%)	3	4
26	14	59/63 (94%)	50 (85%)	9 (15%)	2	3
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	3
27	15	50/52 (96%)	44 (88%)	6 (12%)	5	6
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	31
28	16	51/52 (98%)	47 (92%)	4 (8%)	12	19
28	26	50/52 (96%)	47 (94%)	3 (6%)	19	31
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	11
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	22
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	22
30	28	54/55 (98%)	48 (89%)	6 (11%)	6	8
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	62
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	175 (91%)	17 (9%)	9	14
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4	4
34	1c	142/188 (76%)	129 (91%)	13 (9%)	9	13
34	2c	140/188 (74%)	128 (91%)	12 (9%)	10	16
35	1d	169/181 (93%)	147 (87%)	22 (13%)	4	4
35	2d	173/181 (96%)	158 (91%)	15 (9%)	10	15
36	1e	113/123 (92%)	103 (91%)	10 (9%)	10	15
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	1f	84/90 (93%)	78 (93%)	6 (7%)	14	23
37	2f	85/90 (94%)	80 (94%)	5 (6%)	19	32
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7	11
38	2g	120/127 (94%)	107 (89%)	13 (11%)	6	9
39	1h	114/119 (96%)	108 (95%)	6 (5%)	22	37
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	12
40	1i	90/99 (91%)	81 (90%)	9 (10%)	7	11
40	2i	89/99 (90%)	72 (81%)	17 (19%)	1	1
41	1j	66/92 (72%)	61 (92%)	5 (8%)	13	20
41	2j	69/92 (75%)	64 (93%)	5 (7%)	14	23
42	1k	82/99 (83%)	75 (92%)	7 (8%)	10	16
42	2k	83/99 (84%)	78 (94%)	5 (6%)	19	31
43	1l	96/108 (89%)	90 (94%)	6 (6%)	18	28
43	2l	96/108 (89%)	87 (91%)	9 (9%)	8	13
44	1m	93/101 (92%)	84 (90%)	9 (10%)	8	12
44	2m	92/101 (91%)	83 (90%)	9 (10%)	8	11
45	1n	49/50 (98%)	42 (86%)	7 (14%)	3	4
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	6
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9	14
46	2o	78/80 (98%)	75 (96%)	3 (4%)	33	51
47	1p	69/74 (93%)	58 (84%)	11 (16%)	2	3
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	4
48	1q	94/97 (97%)	90 (96%)	4 (4%)	29	46
48	2q	94/97 (97%)	90 (96%)	4 (4%)	29	46
49	1r	59/77 (77%)	52 (88%)	7 (12%)	5	6
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	65 (94%)	4 (6%)	20	32
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	14
51	1t	70/82 (85%)	66 (94%)	4 (6%)	20	33
51	2t	70/82 (85%)	67 (96%)	3 (4%)	29	46
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8534 (92%)	769 (8%)	11	17

All (769) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	14	ARG
3	1D	32	SER
3	1D	71	ASP
3	1D	99	ASP
3	1D	142	VAL
3	1D	211	ARG
3	1D	242	ARG
3	1D	260	ARG
3	1D	273	ARG
4	1E	21	VAL
4	1E	34	VAL
4	1E	47	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	101	ARG
4	1E	116	VAL
4	1E	163	GLU
4	1E	178	GLU
4	1E	181	LEU
4	1E	184	VAL
5	1F	17	ARG
5	1F	24	LEU
5	1F	43	LYS
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	132	VAL
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	21	ARG
6	1G	31	VAL
6	1G	45	GLU
6	1G	49	ASP
6	1G	82	LEU

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Mol	Chain	Res	Type
6	1G	91	ARG
6	1G	115	ARG
6	1G	133	LEU
6	1G	139	LEU
6	1G	140	ILE
6	1G	150	ASP
6	1G	159	VAL
6	1G	165	THR
6	1G	170	ARG
6	1G	175	LEU
7	1H	56	SER
7	1H	81	GLU
7	1H	84	SER
7	1H	107	VAL
8	1I	10	GLU
8	1I	40	THR
8	1I	41	GLU
8	1I	47	LEU
8	1I	50	ARG
8	1I	86	THR
8	1I	92	VAL
8	1I	108	THR
8	1I	116	LEU
8	1I	123	LEU
8	1I	133	HIS
8	1I	140	LEU
9	1N	9	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	46	VAL
9	1N	62	VAL
9	1N	68	GLU
9	1N	96	GLU
9	1N	99	LEU
10	1O	10	VAL
10	1O	28	SER
10	1O	64	ARG
10	1O	89	ASN
10	1O	98	VAL
11	1P	3	LEU
11	1P	15	ARG
11	1P	45	LEU

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Mol	Chain	Res	Type
11	1P	55	ARG
11	1P	83	VAL
11	1P	95	VAL
11	1P	101	VAL
11	1P	112	LEU
11	1P	119	GLU
11	1P	133	SER
11	1P	147	LEU
11	1P	149	GLU
12	1Q	35	VAL
12	1Q	38	GLU
12	1Q	56	ARG
12	1Q	59	ARG
12	1Q	109	VAL
12	1Q	110	THR
13	1R	15	SER
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	67	LEU
13	1R	79	LEU
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	25	ARG
14	1S	46	VAL
14	1S	49	VAL
14	1S	50	SER
14	1S	53	SER
14	1S	69	VAL
14	1S	73	LEU
14	1S	78	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	21	GLU
15	1T	28	VAL
15	1T	38	ASN
15	1T	48	ILE
15	1T	49	VAL

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Mol	Chain	Res	Type
15	1T	89	VAL
15	1T	96	ARG
15	1T	104	ASN
16	1U	8	VAL
16	1U	17	ILE
16	1U	74	LEU
16	1U	95	LEU
16	1U	111	GLU
17	1V	46	VAL
17	1V	52	VAL
17	1V	56	SER
17	1V	61	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	15	ARG
18	1W	18	ARG
18	1W	24	ILE
18	1W	30	GLU
18	1W	67	ASP
18	1W	68	ARG
19	1X	35	THR
19	1X	45	THR
19	1X	57	LEU
19	1X	68	ARG
19	1X	87	GLN
19	1X	93	GLU
20	1Y	7	VAL
20	1Y	14	LEU
20	1Y	43	ASN
20	1Y	55	TYR
20	1Y	72	VAL
20	1Y	90	LEU
20	1Y	91	GLU
20	1Y	99	CYS
20	1Y	106	LEU
21	1Z	18	LEU
21	1Z	46	LYS
21	1Z	61	LEU
21	1Z	69	THR
21	1Z	91	LEU
21	1Z	104	PHE
21	1Z	124	ILE

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Mol	Chain	Res	Type
21	1Z	149	SER
21	1Z	153	SER
21	1Z	154	ASP
21	1Z	170	THR
21	1Z	171	ILE
24	12	19	VAL
24	12	50	ILE
24	12	53	LEU
24	12	70	GLN
25	13	34	GLU
25	13	35	ARG
25	13	37	LEU
25	13	54	VAL
25	13	60	GLU
26	14	28	LYS
26	14	35	VAL
26	14	49	PHE
26	14	56	VAL
26	14	59	PHE
26	14	61	ARG
26	14	63	TYR
26	14	65	ASP
26	14	67	TYR
27	15	6	VAL
27	15	26	THR
27	15	40	LYS
27	15	55	ARG
27	15	58	LEU
27	15	59	GLU
28	16	6	ARG
28	16	9	LEU
28	16	47	THR
28	16	48	VAL
29	17	41	ARG
29	17	43	THR
29	17	46	VAL
29	17	47	ARG
30	18	14	VAL
30	18	31	HIS
30	18	32	LEU
30	18	58	ILE
31	19	7	VAL

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Mol	Chain	Res	Type
33	1b	8	LYS
33	1b	12	GLU
33	1b	21	ARG
33	1b	24	TRP
33	1b	35	GLU
33	1b	53	ARG
33	1b	64	ARG
33	1b	82	ARG
33	1b	101	MET
33	1b	113	HIS
33	1b	124	SER
33	1b	127	ILE
33	1b	154	LEU
33	1b	189	ASP
33	1b	200	ILE
33	1b	208	ILE
33	1b	217	ARG
34	1c	8	ILE
34	1c	20	SER
34	1c	49	SER
34	1c	72	LYS
34	1c	77	ILE
34	1c	105	GLU
34	1c	110	ASN
34	1c	115	LEU
34	1c	119	ARG
34	1c	192	THR
34	1c	195	VAL
34	1c	201	TYR
34	1c	206	GLU
35	1d	3	ARG
35	1d	31	CYS
35	1d	46	LYS
35	1d	49	ARG
35	1d	59	ARG
35	1d	73	ARG
35	1d	76	ARG
35	1d	127	THR
35	1d	134	ASP
35	1d	141	ARG
35	1d	144	ASP
35	1d	155	LEU

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Mol	Chain	Res	Type
35	1d	157	LEU
35	1d	162	LEU
35	1d	175	SER
35	1d	177	ASP
35	1d	178	VAL
35	1d	190	ASP
35	1d	193	ASP
35	1d	194	LEU
35	1d	200	GLU
35	1d	205	GLU
36	1e	24	ARG
36	1e	31	LEU
36	1e	41	VAL
36	1e	45	PHE
36	1e	56	GLN
36	1e	68	GLU
36	1e	81	GLU
36	1e	91	LEU
36	1e	126	ARG
36	1e	141	GLN
37	1f	10	LEU
37	1f	43	LEU
37	1f	64	GLN
37	1f	70	ASP
37	1f	78	GLU
37	1f	93	SER
38	1g	8	GLU
38	1g	12	LEU
38	1g	13	GLN
38	1g	21	VAL
38	1g	47	CYS
38	1g	59	LEU
38	1g	92	SER
38	1g	94	ARG
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	115	ARG
39	1h	23	SER
39	1h	51	VAL
39	1h	52	ASP
39	1h	91	ARG

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Mol	Chain	Res	Type
39	1h	97	VAL
39	1h	127	LEU
40	1i	23	ASN
40	1i	27	THR
40	1i	41	VAL
40	1i	50	LEU
40	1i	56	LEU
40	1i	86	VAL
40	1i	92	TYR
40	1i	105	ASP
40	1i	128	ARG
41	1j	35	SER
41	1j	46	ARG
41	1j	49	VAL
41	1j	98	ILE
41	1j	100	THR
42	1k	25	TYR
42	1k	26	ASN
42	1k	30	VAL
42	1k	31	THR
42	1k	48	ILE
42	1k	109	VAL
42	1k	114	VAL
43	1l	13	LYS
43	1l	36	VAL
43	1l	54	LYS
43	1l	55	VAL
43	1l	83	VAL
43	1l	114	LYS
44	1m	4	ILE
44	1m	8	GLU
44	1m	17	VAL
44	1m	49	THR
44	1m	61	GLU
44	1m	64	TRP
44	1m	94	ARG
44	1m	108	ARG
44	1m	109	THR
45	1n	3	ARG
45	1n	7	ILE
45	1n	9	LYS
45	1n	13	THR

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Mol	Chain	Res	Type
45	1n	18	VAL
45	1n	33	VAL
45	1n	56	VAL
46	1o	21	ASP
46	1o	39	LEU
46	1o	48	LYS
46	1o	76	GLU
46	1o	77	ARG
46	1o	84	LYS
46	1o	88	ARG
47	1p	2	VAL
47	1p	16	HIS
47	1p	21	VAL
47	1p	27	LYS
47	1p	31	LYS
47	1p	45	THR
47	1p	50	LYS
47	1p	60	LEU
47	1p	62	VAL
47	1p	67	THR
47	1p	72	ARG
48	1q	11	VAL
48	1q	39	SER
48	1q	45	HIS
48	1q	76	LEU
49	1r	26	LEU
49	1r	31	LEU
49	1r	38	GLU
49	1r	46	GLU
49	1r	54	ARG
49	1r	66	LEU
49	1r	76	LEU
50	1s	7	LYS
50	1s	32	LYS
50	1s	37	ARG
50	1s	41	VAL
51	1t	10	LEU
51	1t	19	SER
51	1t	24	LEU
51	1t	53	LEU
52	1u	15	ARG
3	2D	14	ARG

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Mol	Chain	Res	Type
3	2D	22	SER
3	2D	26	LYS
3	2D	71	ASP
3	2D	88	ARG
3	2D	99	ASP
3	2D	141	VAL
3	2D	142	VAL
3	2D	204	ILE
3	2D	229	VAL
3	2D	242	ARG
4	2E	12	THR
4	2E	21	VAL
4	2E	27	LEU
4	2E	75	VAL
4	2E	90	THR
4	2E	93	VAL
4	2E	100	GLU
4	2E	101	ARG
4	2E	116	VAL
4	2E	119	ARG
4	2E	145	LYS
4	2E	175	VAL
4	2E	181	LEU
4	2E	184	VAL
4	2E	195	LEU
5	2F	15	SER
5	2F	24	LEU
5	2F	33	LEU
5	2F	57	VAL
5	2F	74	ARG
5	2F	88	VAL
5	2F	98	SER
5	2F	125	LEU
5	2F	132	VAL
5	2F	144	LYS
5	2F	145	GLU
5	2F	158	THR
5	2F	165	ARG
5	2F	170	LEU
5	2F	192	LEU
5	2F	195	ASP
6	2G	3	LEU

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Mol	Chain	Res	Type
6	2G	4	ASP
6	2G	9	ARG
6	2G	19	LEU
6	2G	28	VAL
6	2G	51	ARG
6	2G	53	LEU
6	2G	79	ASN
6	2G	91	ARG
6	2G	115	ARG
6	2G	124	SER
6	2G	133	LEU
6	2G	140	ILE
6	2G	152	LEU
6	2G	159	VAL
6	2G	162	THR
6	2G	165	THR
6	2G	170	ARG
6	2G	175	LEU
7	2H	15	VAL
7	2H	44	VAL
7	2H	70	THR
7	2H	88	LEU
7	2H	106	THR
7	2H	114	VAL
7	2H	125	VAL
7	2H	130	ARG
8	2I	12	LEU
8	2I	38	LEU
8	2I	40	THR
8	2I	44	LEU
8	2I	45	LYS
8	2I	48	GLU
8	2I	50	ARG
8	2I	58	LEU
8	2I	61	ARG
8	2I	68	LEU
8	2I	74	ASN
8	2I	75	LEU
8	2I	87	LYS
8	2I	91	SER
8	2I	101	LEU
8	2I	102	SER

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Mol	Chain	Res	Type
8	2I	127	VAL
8	2I	139	GLN
8	2I	142	VAL
8	2I	143	SER
8	2I	144	VAL
9	2N	9	VAL
9	2N	14	VAL
9	2N	28	THR
9	2N	33	LEU
9	2N	38	HIS
9	2N	46	VAL
9	2N	48	MET
9	2N	62	VAL
9	2N	68	GLU
10	2O	24	VAL
10	2O	57	VAL
10	2O	64	ARG
10	2O	65	THR
10	2O	78	ARG
10	2O	108	GLU
11	2P	15	ARG
11	2P	45	LEU
11	2P	55	ARG
11	2P	77	ARG
11	2P	95	VAL
11	2P	96	THR
11	2P	112	LEU
11	2P	121	LYS
11	2P	123	LEU
11	2P	148	LEU
12	2Q	1	MET
12	2Q	5	ARG
12	2Q	71	ASP
12	2Q	109	VAL
13	2R	29	LEU
13	2R	44	LEU
13	2R	60	LEU
13	2R	67	LEU
13	2R	79	LEU
13	2R	100	LEU
13	2R	114	VAL
14	2S	8	GLU

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Mol	Chain	Res	Type
14	2S	12	PHE
14	2S	26	LEU
14	2S	27	SER
14	2S	52	SER
14	2S	58	LEU
14	2S	63	THR
14	2S	64	GLU
14	2S	80	LEU
14	2S	93	LYS
14	2S	97	ARG
14	2S	110	LEU
15	2T	9	LEU
15	2T	40	THR
15	2T	46	GLU
15	2T	49	VAL
15	2T	72	VAL
15	2T	74	ARG
15	2T	85	LYS
15	2T	89	VAL
15	2T	96	ARG
15	2T	107	ASP
16	2U	5	LYS
16	2U	74	LEU
16	2U	78	THR
16	2U	95	LEU
16	2U	111	GLU
16	2U	117	GLN
17	2V	7	THR
17	2V	18	LEU
17	2V	46	VAL
17	2V	53	GLU
17	2V	61	VAL
17	2V	85	LYS
17	2V	93	GLU
17	2V	98	GLU
18	2W	11	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	67	ASP
19	2X	45	THR
19	2X	81	VAL
19	2X	90	GLU

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Mol	Chain	Res	Type
19	2X	93	GLU
20	2Y	14	LEU
20	2Y	55	TYR
20	2Y	72	VAL
20	2Y	91	GLU
20	2Y	97	ARG
20	2Y	99	CYS
20	2Y	106	LEU
21	2Z	24	LEU
21	2Z	35	ARG
21	2Z	37	VAL
21	2Z	42	VAL
21	2Z	66	SER
21	2Z	69	THR
21	2Z	84	GLU
21	2Z	90	VAL
21	2Z	91	LEU
21	2Z	121	HIS
21	2Z	122	ARG
21	2Z	124	ILE
21	2Z	126	VAL
21	2Z	136	PHE
21	2Z	144	LEU
21	2Z	145	GLU
21	2Z	148	ASP
21	2Z	154	ASP
22	20	14	ARG
23	21	21	ARG
23	21	58	ILE
23	21	65	SER
24	22	19	VAL
25	23	3	ARG
25	23	7	LYS
25	23	28	LEU
25	23	30	ARG
25	23	34	GLU
25	23	35	ARG
25	23	54	VAL
26	24	1	MET
26	24	26	SER
26	24	27	THR
26	24	34	GLU

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Mol	Chain	Res	Type
26	24	49	PHE
26	24	59	PHE
26	24	67	TYR
26	24	68	ARG
27	25	6	VAL
27	25	58	LEU
27	25	59	GLU
28	26	9	LEU
28	26	14	THR
28	26	30	THR
29	27	1	MET
29	27	43	THR
29	27	46	VAL
30	28	3	LYS
30	28	14	VAL
30	28	23	VAL
30	28	31	HIS
30	28	32	LEU
30	28	46	ARG
33	2b	9	GLU
33	2b	16	HIS
33	2b	24	TRP
33	2b	30	ARG
33	2b	39	ILE
33	2b	76	GLN
33	2b	78	GLN
33	2b	90	MET
33	2b	94	ASN
33	2b	110	GLN
33	2b	112	VAL
33	2b	115	LEU
33	2b	118	LEU
33	2b	126	GLU
33	2b	127	ILE
33	2b	135	GLN
33	2b	142	LEU
33	2b	144	ARG
33	2b	158	LEU
33	2b	163	PHE
33	2b	168	THR
33	2b	185	ILE
33	2b	187	LEU

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Mol	Chain	Res	Type
33	2b	189	ASP
33	2b	198	ASP
34	2c	49	SER
34	2c	57	ILE
34	2c	58	GLU
34	2c	70	VAL
34	2c	77	ILE
34	2c	101	LEU
34	2c	105	GLU
34	2c	164	ARG
34	2c	166	GLU
34	2c	172	ARG
34	2c	190	ARG
34	2c	196	LEU
35	2d	5	ILE
35	2d	8	VAL
35	2d	28	SER
35	2d	31	CYS
35	2d	83	SER
35	2d	86	LYS
35	2d	96	LEU
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	158	ILE
35	2d	175	SER
35	2d	181	MET
35	2d	196	LEU
36	2e	13	ILE
36	2e	20	GLN
36	2e	24	ARG
36	2e	25	ARG
36	2e	41	VAL
36	2e	51	VAL
36	2e	53	LEU
36	2e	64	ARG
36	2e	139	LEU
36	2e	144	THR
36	2e	149	GLU
37	2f	19	LEU
37	2f	45	LEU

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Mol	Chain	Res	Type
37	2f	69	GLU
37	2f	93	SER
37	2f	94	GLN
38	2g	9	VAL
38	2g	15	ASP
38	2g	16	LEU
38	2g	32	ARG
38	2g	77	SER
38	2g	78	ARG
38	2g	79	ARG
38	2g	90	GLU
38	2g	98	SER
38	2g	106	GLN
38	2g	113	GLU
38	2g	115	ARG
38	2g	140	ASP
39	2h	8	ASP
39	2h	11	THR
39	2h	22	GLU
39	2h	24	THR
39	2h	26	VAL
39	2h	29	SER
39	2h	51	VAL
39	2h	52	ASP
39	2h	91	ARG
39	2h	99	GLU
39	2h	114	THR
40	2i	7	THR
40	2i	14	VAL
40	2i	47	LEU
40	2i	50	LEU
40	2i	51	ARG
40	2i	53	VAL
40	2i	65	VAL
40	2i	75	ASP
40	2i	83	ARG
40	2i	89	ASN
40	2i	92	TYR
40	2i	102	LEU
40	2i	103	THR
40	2i	105	ASP
40	2i	108	VAL

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Mol	Chain	Res	Type
40	2i	113	LYS
40	2i	125	TYR
41	2j	23	ILE
41	2j	38	ILE
41	2j	45	ARG
41	2j	55	LYS
41	2j	100	THR
42	2k	14	VAL
42	2k	41	THR
42	2k	78	GLN
42	2k	79	SER
42	2k	81	ASP
43	2l	18	VAL
43	2l	40	VAL
43	2l	53	ARG
43	2l	62	SER
43	2l	67	THR
43	2l	83	VAL
43	2l	91	LYS
43	2l	97	ARG
43	2l	112	ASP
44	2m	27	LYS
44	2m	47	ASP
44	2m	62	ASN
44	2m	73	GLU
44	2m	80	ARG
44	2m	90	LEU
44	2m	103	THR
44	2m	108	ARG
44	2m	117	VAL
45	2n	3	ARG
45	2n	4	LYS
45	2n	18	VAL
45	2n	33	VAL
45	2n	50	LYS
45	2n	56	VAL
46	2o	7	GLU
46	2o	39	LEU
46	2o	87	ILE
47	2p	1	MET
47	2p	5	ARG
47	2p	8	ARG

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Mol	Chain	Res	Type
47	2p	27	LYS
47	2p	45	THR
47	2p	60	LEU
47	2p	62	VAL
47	2p	67	THR
47	2p	71	ARG
48	2q	37	LYS
48	2q	45	HIS
48	2q	63	ARG
48	2q	83	ASP
50	2s	9	VAL
50	2s	37	ARG
50	2s	41	VAL
50	2s	49	ILE
50	2s	57	HIS
50	2s	77	THR
51	2t	15	ARG
51	2t	24	LEU
51	2t	71	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
4	1E	48	GLN
4	1E	180	ASN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
8	1I	133	HIS
9	1N	8	GLN
10	1O	3	GLN
10	1O	5	GLN
11	1P	27	HIS
12	1Q	12	GLN
14	1S	61	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	73	GLN
22	10	50	ASN

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Mol	Chain	Res	Type
24	12	46	GLN
25	13	32	GLN
27	15	23	HIS
33	1b	95	GLN
33	1b	212	GLN
34	1c	6	HIS
34	1c	162	GLN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	161	ASN
36	1e	20	GLN
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
40	1i	3	GLN
40	1i	23	ASN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	73	GLN
40	1i	124	GLN
42	1k	22	HIS
42	1k	117	ASN
43	1l	99	HIS
44	1m	77	ASN
44	1m	92	HIS
44	1m	106	ASN
46	1o	46	HIS
47	1p	13	HIS
48	1q	93	GLN
49	1r	63	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	83	HIS
51	1t	90	GLN
3	2D	87	ASN
5	2F	69	HIS
5	2F	75	HIS
6	2G	58	GLN

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Mol	Chain	Res	Type
8	2I	139	GLN
9	2N	8	GLN
9	2N	131	GLN
10	2O	5	GLN
11	2P	27	HIS
12	2Q	12	GLN
13	2R	13	HIS
13	2R	24	GLN
14	2S	38	GLN
15	2T	58	ASN
16	2U	117	GLN
19	2X	31	HIS
21	2Z	55	HIS
21	2Z	73	GLN
22	20	17	GLN
22	20	35	ASN
22	20	50	ASN
33	2b	212	GLN
34	2c	162	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	201	GLN
36	2e	20	GLN
36	2e	56	GLN
36	2e	78	HIS
37	2f	73	ASN
37	2f	100	ASN
38	2g	68	ASN
40	2i	3	GLN
40	2i	58	HIS
41	2j	62	HIS
42	2k	78	GLN
48	2q	93	GLN
49	2r	63	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	57	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2860/2915 (98%)	472 (16%)	34 (1%)
1	2A	2787/2915 (95%)	502 (18%)	25 (0%)
2	1B	119/121 (98%)	8 (6%)	0
2	2B	118/121 (97%)	28 (23%)	0
32	1a	1494/1521 (98%)	262 (17%)	0
32	2a	1498/1521 (98%)	290 (19%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	70/76 (92%)	23 (32%)	0
54	2w	67/76 (88%)	25 (37%)	0
55	1x	74/77 (96%)	10 (13%)	0
55	2x	74/77 (96%)	7 (9%)	0
56	1y	71/76 (93%)	26 (36%)	0
56	2y	69/76 (90%)	25 (36%)	0
All	All	9325/9620 (96%)	1680 (18%)	59 (0%)

All (1680) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	14	A
1	1A	34	C
1	1A	45	C
1	1A	55	G
1	1A	63	U
1	1A	71	A
1	1A	72	U
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	154	G
1	1A	154(A)	C
1	1A	181	A
1	1A	182	A
1	1A	188	G
1	1A	196	A
1	1A	205	G

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Mol	Chain	Res	Type
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(P)	C
1	1A	271(S)	G
1	1A	271(X)	G
1	1A	272(B)	G
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	283	A
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	342	G
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	370	G
1	1A	372	G
1	1A	380	U
1	1A	386	G
1	1A	389	G
1	1A	396	G
1	1A	404	C
1	1A	405	U
1	1A	411	G
1	1A	418	G
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C

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Mol	Chain	Res	Type
1	1A	456	C
1	1A	467	G
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	568	U
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G

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Mol	Chain	Res	Type
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	857	C
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	892	G
1	1A	893	C
1	1A	894	C
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	899	A
1	1A	900	A
1	1A	910	A
1	1A	914	C
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	989	G
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1017	G

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Mol	Chain	Res	Type
1	1A	1018	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1041	C
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1063	G
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1072	C
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1098	A
1	1A	1099	G
1	1A	1101	U
1	1A	1102	C
1	1A	1103	A
1	1A	1108	U
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C

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Mol	Chain	Res	Type
1	1A	1117	G
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1142	U
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1211	U
1	1A	1220	A
1	1A	1229	G
1	1A	1236	G
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1281	G
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1306	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1372	U
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1427	A

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Mol	Chain	Res	Type
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1473	G
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1540	U
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1719	G
1	1A	1722	A
1	1A	1739	U
1	1A	1740	G
1	1A	1746	G
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A

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Mol	Chain	Res	Type
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1817	G
1	1A	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1852	C
1	1A	1861	G
1	1A	1877	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1984	G
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2098	U
1	1A	2102	U

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Mol	Chain	Res	Type
1	1A	2104	G
1	1A	2105	C
1	1A	2108	C
1	1A	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2120	G
1	1A	2121	G
1	1A	2122	U
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2147	G
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2163	C
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C

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Mol	Chain	Res	Type
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2218	U
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2313	C
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2358	G
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G
1	1A	2400	G
1	1A	2406	U
1	1A	2424	C
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A

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Mol	Chain	Res	Type
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2449	U
1	1A	2468	G
1	1A	2469	A
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2578	G
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2634	G
1	1A	2654	A
1	1A	2663	G
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2726	U
1	1A	2733	A

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Mol	Chain	Res	Type
1	1A	2744	G
1	1A	2757	A
1	1A	2758	A
1	1A	2761	G
1	1A	2765	A
1	1A	2766	G
1	1A	2769	C
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2792	G
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2803	C
1	1A	2807	G
1	1A	2820	A
1	1A	2821	A
1	1A	2825	C
1	1A	2834	G
1	1A	2835	A
1	1A	2872	G
1	1A	2876	G
1	1A	2880	C
1	1A	2891	G
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	13	A
2	1B	15	A
2	1B	35	U
2	1B	45	A
2	1B	56	G
2	1B	73	A
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	48	C

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Mol	Chain	Res	Type
32	1a	50	A
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	69	G
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	93	G
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	129(A)	G
32	1a	131	C
32	1a	144	G
32	1a	145	G
32	1a	151	A
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(F)	U
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	221	C
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A

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Mol	Chain	Res	Type
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	342	C
32	1a	344	A
32	1a	345	C
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	388	G
32	1a	392	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	451	A
32	1a	452	A
32	1a	457	C
32	1a	461	A
32	1a	470	C
32	1a	474	G
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	508	C
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C

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Mol	Chain	Res	Type
32	1a	521	G
32	1a	524	G
32	1a	527	7MG
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	574	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	608	A
32	1a	616	G
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	684	A
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	709	G
32	1a	722	A
32	1a	723	U
32	1a	731	G
32	1a	748	C
32	1a	749	C
32	1a	752	G
32	1a	753	A
32	1a	755	G
32	1a	766	A
32	1a	787	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	806	C
32	1a	815	A
32	1a	816	A

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Mol	Chain	Res	Type
32	1a	817	C
32	1a	821	G
32	1a	827	U
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	852	G
32	1a	872	A
32	1a	874	G
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	960	U
32	1a	961	U
32	1a	964	A
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	991	U
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	997	U
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1011	G
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G

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Mol	Chain	Res	Type
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	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1037	C
32	1a	1039	C
32	1a	1040	U
32	1a	1054	C
32	1a	1066	C
32	1a	1068	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1125	U
32	1a	1134	G
32	1a	1135	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1159	U
32	1a	1160	G
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A

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Mol	Chain	Res	Type
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1269	A
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	1320	C
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1435	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1475	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

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Mol	Chain	Res	Type
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
54	1w	2	C
54	1w	3	C
54	1w	6	G
54	1w	8	4SU
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	66	U
54	1w	67	C
54	1w	68	C
54	1w	69	G
54	1w	71	G
54	1w	73	A
54	1w	74	C
55	1x	7	G
55	1x	9	G
55	1x	14	A
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	48	C
55	1x	61	C
55	1x	64	G
56	1y	5	G
56	1y	8	4SU
56	1y	12	U
56	1y	13	C

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Mol	Chain	Res	Type
56	1y	14	A
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	35	A
56	1y	36	A
56	1y	44	G
56	1y	45	U
56	1y	46	7MG
56	1y	47	U
56	1y	48	C
56	1y	49	C
56	1y	53	G
56	1y	54	5MU
56	1y	57	G
56	1y	59	U
56	1y	61	C
56	1y	65	G
56	1y	66	U
56	1y	67	C
56	1y	69	G
56	1y	72	C
1	2A	10	G
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	73	A
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	119	A
1	2A	120	U

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Mol	Chain	Res	Type
1	2A	131	G
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
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	232	G
1	2A	233	A
1	2A	245	G
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	346	A
1	2A	348	G
1	2A	352	G
1	2A	354	G
1	2A	360	G
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	386	G
1	2A	389	G
1	2A	396	G
1	2A	403	U

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Mol	Chain	Res	Type
1	2A	411	G
1	2A	421	U
1	2A	422	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	479	A
1	2A	481	G
1	2A	488	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	592	G
1	2A	595	C
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	652(B)	A
1	2A	652(C)	G
1	2A	668	G

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Mol	Chain	Res	Type
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	740	U
1	2A	751	A
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
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
1	2A	854	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	875	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	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A

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Mol	Chain	Res	Type
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	907	U
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	928	G
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1008	C
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1040	C
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1117	G
1	2A	1126	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1144	G

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Mol	Chain	Res	Type
1	2A	1151	G
1	2A	1171	G
1	2A	1195	G
1	2A	1205	U
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1230	C
1	2A	1236	G
1	2A	1244	G
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
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
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1395	A
1	2A	1416	G
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G

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Mol	Chain	Res	Type
1	2A	1460	A
1	2A	1461	G
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A
1	2A	1478	G
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	1531	C
1	2A	1532	C
1	2A	1543	C
1	2A	1544	A
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1620	G
1	2A	1633	G
1	2A	1639	U
1	2A	1648	C
1	2A	1654	A
1	2A	1667	G
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G

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Mol	Chain	Res	Type
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1747	G
1	2A	1747(A)	G
1	2A	1756	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	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1817	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1857	G
1	2A	1858	G
1	2A	1877	A
1	2A	1878	G
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
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A

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Mol	Chain	Res	Type
1	2A	1972	A
1	2A	1983	C
1	2A	1984	G
1	2A	1991	U
1	2A	1992	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	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2074	U
1	2A	2093	G
1	2A	2096	U
1	2A	2097	C
1	2A	2099	U
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2114	A
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
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	2130	U
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	2140	C
1	2A	2141	G
1	2A	2146	C
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2157	G
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2185	C
1	2A	2186	G
1	2A	2188	C
1	2A	2189	U
1	2A	2190	G
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	2267	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2298	A

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Mol	Chain	Res	Type
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2414	G
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	2447	G
1	2A	2448	A
1	2A	2459	A
1	2A	2460	U
1	2A	2469	A
1	2A	2476	A
1	2A	2477	C
1	2A	2478	A
1	2A	2484	G
1	2A	2487	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A

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Mol	Chain	Res	Type
1	2A	2520	C
1	2A	2529	G
1	2A	2530	A
1	2A	2532	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2569	G
1	2A	2573	C
1	2A	2578	G
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2651	C
1	2A	2654	A
1	2A	2658	C
1	2A	2673	G
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2731	G
1	2A	2733	A
1	2A	2748	A
1	2A	2751	G
1	2A	2754	U
1	2A	2757	A
1	2A	2759	G
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A

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Mol	Chain	Res	Type
1	2A	2789	C
1	2A	2793	G
1	2A	2794	C
1	2A	2803	C
1	2A	2805	G
1	2A	2807	G
1	2A	2808	U
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2839	G
1	2A	2872	G
1	2A	2880	C
1	2A	2894	G
1	2A	2895	U
1	2A	2896	C
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	13	A
2	2B	32	C
2	2B	40	U
2	2B	41	U
2	2B	42	C
2	2B	45	A
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	59	A
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	91	C
2	2B	94	C
2	2B	97	G
2	2B	106	G

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Mol	Chain	Res	Type
2	2B	108	U
2	2B	109	C
2	2B	110	G
2	2B	113	G
2	2B	119	G
2	2B	120	A
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	78	G
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	143	A
32	2a	144	G
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	188	C
32	2a	189(C)	C
32	2a	189(E)	U
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	227	G
32	2a	238	G
32	2a	244	U

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Mol	Chain	Res	Type
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	269	C
32	2a	279	A
32	2a	289	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	350	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
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	447	G
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	476	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A

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Mol	Chain	Res	Type
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	527	7MG
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	536	C
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	562	C
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	575	G
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	651	C
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	701	C
32	2a	703	G
32	2a	712	A
32	2a	723	U
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	759	A
32	2a	787	A
32	2a	793	U
32	2a	794	A
32	2a	815	A

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Mol	Chain	Res	Type
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	836	G
32	2a	839	U
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1001	A
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A

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Mol	Chain	Res	Type
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1024	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1030(C)	G
32	2a	1031	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1089	G
32	2a	1091	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U

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Mol	Chain	Res	Type
32	2a	1126	U
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1172	C
32	2a	1182	G
32	2a	1184	G
32	2a	1186	G
32	2a	1191	A
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1218	C
32	2a	1220	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1241	G
32	2a	1246	C
32	2a	1248	A
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1261	A
32	2a	1262	C

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Mol	Chain	Res	Type
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1285	A
32	2a	1287	A
32	2a	1299	A
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1312	G
32	2a	1321	C
32	2a	1323	G
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1357	A
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1364	U
32	2a	1370	G
32	2a	1381	U
32	2a	1394	A
32	2a	1404	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1492	A
32	2a	1494	G
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

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Mol	Chain	Res	Type
32	2a	1531	A
32	2a	1532	U
53	2v	15	A
54	2w	3	C
54	2w	4	C
54	2w	6	G
54	2w	7	A
54	2w	8	4SU
54	2w	9	A
54	2w	11	C
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	26	A
54	2w	46	7MG
54	2w	48	C
54	2w	54	5MU
54	2w	62	C
54	2w	63	G
54	2w	65	G
54	2w	66	U
54	2w	67	C
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	73	A
54	2w	74	C
55	2x	9	G
55	2x	18	G
55	2x	19	G
55	2x	21	A
55	2x	47	U
55	2x	56	C
55	2x	59	A
56	2y	15	G
56	2y	19	G
56	2y	27	G
56	2y	34	G
56	2y	36	A
56	2y	40	C
56	2y	41	C

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Mol	Chain	Res	Type
56	2y	43	C
56	2y	45	U
56	2y	46	7MG
56	2y	49	C
56	2y	50	U
56	2y	52	G
56	2y	53	G
56	2y	55	PSU
56	2y	57	G
56	2y	58	A
56	2y	59	U
56	2y	61	C
56	2y	62	C
56	2y	63	G
56	2y	65	G
56	2y	69	G
56	2y	70	G
56	2y	73	A

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	90	U
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	764	A
1	1A	974	G
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1078	U
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1210	A
1	1A	1301	A
1	1A	1379	A

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Mol	Chain	Res	Type
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1653	G
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
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	827	U
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1142(A)	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1608	A
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2A	1911	1	17,21,22	1.69	3 (17%)	20,30,33	3.00	6 (30%)
55	5MC	2x	32	55	15,22,23	1.34	1 (6%)	19,32,35	1.36	3 (15%)
54	PSU	2w	32	54	17,21,22	1.50	2 (11%)	20,30,33	3.29	6 (30%)
1	PSU	2A	1917	1	17,21,22	1.60	2 (11%)	20,30,33	3.15	6 (30%)
54	PSU	2w	55	54	17,21,22	1.40	2 (11%)	20,30,33	3.35	6 (30%)
55	5MU	2x	54	55	15,22,23	1.07	1 (6%)	16,32,35	1.81	2 (12%)
32	5MC	2a	1400	32	15,22,23	1.34	1 (6%)	19,32,35	1.33	3 (15%)
1	2MA	2A	2503	1,57	17,25,26	1.32	2 (11%)	19,37,40	1.99	3 (15%)
1	MA6	2A	2058	1	19,26,27	0.79	0	18,38,41	1.71	3 (16%)
32	5MC	2a	1404	32	15,22,23	1.30	1 (6%)	19,32,35	1.41	3 (15%)
54	7MG	2w	46	54	22,26,27	1.77	4 (18%)	28,39,42	2.70	9 (32%)
56	MIA	2y	37	56	18,24,32	1.17	2 (11%)	18,35,47	1.33	2 (11%)
1	5MU	2A	1939	1,57	15,22,23	1.04	1 (6%)	16,32,35	1.80	2 (12%)
32	MA6	1a	1519	32	19,26,27	0.84	0	18,38,41	1.68	3 (16%)
32	2MG	2a	1207	32	19,26,27	1.23	2 (10%)	21,38,41	2.11	6 (28%)
54	PSU	1w	55	54	17,21,22	1.52	2 (11%)	20,30,33	3.29	6 (30%)
32	2MG	1a	1207	32	19,26,27	1.22	2 (10%)	21,38,41	2.38	9 (42%)
1	PSU	1A	1917	1	17,21,22	1.53	3 (17%)	20,30,33	3.19	6 (30%)
54	5MU	2w	54	54	15,22,23	1.07	1 (6%)	16,32,35	2.06	2 (12%)
1	PSU	2A	2605	1	17,21,22	1.55	4 (23%)	20,30,33	3.23	7 (35%)
1	PSU	1A	1911	1	17,21,22	1.58	3 (17%)	20,30,33	3.07	6 (30%)
55	31H	2x	76	55,57	28,34,35	1.02	3 (10%)	23,47,50	1.50	2 (8%)
56	7MG	2y	46	56	22,26,27	1.79	3 (13%)	28,39,42	3.09	10 (35%)
55	5MC	1x	32	55	15,22,23	1.28	1 (6%)	19,32,35	1.44	3 (15%)
32	MA6	2a	1519	32	19,26,27	0.80	0	18,38,41	1.59	3 (16%)
56	PSU	2y	32	56	17,21,22	1.35	3 (17%)	20,30,33	3.20	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	4OC	1a	1402	32	16,23,24	0.69	0	17,32,35	1.29	1 (5%)
32	5MC	1a	1404	32	15,22,23	1.39	1 (6%)	19,32,35	1.29	3 (15%)
32	5MC	2a	967	32,57	15,22,23	1.39	1 (6%)	19,32,35	1.30	3 (15%)
54	F3N	2w	76	1,54	30,36,37	1.46	6 (20%)	29,51,54	1.23	2 (6%)
1	5MU	1A	1915	1	15,22,23	1.04	1 (6%)	16,32,35	1.61	2 (12%)
43	0TD	1l	92	43	4,9,10	3.17	1 (25%)	3,11,13	11.93	1 (33%)
32	4OC	2a	1402	32	16,23,24	0.64	0	17,32,35	1.53	1 (5%)
56	PSU	2y	39	56	17,21,22	1.56	2 (11%)	20,30,33	3.51	7 (35%)
1	5MU	1A	1939	1	15,22,23	1.10	1 (6%)	16,32,35	1.81	2 (12%)
1	PSU	1A	2605	1,57	17,21,22	1.62	3 (17%)	20,30,33	3.07	6 (30%)
32	PSU	1a	516	32	17,21,22	1.58	3 (17%)	20,30,33	3.06	6 (30%)
54	PSU	1w	39	54	17,21,22	1.47	2 (11%)	20,30,33	3.15	6 (30%)
32	M2G	2a	966	32	20,27,28	1.40	3 (15%)	22,40,43	2.12	5 (22%)
56	MIA	1y	37	56	18,24,32	1.12	2 (11%)	18,35,47	1.25	2 (11%)
1	4OC	2A	1920	1	15,22,24	0.67	0	17,31,35	1.40	2 (11%)
55	PSU	1x	55	55	17,21,22	1.48	2 (11%)	20,30,33	3.24	6 (30%)
56	PSU	1y	55	56	17,21,22	1.49	2 (11%)	20,30,33	3.16	6 (30%)
54	4SU	1w	8	54	14,21,22	1.31	2 (14%)	15,30,33	1.60	2 (13%)
54	MIA	2w	37	54	20,27,32	1.74	2 (10%)	22,39,47	1.93	7 (31%)
43	0TD	2l	92	43	4,9,10	3.11	1 (25%)	3,11,13	10.93	1 (33%)
54	5MU	1w	54	54	15,22,23	1.08	1 (6%)	16,32,35	1.93	1 (6%)
56	PSU	2y	55	56	17,21,22	1.59	4 (23%)	20,30,33	3.27	8 (40%)
56	5MU	2y	54	56	15,22,23	1.13	1 (6%)	16,32,35	1.82	2 (12%)
56	4SU	1y	8	56	14,21,22	1.23	1 (7%)	15,30,33	1.68	2 (13%)
1	5MC	2A	1942	1	15,22,23	1.37	1 (6%)	19,32,35	1.32	2 (10%)
1	5MC	1A	1942	1	15,22,23	1.31	1 (6%)	19,32,35	1.40	3 (15%)
32	5MC	2a	1407	32	15,22,23	1.28	1 (6%)	19,32,35	1.37	2 (10%)
32	7MG	2a	527	32,57	22,26,27	1.74	4 (18%)	28,39,42	2.75	9 (32%)
1	OMG	2A	2251	1,55,57	18,26,27	1.08	2 (11%)	20,38,41	2.14	6 (30%)
56	PSU	1y	39	56	17,21,22	1.38	2 (11%)	20,30,33	3.14	5 (25%)
56	PSU	1y	32	56	17,21,22	1.44	2 (11%)	20,30,33	3.21	6 (30%)
56	5MU	1y	54	56	15,22,23	1.07	2 (13%)	16,32,35	2.14	2 (12%)
54	7MG	1w	46	54	22,26,27	1.76	4 (18%)	28,39,42	2.72	8 (28%)
32	5MC	1a	967	32	15,22,23	1.26	1 (6%)	19,32,35	1.29	2 (10%)
54	F3N	1w	76	1,54	30,36,37	1.52	5 (16%)	29,51,54	1.24	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	UR3	1a	1498	32	14,22,23	0.77	1 (7%)	15,32,35	0.69	0
32	7MG	1a	527	32	22,26,27	1.72	4 (18%)	28,39,42	2.65	10 (35%)
1	OMG	1A	2251	1,55,57	18,26,27	1.15	2 (11%)	20,38,41	2.16	6 (30%)
32	5MC	1a	1400	32	15,22,23	1.37	1 (6%)	19,32,35	1.31	3 (15%)
1	5MU	2A	1915	1	15,22,23	1.07	1 (6%)	16,32,35	1.77	1 (6%)
56	4SU	2y	8	56	14,21,22	1.34	1 (7%)	15,30,33	1.63	2 (13%)
54	PSU	1w	32	54,57	17,21,22	1.54	2 (11%)	20,30,33	3.17	6 (30%)
1	2MA	1A	2503	1,57	17,25,26	1.28	2 (11%)	19,37,40	2.16	3 (15%)
54	PSU	2w	39	54	17,21,22	1.52	3 (17%)	20,30,33	3.44	6 (30%)
32	M2G	1a	966	32	20,27,28	1.42	3 (15%)	22,40,43	2.16	6 (27%)
56	7MG	1y	46	56	22,26,27	1.88	3 (13%)	28,39,42	2.97	9 (32%)
32	UR3	2a	1498	32	14,22,23	0.83	1 (7%)	15,32,35	0.75	0
1	2MU	1A	2552	1,57	14,22,24	0.85	1 (7%)	14,31,36	0.81	0
1	5MC	2A	1962	1,57	15,22,23	1.39	1 (6%)	19,32,35	1.29	2 (10%)
1	2MU	2A	2552	1,57	14,22,24	0.90	0	14,31,36	0.91	1 (7%)
55	4SU	2x	8	55	14,21,22	1.40	2 (14%)	15,30,33	2.44	2 (13%)
1	4OC	1A	1920	1	15,22,24	0.70	0	17,31,35	1.51	2 (11%)
55	PSU	2x	55	55	17,21,22	1.60	2 (11%)	20,30,33	3.09	6 (30%)
32	PSU	2a	516	32	17,21,22	1.56	2 (11%)	20,30,33	3.17	7 (35%)
54	MIA	1w	37	54	24,31,32	2.34	3 (12%)	26,44,47	2.73	9 (34%)
32	MA6	2a	1518	32	19,26,27	0.82	0	18,38,41	1.47	2 (11%)
32	MA6	1a	1518	32	19,26,27	0.82	0	18,38,41	1.43	2 (11%)
55	4SU	1x	8	55	14,21,22	1.46	2 (14%)	15,30,33	2.75	2 (13%)
1	5MC	1A	1962	1	15,22,23	1.49	1 (6%)	19,32,35	1.21	2 (10%)
54	4SU	2w	8	54	14,21,22	1.26	1 (7%)	15,30,33	1.20	2 (13%)
32	5MC	1a	1407	32	15,22,23	1.32	1 (6%)	19,32,35	1.39	3 (15%)
55	31H	1x	76	55,57	28,34,35	1.03	3 (10%)	23,47,50	1.77	4 (17%)
55	5MU	1x	54	55	15,22,23	1.06	1 (6%)	16,32,35	2.01	1 (6%)
1	MA6	1A	2058	1,57	19,26,27	0.79	0	18,38,41	1.74	3 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
54	PSU	2w	32	54	-	3/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	1/3/25/26	0/3/3/3
1	MA6	2A	2058	1	-	0/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	2/5/25/26	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
56	MIA	2y	37	56	-	3/3/25/34	0/3/3/3
1	5MU	2A	1939	1,57	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	2/5/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,57	-	3/18/40/41	0/3/3/3
56	7MG	2y	46	56	-	6/7/37/38	0/3/3/3
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
56	PSU	2y	32	56	-	3/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	5MC	2a	967	32,57	-	1/5/25/26	0/2/2/2
54	F3N	2w	76	1,54	-	2/15/37/38	0/4/4/4
1	5MU	1A	1915	1	-	0/5/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/3/12/14	-
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/5/25/26	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
56	MIA	1y	37	56	-	0/3/25/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
43	0TD	2l	92	43	-	2/3/12/14	-
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
56	PSU	2y	55	56	-	6/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	0/5/25/26	0/2/2/2
56	4SU	1y	8	56	-	3/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
32	7MG	2a	527	32,57	-	3/7/37/38	0/3/3/3
1	OMG	2A	2251	1,55,57	-	1/5/27/28	0/3/3/3
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	2/5/25/26	0/2/2/2
54	7MG	1w	46	54	-	1/7/37/38	0/3/3/3
32	5MC	1a	967	32	-	1/5/25/26	0/2/2/2
54	F3N	1w	76	1,54	-	0/15/37/38	0/4/4/4
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32	-	3/7/37/38	0/3/3/3
1	OMG	1A	2251	1,55,57	-	0/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	0/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
56	4SU	2y	8	56	-	1/5/25/26	0/2/2/2
54	PSU	1w	32	54,57	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,57	-	2/3/25/26	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
56	7MG	1y	46	56	-	1/7/37/38	0/3/3/3
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
1	2MU	1A	2552	1,57	-	0/7/27/28	0/2/2/2
1	5MC	2A	1962	1,57	-	2/5/25/26	0/2/2/2
1	2MU	2A	2552	1,57	-	0/7/27/28	0/2/2/2
55	4SU	2x	8	55	-	0/5/25/26	0/2/2/2
1	4OC	1A	1920	1	-	0/7/27/30	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	MIA	1w	37	54	-	2/11/33/34	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
1	5MC	1A	1962	1	-	2/5/25/26	0/2/2/2
54	4SU	2w	8	54	-	1/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
55	31H	1x	76	55,57	-	5/18/40/41	0/3/3/3
55	5MU	1x	54	55	-	0/5/25/26	0/2/2/2
1	MA6	1A	2058	1,57	-	0/7/29/30	0/3/3/3

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C2-S10	-7.90	1.69	1.75
54	1w	37	MIA	C13-C14	7.14	1.52	1.32
54	2w	37	MIA	C2-S10	-6.49	1.70	1.75
43	1l	92	0TD	CB-SB	-5.93	1.69	1.84
43	2l	92	0TD	CB-SB	-5.93	1.69	1.84
1	1A	1962	5MC	C5-C4	5.38	1.49	1.41
54	1w	76	F3N	CB-CG	-5.19	1.38	1.51
56	1y	46	7MG	C6-C5	5.12	1.48	1.41
32	2a	967	5MC	C5-C4	5.03	1.49	1.41
32	2a	527	7MG	C6-C5	5.00	1.48	1.41
1	2A	1962	5MC	C5-C4	4.99	1.49	1.41
32	1a	1404	5MC	C5-C4	4.97	1.49	1.41
54	2w	76	F3N	CB-CG	-4.90	1.39	1.51
56	1y	46	7MG	C5-C4	4.89	1.48	1.39
54	2w	46	7MG	C6-C5	4.89	1.48	1.41
1	2A	1942	5MC	C5-C4	4.88	1.48	1.41
32	1a	1400	5MC	C5-C4	4.85	1.48	1.41
55	2x	32	5MC	C5-C4	4.81	1.48	1.41
1	1A	1942	5MC	C5-C4	4.76	1.48	1.41
1	2A	1911	PSU	C5-C1'	-4.76	1.48	1.52
56	2y	46	7MG	C5-C4	4.75	1.48	1.39
32	2a	1400	5MC	C5-C4	4.74	1.48	1.41
32	1a	1407	5MC	C5-C4	4.62	1.48	1.41
54	1w	46	7MG	C6-C5	4.57	1.47	1.41
1	1A	2605	PSU	C5-C1'	-4.56	1.48	1.52
32	1a	967	5MC	C5-C4	4.56	1.48	1.41
54	1w	46	7MG	C5-C4	4.55	1.48	1.39
32	2a	1404	5MC	C5-C4	4.53	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	46	7MG	C5-C4	4.51	1.48	1.39
32	2a	1407	5MC	C5-C4	4.45	1.48	1.41
55	2x	55	PSU	C5-C1'	-4.45	1.48	1.52
1	2A	1917	PSU	C5-C1'	-4.45	1.48	1.52
32	1a	516	PSU	C5-C1'	-4.42	1.48	1.52
55	1x	32	5MC	C5-C4	4.41	1.48	1.41
56	2y	46	7MG	C6-C5	4.41	1.47	1.41
32	1a	527	7MG	C6-C5	4.41	1.47	1.41
32	2a	516	PSU	C5-C1'	-4.36	1.48	1.52
1	2A	2503	2MA	C6-C5	4.35	1.48	1.41
32	1a	966	M2G	C6-C5	4.34	1.48	1.41
54	1w	32	PSU	C5-C1'	-4.34	1.48	1.52
32	1a	1207	2MG	C6-C5	4.31	1.48	1.41
1	1A	2503	2MA	C6-C5	4.31	1.47	1.41
1	1A	1911	PSU	C5-C1'	-4.29	1.48	1.52
32	2a	1207	2MG	C6-C5	4.23	1.48	1.41
32	1a	527	7MG	C5-C4	4.22	1.47	1.39
54	1w	55	PSU	C5-C1'	-4.19	1.48	1.52
32	2a	966	M2G	C6-C5	4.14	1.48	1.41
56	2y	39	PSU	C5-C1'	-4.14	1.48	1.52
54	2w	39	PSU	C5-C1'	-4.14	1.48	1.52
56	2y	55	PSU	C5-C1'	-4.09	1.48	1.52
32	2a	527	7MG	C5-C4	4.09	1.47	1.39
54	1w	8	4SU	C4-S4	-4.06	1.60	1.67
56	2y	8	4SU	C4-S4	-4.05	1.60	1.67
1	2A	2605	PSU	C5-C1'	-4.02	1.48	1.52
54	2w	8	4SU	C4-S4	-4.00	1.60	1.67
56	1y	55	PSU	C5-C1'	-3.88	1.48	1.52
55	2x	8	4SU	C4-S4	-3.76	1.60	1.67
56	2y	39	PSU	C4-C5	3.75	1.49	1.41
56	2y	32	PSU	C4-C5	3.75	1.49	1.41
54	1w	39	PSU	C5-C1'	-3.74	1.49	1.52
55	1x	8	4SU	C2-N3	-3.71	1.30	1.38
56	2y	46	7MG	C5-N7	-3.71	1.33	1.39
54	1w	76	F3N	O4'-C1'	3.71	1.46	1.41
56	1y	8	4SU	C4-S4	-3.67	1.60	1.67
56	1y	32	PSU	C5-C1'	-3.67	1.49	1.52
32	1a	527	7MG	C5-N7	-3.65	1.33	1.39
54	2w	32	PSU	C5-C1'	-3.65	1.49	1.52
54	2w	32	PSU	C4-C5	3.64	1.49	1.41
1	1A	1917	PSU	C5-C1'	-3.61	1.49	1.52
56	1y	39	PSU	C4-C5	3.60	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	8	4SU	C4-S4	-3.59	1.60	1.67
55	2x	55	PSU	C4-C5	3.57	1.49	1.41
56	2y	55	PSU	C4-C5	3.56	1.49	1.41
56	2y	54	5MU	C4-C5	3.55	1.49	1.41
55	1x	55	PSU	C5-C1'	-3.53	1.49	1.52
1	2A	1911	PSU	C4-C5	3.52	1.49	1.41
1	1A	2251	OMG	C6-C5	3.52	1.47	1.41
32	2a	966	M2G	C2-N2	3.45	1.40	1.34
1	2A	2251	OMG	C6-C5	3.43	1.47	1.41
1	2A	1917	PSU	C4-C5	3.43	1.48	1.41
1	1A	1917	PSU	C4-C5	3.43	1.48	1.41
55	1x	55	PSU	C4-C5	3.42	1.48	1.41
54	2w	55	PSU	C4-C5	3.42	1.48	1.41
1	2A	1915	5MU	C4-C5	3.42	1.48	1.41
54	1w	46	7MG	C5-N7	-3.40	1.34	1.39
56	1y	32	PSU	C4-C5	3.40	1.48	1.41
32	2a	527	7MG	C5-N7	-3.39	1.34	1.39
56	1y	54	5MU	C4-C5	3.36	1.48	1.41
56	1y	46	7MG	C5-N7	-3.36	1.34	1.39
54	1w	32	PSU	C4-C5	3.35	1.48	1.41
1	1A	1939	5MU	C4-C5	3.35	1.48	1.41
54	2w	54	5MU	C4-C5	3.31	1.48	1.41
56	1y	55	PSU	C4-C5	3.30	1.48	1.41
54	2w	46	7MG	C5-N7	-3.30	1.34	1.39
32	2a	516	PSU	C4-C5	3.28	1.48	1.41
55	2x	8	4SU	C2-N3	-3.26	1.31	1.38
55	2x	54	5MU	C4-C5	3.25	1.48	1.41
55	1x	54	5MU	C4-C5	3.24	1.48	1.41
1	1A	1911	PSU	C4-C5	3.23	1.48	1.41
54	2w	55	PSU	C5-C1'	-3.22	1.49	1.52
54	1w	39	PSU	C4-C5	3.22	1.48	1.41
54	1w	54	5MU	C4-C5	3.21	1.48	1.41
32	1a	966	M2G	C2-N2	3.20	1.40	1.34
54	1w	55	PSU	C4-C5	3.17	1.48	1.41
1	1A	1915	5MU	C4-C5	3.07	1.48	1.41
32	1a	516	PSU	C4-C5	3.06	1.48	1.41
1	2A	2605	PSU	C4-C5	3.06	1.48	1.41
1	2A	1939	5MU	C4-C5	3.06	1.48	1.41
1	1A	2605	PSU	C4-C5	3.01	1.47	1.41
54	2w	39	PSU	C4-C5	2.98	1.47	1.41
54	2w	76	F3N	O4'-C1'	2.94	1.45	1.41
54	2w	76	F3N	C5-C4	-2.89	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1y	39	PSU	C5-C1'	-2.89	1.49	1.52
55	2x	76	31H	C5-C4	-2.82	1.33	1.40
56	2y	37	MIA	C5-C4	2.80	1.48	1.40
32	1a	527	7MG	C4-N9	-2.76	1.33	1.38
54	1w	46	7MG	C4-N9	-2.75	1.33	1.38
56	1y	37	MIA	C5-C4	2.74	1.48	1.40
56	2y	37	MIA	C2-N3	2.72	1.36	1.32
55	1x	76	31H	C5-C4	-2.66	1.33	1.40
56	1y	37	MIA	C2-N3	2.66	1.36	1.32
54	1w	76	F3N	C5-C4	-2.65	1.33	1.40
32	2a	1207	2MG	C5-C4	2.57	1.47	1.40
54	2w	37	MIA	C5-C4	2.57	1.47	1.40
55	1x	76	31H	C6-C5	-2.57	1.33	1.43
32	2a	966	M2G	C5-C4	2.55	1.47	1.40
32	1a	966	M2G	C5-C4	2.55	1.47	1.40
54	1w	76	F3N	C6-C5	-2.53	1.33	1.43
55	2x	76	31H	C6-C5	-2.53	1.33	1.43
1	1A	2251	OMG	C5-C4	2.48	1.47	1.40
54	2w	76	F3N	C6-C5	-2.47	1.34	1.43
54	2w	46	7MG	C4-N9	-2.42	1.33	1.38
32	2a	527	7MG	C4-N9	-2.40	1.33	1.38
54	1w	37	MIA	C5-C4	2.40	1.47	1.40
1	2A	2605	PSU	C2-N3	-2.40	1.33	1.38
54	2w	39	PSU	O4'-C1'	-2.33	1.41	1.44
1	2A	2503	2MA	C5-C4	2.32	1.47	1.40
32	1a	1207	2MG	C5-C4	2.32	1.47	1.40
56	2y	32	PSU	C5-C1'	-2.31	1.50	1.52
1	1A	1911	PSU	O4'-C1'	-2.27	1.41	1.44
32	1a	516	PSU	O4'-C1'	-2.26	1.41	1.44
1	1A	2605	PSU	C2-N3	-2.26	1.33	1.38
1	2A	2251	OMG	C5-C4	2.18	1.46	1.40
32	2a	1498	UR3	C4-N3	2.15	1.41	1.38
1	1A	1917	PSU	O4'-C1'	-2.11	1.41	1.44
54	1w	8	4SU	C2-N3	-2.11	1.34	1.38
54	1w	76	F3N	C5-N7	-2.11	1.32	1.39
55	2x	76	31H	C5-N7	-2.10	1.32	1.39
54	2w	76	F3N	C5-N7	-2.10	1.32	1.39
1	1A	2552	2MU	C2-N3	-2.09	1.34	1.38
56	2y	55	PSU	O4'-C1'	-2.08	1.41	1.44
56	1y	54	5MU	C2-N3	-2.07	1.34	1.38
54	2w	76	F3N	C2'-C3'	-2.06	1.50	1.53
55	1x	76	31H	C5-N7	-2.05	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	55	PSU	C2-N1	-2.05	1.34	1.38
1	2A	1911	PSU	C2-N3	-2.04	1.34	1.38
1	2A	2605	PSU	C2-N1	-2.04	1.34	1.38
1	1A	2503	2MA	C5-C4	2.03	1.46	1.40
32	1a	1498	UR3	C4-N3	2.03	1.41	1.38
56	2y	32	PSU	O4'-C1'	-2.01	1.41	1.44

All (354) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-20.62	61.30	101.85
43	2l	92	0TD	CSB-SB-CB	-18.87	64.73	101.85
56	2y	46	7MG	N3-C4-N9	10.22	140.04	126.91
56	1y	46	7MG	N3-C4-N9	9.88	139.59	126.91
54	2w	39	PSU	N1-C2-N3	-9.64	120.76	128.43
54	2w	32	PSU	N1-C2-N3	-9.42	120.94	128.43
55	1x	8	4SU	C2-N3-C4	9.27	128.59	115.15
56	2y	32	PSU	N1-C2-N3	-9.23	121.09	128.43
56	1y	39	PSU	N1-C2-N3	-9.06	121.23	128.43
54	2w	55	PSU	N1-C2-N3	-9.05	121.23	128.43
56	1y	32	PSU	N1-C2-N3	-9.05	121.23	128.43
54	1w	37	MIA	C12-C13-C14	-8.83	109.96	127.14
32	2a	527	7MG	N3-C4-N9	8.83	138.25	126.91
54	2w	46	7MG	N3-C4-N9	8.77	138.18	126.91
54	1w	32	PSU	N1-C2-N3	-8.77	121.46	128.43
54	1w	39	PSU	N1-C2-N3	-8.71	121.51	128.43
55	1x	55	PSU	N1-C2-N3	-8.69	121.52	128.43
54	1w	46	7MG	N3-C4-N9	8.64	138.01	126.91
32	1a	527	7MG	N3-C4-N9	8.59	137.94	126.91
1	2A	2605	PSU	N1-C2-N3	-8.58	121.61	128.43
1	1A	1917	PSU	N1-C2-N3	-8.52	121.66	128.43
56	2y	39	PSU	N1-C2-N3	-8.50	121.67	128.43
56	2y	55	PSU	N1-C2-N3	-8.50	121.67	128.43
54	2w	39	PSU	C4-N3-C2	8.49	122.31	115.14
54	1w	55	PSU	N1-C2-N3	-8.36	121.78	128.43
32	1a	516	PSU	N1-C2-N3	-8.35	121.79	128.43
32	2a	516	PSU	N1-C2-N3	-8.34	121.80	128.43
55	2x	55	PSU	N1-C2-N3	-8.32	121.81	128.43
56	1y	55	PSU	N1-C2-N3	-8.32	121.81	128.43
55	2x	8	4SU	C2-N3-C4	8.22	127.07	115.15
1	2A	1917	PSU	N1-C2-N3	-8.14	121.96	128.43
1	1A	1911	PSU	N1-C2-N3	-8.08	122.01	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1y	54	5MU	C4-N3-C2	7.84	121.77	115.14
1	2A	1911	PSU	N1-C2-N3	-7.75	122.27	128.43
1	1A	2605	PSU	N1-C2-N3	-7.70	122.31	128.43
55	1x	54	5MU	C4-N3-C2	7.50	121.47	115.14
56	2y	32	PSU	C4-N3-C2	7.49	121.47	115.14
54	2w	54	5MU	C4-N3-C2	7.45	121.43	115.14
54	2w	32	PSU	C4-N3-C2	7.30	121.30	115.14
54	1w	54	5MU	C4-N3-C2	7.18	121.20	115.14
1	2A	2605	PSU	C4-N3-C2	7.16	121.19	115.14
56	2y	55	PSU	C4-N3-C2	7.10	121.14	115.14
56	1y	39	PSU	C4-N3-C2	7.09	121.13	115.14
54	2w	55	PSU	C4-N3-C2	7.09	121.13	115.14
55	1x	55	PSU	C4-N3-C2	7.08	121.12	115.14
54	1w	55	PSU	C4-N3-C2	7.06	121.10	115.14
56	1y	32	PSU	C4-N3-C2	6.95	121.01	115.14
1	1A	2503	2MA	C2-N3-C4	6.92	121.14	115.52
56	1y	55	PSU	C4-N3-C2	6.90	120.97	115.14
54	1w	32	PSU	C4-N3-C2	6.88	120.95	115.14
56	2y	39	PSU	C5-C1'-C2'	-6.78	103.23	115.32
1	1A	1917	PSU	C4-N3-C2	6.77	120.86	115.14
1	2A	1917	PSU	C4-N3-C2	6.69	120.79	115.14
56	2y	39	PSU	C4-N3-C2	6.65	120.75	115.14
1	1A	2605	PSU	C4-N3-C2	6.65	120.75	115.14
32	2a	516	PSU	C4-N3-C2	6.64	120.75	115.14
32	1a	516	PSU	C4-N3-C2	6.60	120.71	115.14
56	2y	54	5MU	C4-N3-C2	6.56	120.69	115.14
1	2A	1915	5MU	C4-N3-C2	6.51	120.64	115.14
55	2x	54	5MU	C4-N3-C2	6.46	120.59	115.14
55	2x	55	PSU	C4-N3-C2	6.44	120.58	115.14
1	1A	1911	PSU	C4-N3-C2	6.42	120.56	115.14
54	1w	39	PSU	C4-N3-C2	6.35	120.50	115.14
1	2A	2503	2MA	C2-N3-C4	5.92	120.34	115.52
54	1w	55	PSU	C5-C4-N3	-5.90	117.76	125.36
1	2A	1939	5MU	C4-N3-C2	5.88	120.11	115.14
56	2y	46	7MG	C5-C4-N3	-5.81	117.01	126.49
56	2y	55	PSU	C5-C4-N3	-5.80	117.88	125.36
32	2a	527	7MG	N7-C8-N9	-5.80	95.08	103.38
1	2A	1911	PSU	C4-N3-C2	5.80	120.04	115.14
55	1x	76	31H	N3-C2-N1	-5.78	119.65	128.68
1	1A	1939	5MU	C4-N3-C2	5.77	120.02	115.14
54	1w	76	F3N	N3-C2-N1	-5.77	119.66	128.68
1	1A	1915	5MU	C4-N3-C2	5.76	120.00	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	76	31H	N3-C2-N1	-5.72	119.74	128.68
54	2w	39	PSU	C5-C4-N3	-5.67	118.05	125.36
54	2w	76	F3N	N3-C2-N1	-5.60	119.92	128.68
1	1A	2605	PSU	C5-C4-N3	-5.51	118.25	125.36
32	2a	516	PSU	C5-C4-N3	-5.51	118.26	125.36
55	1x	55	PSU	C5-C4-N3	-5.48	118.30	125.36
56	1y	55	PSU	C5-C4-N3	-5.46	118.33	125.36
1	1A	2058	MA6	N3-C2-N1	-5.43	120.19	128.68
56	1y	46	7MG	C5-C4-N3	-5.42	117.65	126.49
32	2a	966	M2G	C6-N1-C2	5.40	122.61	116.18
32	2a	1402	4OC	CM4-N4-C4	-5.39	118.33	122.97
1	2A	1917	PSU	C5-C4-N3	-5.38	118.43	125.36
54	1w	32	PSU	C5-C4-N3	-5.38	118.43	125.36
54	2w	46	7MG	N7-C8-N9	-5.35	95.73	103.38
56	2y	39	PSU	C5-C4-N3	-5.33	118.50	125.36
32	1a	516	PSU	C5-C4-N3	-5.31	118.51	125.36
54	1w	46	7MG	N7-C8-N9	-5.27	95.83	103.38
54	2w	32	PSU	C5-C4-N3	-5.27	118.58	125.36
1	1A	1917	PSU	C5-C4-N3	-5.26	118.58	125.36
32	1a	527	7MG	N7-C8-N9	-5.26	95.86	103.38
32	1a	966	M2G	C6-N1-C2	5.23	122.41	116.18
56	2y	32	PSU	C5-C4-N3	-5.23	118.63	125.36
55	2x	55	PSU	C5-C4-N3	-5.21	118.65	125.36
1	2A	2058	MA6	N3-C2-N1	-5.20	120.56	128.68
1	2A	1911	PSU	C5-C4-N3	-5.16	118.71	125.36
56	1y	46	7MG	C6-N1-C2	5.16	124.13	115.93
32	2a	1518	MA6	N3-C2-N1	-5.12	120.68	128.68
56	1y	8	4SU	C2-N3-C4	5.11	122.56	115.15
1	1A	1911	PSU	C5-C4-N3	-5.10	118.78	125.36
32	1a	1518	MA6	N3-C2-N1	-5.10	120.71	128.68
54	2w	55	PSU	C5-C4-N3	-5.10	118.80	125.36
54	1w	8	4SU	C2-N3-C4	5.07	122.50	115.15
56	2y	46	7MG	C6-N1-C2	5.05	123.96	115.93
56	1y	32	PSU	C5-C4-N3	-5.04	118.87	125.36
56	2y	46	7MG	C6-C5-C4	5.04	120.61	115.20
32	2a	1519	MA6	N3-C2-N1	-5.03	120.82	128.68
56	1y	39	PSU	C5-C4-N3	-5.02	118.89	125.36
54	1w	39	PSU	C5-C4-N3	-4.98	118.95	125.36
54	2w	46	7MG	C5-C4-N3	-4.94	118.43	126.49
32	2a	527	7MG	C5-C4-N3	-4.94	118.43	126.49
54	1w	37	MIA	C12-N6-C6	-4.89	115.31	122.55
1	2A	2503	2MA	C5-C6-N1	-4.88	117.94	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2605	PSU	C5-C4-N3	-4.87	119.09	125.36
56	1y	46	7MG	N7-C8-N9	-4.86	96.42	103.38
32	1a	1519	MA6	N3-C2-N1	-4.86	121.08	128.68
32	1a	966	M2G	C2-N3-C4	4.85	120.78	115.28
32	1a	527	7MG	C5-C4-N3	-4.79	118.67	126.49
32	1a	1207	2MG	C2-N3-C4	4.77	120.70	115.28
55	1x	8	4SU	C5-C4-N3	-4.77	117.44	123.83
56	2y	8	4SU	C2-N3-C4	4.77	122.06	115.15
54	1w	46	7MG	C6-N1-C2	4.76	123.49	115.93
1	1A	2251	OMG	C2-N3-C4	4.73	120.75	115.36
54	2w	55	PSU	C5-C1'-C2'	-4.68	106.97	115.32
32	2a	966	M2G	C2-N3-C4	4.63	120.54	115.28
1	1A	1920	4OC	C2-N3-C4	4.62	121.02	116.34
1	2A	1911	PSU	C5-C6-N1	-4.62	118.77	124.44
1	1A	2503	2MA	C5-C6-N1	-4.58	118.26	123.06
32	2a	1207	2MG	C2-N3-C4	4.56	120.46	115.28
55	2x	55	PSU	C5-C6-N1	-4.55	118.84	124.44
54	1w	55	PSU	C5-C1'-C2'	-4.53	107.25	115.32
56	2y	46	7MG	N7-C8-N9	-4.52	96.91	103.38
54	1w	46	7MG	C5-C4-N3	-4.49	119.16	126.49
32	2a	1207	2MG	C5-C6-N1	-4.42	117.38	123.43
56	1y	46	7MG	C6-C5-C4	4.41	119.93	115.20
1	2A	1920	4OC	C2-N3-C4	4.40	120.80	116.34
32	2a	527	7MG	C6-N1-C2	4.40	122.91	115.93
32	1a	527	7MG	C6-N1-C2	4.37	122.87	115.93
54	2w	37	MIA	C2-N3-C4	4.36	121.34	115.32
54	2w	32	PSU	C6-N1-C2	4.34	122.52	115.36
32	1a	516	PSU	C5-C6-N1	-4.33	119.12	124.44
32	1a	1402	4OC	CM4-N4-C4	-4.32	119.26	122.97
1	2A	1917	PSU	C5-C6-N1	-4.31	119.14	124.44
54	1w	39	PSU	C6-N1-C2	4.31	122.47	115.36
32	2a	516	PSU	C5-C6-N1	-4.31	119.14	124.44
32	1a	1207	2MG	C5-C6-N1	-4.30	117.55	123.43
1	2A	2251	OMG	C6-C5-C4	-4.30	116.69	120.80
1	1A	2251	OMG	C6-N1-C2	4.29	122.74	115.93
1	2A	1911	PSU	C6-N1-C2	4.29	122.43	115.36
1	1A	1911	PSU	C5-C6-N1	-4.26	119.20	124.44
32	1a	966	M2G	C5-C6-N1	-4.26	117.61	123.43
1	1A	2605	PSU	C5-C6-N1	-4.26	119.21	124.44
56	2y	39	PSU	C5-C6-N1	-4.25	119.21	124.44
32	2a	966	M2G	C5-C6-N1	-4.25	117.62	123.43
54	2w	46	7MG	C6-N1-C2	4.25	122.68	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	C6-N1-C2	4.24	122.77	115.18
32	1a	1207	2MG	C6-C5-C4	-4.22	116.77	120.80
55	2x	55	PSU	C6-N1-C2	4.22	122.32	115.36
56	2y	55	PSU	C6-N1-C2	4.20	122.29	115.36
1	2A	2251	OMG	C2-N3-C4	4.19	120.15	115.36
54	1w	37	MIA	C15-C14-C13	-4.19	110.53	122.65
55	2x	8	4SU	C5-C4-N3	-4.19	118.22	123.83
56	2y	39	PSU	C6-N1-C2	4.18	122.26	115.36
56	1y	32	PSU	C6-N1-C2	4.18	122.25	115.36
54	1w	39	PSU	C5-C6-N1	-4.15	119.34	124.44
1	1A	1917	PSU	C6-N1-C2	4.14	122.19	115.36
54	2w	55	PSU	C6-N1-C2	4.13	122.17	115.36
32	2a	516	PSU	C6-N1-C2	4.12	122.16	115.36
54	1w	46	7MG	C6-C5-C4	4.12	119.62	115.20
56	1y	39	PSU	C6-N1-C2	4.12	122.15	115.36
1	2A	2251	OMG	C6-N1-C2	4.11	122.46	115.93
1	1A	1917	PSU	C5-C1'-C2'	-4.11	107.99	115.32
32	1a	516	PSU	C6-N1-C2	4.09	122.10	115.36
1	1A	2251	OMG	C6-C5-C4	-4.07	116.91	120.80
56	2y	55	PSU	C5-C6-N1	-4.07	119.44	124.44
54	1w	46	7MG	C5-C6-N1	-4.06	114.80	123.14
54	1w	32	PSU	C6-N1-C2	4.05	122.03	115.36
54	1w	37	MIA	C2-N3-C4	4.03	120.87	115.32
55	1x	55	PSU	C6-N1-C2	4.02	121.99	115.36
1	2A	1917	PSU	C6-N1-C2	4.02	121.98	115.36
54	2w	46	7MG	C6-C5-C4	4.01	119.51	115.20
56	2y	32	PSU	C6-N1-C2	4.01	121.98	115.36
32	2a	527	7MG	C6-C5-C4	3.99	119.48	115.20
1	1A	1911	PSU	C6-N1-C2	3.99	121.94	115.36
1	2A	1917	PSU	C5-C1'-C2'	-3.99	108.20	115.32
56	1y	32	PSU	C5-C6-N1	-3.98	119.55	124.44
1	2A	2605	PSU	C6-N1-C2	3.96	121.89	115.36
56	1y	55	PSU	C5-C1'-C2'	-3.95	108.28	115.32
32	1a	1404	5MC	C2-N3-C4	3.91	120.74	116.02
1	1A	1917	PSU	C5-C6-N1	-3.89	119.66	124.44
32	1a	527	7MG	C6-C5-C4	3.89	119.37	115.20
54	1w	32	PSU	C5-C6-N1	-3.89	119.66	124.44
54	2w	32	PSU	C5-C6-N1	-3.87	119.69	124.44
55	1x	55	PSU	C5-C6-N1	-3.85	119.70	124.44
56	2y	46	7MG	C5-C6-N1	-3.85	115.22	123.14
32	2a	1207	2MG	C6-N1-C2	3.85	122.07	115.18
1	2A	1962	5MC	C2-N3-C4	3.84	120.65	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1942	5MC	C2-N3-C4	3.84	120.65	116.02
54	1w	37	MIA	C16-C14-C13	-3.84	111.56	122.65
56	1y	46	7MG	C5-C6-N1	-3.83	115.27	123.14
56	1y	55	PSU	C6-N1-C2	3.82	121.67	115.36
1	1A	1911	PSU	C5-C1'-C2'	-3.82	108.51	115.32
1	2A	2605	PSU	C5-C6-N1	-3.81	119.75	124.44
32	2a	967	5MC	C2-N3-C4	3.80	120.61	116.02
54	2w	39	PSU	C6-N1-C2	3.80	121.62	115.36
54	1w	55	PSU	C5-C6-N1	-3.79	119.79	124.44
54	1w	55	PSU	C6-N1-C2	3.76	121.56	115.36
54	2w	37	MIA	C12-N6-C6	-3.75	119.64	122.87
54	1w	39	PSU	C5-C1'-C2'	-3.75	108.64	115.32
32	2a	516	PSU	C5-C1'-C2'	-3.74	108.64	115.32
1	2A	2251	OMG	C5-C6-N1	-3.74	118.31	123.43
1	1A	2605	PSU	C6-N1-C2	3.74	121.53	115.36
32	1a	1400	5MC	C2-N3-C4	3.73	120.52	116.02
32	2a	1404	5MC	C2-N3-C4	3.72	120.50	116.02
32	2a	527	7MG	C5-C6-N1	-3.71	115.51	123.14
32	2a	1407	5MC	C2-N3-C4	3.71	120.49	116.02
56	1y	55	PSU	C5-C6-N1	-3.69	119.90	124.44
32	2a	1400	5MC	C2-N3-C4	3.69	120.47	116.02
1	1A	2251	OMG	C5-C6-N1	-3.69	118.38	123.43
54	2w	55	PSU	C5-C6-N1	-3.68	119.92	124.44
56	1y	39	PSU	C5-C6-N1	-3.65	119.95	124.44
54	2w	46	7MG	C5-C6-N1	-3.65	115.64	123.14
1	2A	1942	5MC	C2-N3-C4	3.65	120.42	116.02
32	1a	527	7MG	C5-C6-N1	-3.64	115.67	123.14
1	2A	2605	PSU	C5-C1'-C2'	-3.62	108.86	115.32
54	2w	39	PSU	C5-C6-N1	-3.62	120.00	124.44
1	1A	1939	5MU	C5-C6-N1	-3.61	118.31	122.19
54	2w	37	MIA	C5-C6-N1	-3.60	117.82	120.81
55	1x	32	5MC	C2-N3-C4	3.59	120.35	116.02
32	1a	1407	5MC	C2-N3-C4	3.58	120.34	116.02
1	1A	2605	PSU	C5-C1'-C2'	-3.57	108.94	115.32
55	1x	76	31H	CA-N-CN	-3.55	117.36	122.82
32	1a	1207	2MG	CM2-N2-C2	-3.52	119.35	123.59
32	2a	966	M2G	C6-C5-C4	-3.51	117.45	120.80
1	1A	2251	OMG	N3-C2-N1	-3.51	122.55	127.22
32	1a	967	5MC	C2-N3-C4	3.50	120.24	116.02
1	1A	1962	5MC	C2-N3-C4	3.50	120.24	116.02
32	1a	966	M2G	C6-C5-C4	-3.49	117.47	120.80
55	1x	55	PSU	C5-C1'-C2'	-3.48	109.11	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2251	OMG	N3-C2-N1	-3.45	122.62	127.22
54	1w	37	MIA	C5-C6-N1	-3.45	117.95	120.81
56	1y	8	4SU	C5-C4-N3	-3.44	119.22	123.83
1	2A	1911	PSU	C5-C1'-C2'	-3.43	109.20	115.32
55	2x	32	5MC	C2-N3-C4	3.42	120.15	116.02
1	1A	2058	MA6	C4-C5-N7	-3.41	105.85	109.40
32	2a	1207	2MG	C6-C5-C4	-3.39	117.56	120.80
32	1a	1207	2MG	C4-C5-N7	-3.37	105.89	109.40
55	1x	32	5MC	N4-C4-N3	3.34	121.75	117.03
56	1y	37	MIA	N3-C2-N1	-3.31	123.50	128.68
32	1a	1519	MA6	C4-C5-N7	-3.27	105.99	109.40
56	2y	32	PSU	C5-C6-N1	-3.26	120.44	124.44
1	2A	2058	MA6	C4-C5-N7	-3.24	106.02	109.40
56	2y	37	MIA	N3-C2-N1	-3.20	123.67	128.68
56	2y	39	PSU	O4'-C1'-C5	3.18	114.86	109.93
56	2y	8	4SU	C5-C4-N3	-3.18	119.57	123.83
54	2w	8	4SU	C2-N3-C4	3.16	119.73	115.15
1	2A	1939	5MU	C5-C6-N1	-3.13	118.82	122.19
54	1w	8	4SU	C5-C4-N3	-3.07	119.72	123.83
32	2a	1519	MA6	C4-C5-N7	-3.04	106.23	109.40
32	2a	1207	2MG	C4-C5-N7	-3.02	106.25	109.40
56	2y	37	MIA	C4-C5-N7	-3.01	106.26	109.40
32	2a	1207	2MG	CM2-N2-C2	-2.98	119.99	123.59
54	2w	37	MIA	C11-S10-C2	-2.98	100.04	102.27
56	2y	55	PSU	C5-C1'-C2'	-2.93	110.09	115.32
1	1A	1942	5MC	N4-C4-N3	2.93	121.17	117.03
32	2a	527	7MG	C8-N7-C5	2.91	116.52	108.94
54	1w	37	MIA	C2-N1-C6	2.89	122.36	117.19
32	1a	966	M2G	C4-C5-N7	-2.88	106.40	109.40
1	1A	1920	4OC	N4-C4-N3	2.88	121.04	116.49
54	1w	37	MIA	C4-C5-N7	-2.87	106.41	109.40
32	1a	967	5MC	N4-C4-N3	2.86	121.08	117.03
56	1y	32	PSU	C5-C1'-C2'	-2.82	110.29	115.32
1	1A	2503	2MA	C4-C5-N7	-2.80	106.48	109.40
54	2w	37	MIA	C4-C5-N7	-2.75	106.53	109.40
54	1w	32	PSU	C5-C1'-C2'	-2.73	110.45	115.32
55	2x	32	5MC	N4-C4-N3	2.72	120.88	117.03
1	2A	2503	2MA	C4-C5-N7	-2.71	106.57	109.40
55	2x	32	5MC	C5-C6-N1	-2.69	119.29	122.19
54	2w	46	7MG	C8-N7-C5	2.67	115.89	108.94
56	1y	46	7MG	C5-C4-N9	-2.63	102.76	106.44
32	2a	1407	5MC	N4-C4-N3	2.60	120.70	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	46	7MG	C5-C4-N9	-2.59	102.81	106.44
56	1y	46	7MG	C8-N7-C5	2.59	115.67	108.94
32	1a	527	7MG	C8-N7-C5	2.58	115.66	108.94
55	1x	76	31H	OCN-CN-N	-2.57	118.49	125.27
32	2a	1518	MA6	C4-C5-N7	-2.56	106.73	109.40
56	1y	37	MIA	C4-C5-N7	-2.54	106.75	109.40
32	2a	1404	5MC	N4-C4-N3	2.54	120.62	117.03
54	2w	8	4SU	C5-C4-N3	-2.54	120.44	123.83
32	1a	1407	5MC	N4-C4-N3	2.52	120.59	117.03
54	2w	37	MIA	C2-N1-C6	2.52	121.69	117.19
56	2y	46	7MG	C5-C4-N9	-2.51	102.92	106.44
1	2A	1962	5MC	N4-C4-N3	2.50	120.56	117.03
56	2y	46	7MG	C8-N7-C5	2.49	115.43	108.94
32	2a	1404	5MC	C5-C6-N1	-2.49	119.51	122.19
54	1w	46	7MG	C8-N7-C5	2.48	115.38	108.94
55	2x	55	PSU	C5-C1'-C2'	-2.47	110.91	115.32
55	2x	76	31H	O4'-C1'-C2'	-2.45	103.35	106.93
32	1a	1519	MA6	C1'-N9-C4	-2.44	122.36	126.64
55	1x	76	31H	O4'-C1'-C2'	-2.43	103.38	106.93
32	1a	1400	5MC	C5-C6-N1	-2.41	119.60	122.19
56	1y	54	5MU	C5-C6-N1	-2.38	119.63	122.19
1	2A	1942	5MC	C5-C6-N1	-2.35	119.66	122.19
1	2A	2251	OMG	C4-C5-N7	-2.33	106.97	109.40
32	1a	1207	2MG	N2-C2-N1	2.32	119.19	116.96
55	2x	54	5MU	C5-C6-N1	-2.32	119.69	122.19
1	1A	1962	5MC	C5-C6-N1	-2.32	119.70	122.19
54	1w	37	MIA	N3-C2-N1	-2.31	122.72	126.98
56	2y	55	PSU	O4'-C1'-C2'	2.30	108.39	104.66
56	2y	46	7MG	C2-N3-C4	2.30	120.25	113.89
32	2a	1400	5MC	C5-C6-N1	-2.29	119.72	122.19
54	2w	76	F3N	C3'-N3'-C	-2.29	119.75	123.21
1	2A	2605	PSU	O4'-C1'-C5	2.29	113.48	109.93
32	1a	516	PSU	O4'-C1'-C2'	2.28	108.36	104.66
56	2y	46	7MG	C4-N9-C1'	2.28	132.01	126.60
1	2A	1920	4OC	N4-C4-N3	2.27	120.08	116.49
32	2a	1400	5MC	N4-C4-N3	2.27	120.24	117.03
56	1y	46	7MG	C2-N3-C4	2.26	120.14	113.89
32	1a	1518	MA6	C4-C5-N7	-2.26	107.05	109.40
54	2w	54	5MU	C5-C6-N1	-2.25	119.77	122.19
32	1a	1404	5MC	N4-C4-N3	2.25	120.21	117.03
54	2w	32	PSU	C5-C1'-C2'	-2.25	111.31	115.32
32	2a	966	M2G	C4-C5-N7	-2.23	107.07	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	C5-C4-N9	-2.23	103.31	106.44
55	1x	32	5MC	C5-C6-N1	-2.23	119.79	122.19
54	2w	46	7MG	C5-C4-N9	-2.20	103.36	106.44
32	1a	527	7MG	C5-C4-N9	-2.20	103.37	106.44
32	1a	1404	5MC	C5-C6-N1	-2.19	119.83	122.19
32	1a	1400	5MC	N4-C4-N3	2.18	120.11	117.03
32	1a	1407	5MC	C5-C6-N1	-2.17	119.86	122.19
32	2a	967	5MC	C5-C6-N1	-2.16	119.86	122.19
32	1a	966	M2G	CM2-N2-C2	-2.16	119.23	121.29
32	2a	527	7MG	C2-N3-C4	2.16	119.87	113.89
56	2y	55	PSU	O4'-C1'-C5	2.16	113.27	109.93
1	1A	1942	5MC	C5-C6-N1	-2.15	119.88	122.19
1	1A	1915	5MU	C5-C6-N1	-2.15	119.88	122.19
32	1a	527	7MG	CM7-N7-C5	2.14	132.25	124.01
1	1A	2251	OMG	C4-C5-N7	-2.13	107.18	109.40
54	2w	37	MIA	N3-C2-N1	-2.11	123.09	126.98
1	2A	2552	2MU	C5-C4-N3	-2.11	118.67	123.31
32	1a	1207	2MG	C1'-N9-C4	-2.11	122.94	126.64
1	1A	2058	MA6	N1-C6-N6	-2.10	114.85	117.06
32	2a	967	5MC	N4-C4-N3	2.09	119.99	117.03
54	2w	46	7MG	C2-N3-C4	2.08	119.65	113.89
32	1a	1207	2MG	N3-C2-N1	-2.08	122.94	126.23
54	2w	39	PSU	O4'-C1'-C2'	2.06	107.99	104.66
56	2y	54	5MU	C5-C6-N1	-2.05	119.98	122.19
1	2A	2058	MA6	C1'-N9-C4	-2.04	123.06	126.64
32	2a	516	PSU	O4'-C1'-C2'	2.04	107.96	104.66
32	2a	1519	MA6	C1'-N9-C4	-2.01	123.10	126.64
32	1a	527	7MG	C2-N3-C4	2.00	119.43	113.89

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
56	2y	37	MIA	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
55	2x	76	31H	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB

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Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
56	2y	55	PSU	C2'-C1'-C5-C4
56	2y	55	PSU	O4'-C1'-C5-C4
56	2y	55	PSU	C2'-C1'-C5-C6
56	2y	55	PSU	O4'-C1'-C5-C6
56	1y	8	4SU	C2'-C1'-N1-C6
56	2y	8	4SU	C2'-C1'-N1-C6
56	1y	46	7MG	C4'-C5'-O5'-P
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
54	1w	37	MIA	C12-C13-C14-C16
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
55	1x	76	31H	C3'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C4'-C5'-O5'
54	2w	46	7MG	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	2w	54	5MU	O4'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
56	2y	55	PSU	C3'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
56	1y	54	5MU	C3'-C4'-C5'-O5'
56	1y	54	5MU	O4'-C4'-C5'-O5'
54	2w	54	5MU	C3'-C4'-C5'-O5'
56	1y	8	4SU	C3'-C4'-C5'-O5'
55	1x	76	31H	CB-CG-SD-CE
56	1y	8	4SU	O4'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
55	1x	76	31H	N-CA-CB-CG
56	2y	37	MIA	O4'-C4'-C5'-O5'
54	2w	32	PSU	O4'-C4'-C5'-O5'
32	2a	1404	5MC	O4'-C4'-C5'-O5'
56	2y	46	7MG	O4'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
54	2w	76	F3N	N-CA-CB-CG
32	2a	1404	5MC	C3'-C4'-C5'-O5'
56	2y	32	PSU	O4'-C4'-C5'-O5'
54	1w	46	7MG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
32	1a	527	7MG	O4'-C4'-C5'-O5'
56	2y	46	7MG	C2'-C1'-N9-C8
55	1x	76	31H	C4'-C5'-O5'-P
56	2y	37	MIA	C4'-C5'-O5'-P
32	2a	527	7MG	C4'-C5'-O5'-P
56	2y	46	7MG	O4'-C1'-N9-C4
1	2A	1917	PSU	O4'-C4'-C5'-O5'
32	1a	527	7MG	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
56	2y	46	7MG	C3'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
54	2w	76	F3N	C-CA-CB-CG
32	2a	967	5MC	O4'-C4'-C5'-O5'
54	2w	32	PSU	C2'-C1'-C5-C6
56	2y	32	PSU	C2'-C1'-C5-C6
54	2w	32	PSU	C3'-C4'-C5'-O5'
56	2y	32	PSU	C3'-C4'-C5'-O5'
56	2y	46	7MG	C2'-C1'-N9-C4
1	2A	2251	OMG	C1'-C2'-O2'-CM2
56	2y	46	7MG	O4'-C1'-N9-C8
55	2x	76	31H	C4'-C5'-O5'-P
54	2w	8	4SU	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	2503	2MA	O4'-C4'-C5'-O5'
54	1w	37	MIA	C5-C6-N6-C12

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2832 ligands modelled in this entry, 2830 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	302	35	0,12,12	0.00	-	-		
60	SF4	2d	303	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	302	35	-	-	0/6/5/5
60	SF4	2d	303	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	1A	2859/2915 (98%)	0.53	88 (3%)	49	47	19, 36, 83, 94	0
1	2A	2788/2915 (95%)	0.39	118 (4%)	36	35	32, 53, 82, 93	0
2	1B	120/121 (99%)	0.22	0	100	100	31, 47, 59, 79	0
2	2B	120/121 (99%)	-0.05	0	100	100	56, 64, 72, 78	0
3	1D	275/276 (99%)	0.63	2 (0%)	87	86	21, 36, 50, 65	0
3	2D	275/276 (99%)	0.70	8 (2%)	51	50	29, 46, 57, 75	0
4	1E	204/206 (99%)	0.58	0	100	100	21, 40, 58, 63	0
4	2E	204/206 (99%)	0.50	6 (2%)	51	50	33, 54, 65, 73	0
5	1F	203/210 (96%)	0.48	0	100	100	21, 42, 64, 71	0
5	2F	203/210 (96%)	0.49	5 (2%)	57	55	33, 59, 70, 77	0
6	1G	181/182 (99%)	0.40	2 (1%)	80	79	39, 54, 66, 75	0
6	2G	181/182 (99%)	0.81	15 (8%)	11	10	57, 66, 73, 81	0
7	1H	174/180 (96%)	0.40	0	100	100	35, 51, 60, 68	0
7	2H	174/180 (96%)	1.33	44 (25%)	0	0	59, 72, 79, 82	0
8	1I	146/148 (98%)	0.27	0	100	100	44, 64, 70, 73	0
8	2I	146/148 (98%)	0.48	5 (3%)	45	44	53, 65, 73, 76	0
9	1N	140/140 (100%)	0.57	0	100	100	25, 37, 54, 65	0
9	2N	140/140 (100%)	0.81	10 (7%)	16	14	43, 57, 69, 73	0
10	1O	122/122 (100%)	0.49	0	100	100	26, 39, 54, 58	0
10	2O	122/122 (100%)	0.58	1 (0%)	86	84	43, 55, 64, 69	0
11	1P	149/150 (99%)	0.42	0	100	100	19, 45, 64, 70	0
11	2P	149/150 (99%)	0.73	9 (6%)	21	20	36, 58, 71, 79	0
12	1Q	141/141 (100%)	0.60	1 (0%)	87	86	24, 38, 51, 62	0
12	2Q	141/141 (100%)	0.75	10 (7%)	16	14	40, 58, 67, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.56	0 100 100	24, 34, 48, 53	0
13	2R	118/118 (100%)	0.57	3 (2%) 57 55	39, 49, 58, 65	0
14	1S	110/112 (98%)	0.43	0 100 100	36, 47, 57, 62	0
14	2S	110/112 (98%)	0.44	5 (4%) 33 31	51, 61, 68, 71	0
15	1T	131/146 (89%)	0.44	1 (0%) 86 84	32, 44, 64, 73	0
15	2T	131/146 (89%)	0.52	3 (2%) 60 58	46, 56, 66, 73	0
16	1U	116/118 (98%)	0.60	1 (0%) 84 82	20, 30, 44, 53	0
16	2U	116/118 (98%)	0.71	5 (4%) 35 33	41, 54, 66, 72	0
17	1V	101/101 (100%)	0.53	0 100 100	22, 39, 54, 63	0
17	2V	101/101 (100%)	0.50	4 (3%) 38 37	42, 62, 68, 76	0
18	1W	112/113 (99%)	0.68	1 (0%) 84 82	24, 32, 49, 77	0
18	2W	112/113 (99%)	0.65	4 (3%) 42 42	35, 48, 61, 78	0
19	1X	95/96 (98%)	0.42	0 100 100	27, 40, 57, 68	0
19	2X	95/96 (98%)	0.73	11 (11%) 4 4	44, 55, 69, 73	0
20	1Y	107/110 (97%)	0.43	0 100 100	35, 49, 62, 68	0
20	2Y	107/110 (97%)	1.02	13 (12%) 4 3	52, 63, 72, 79	0
21	1Z	154/206 (74%)	0.54	6 (3%) 39 38	37, 58, 74, 78	0
21	2Z	160/206 (77%)	0.88	26 (16%) 1 1	57, 69, 78, 84	0
22	10	83/85 (97%)	0.51	0 100 100	27, 36, 47, 61	0
22	20	83/85 (97%)	0.77	4 (4%) 30 29	44, 54, 61, 69	0
23	11	97/98 (98%)	0.65	2 (2%) 63 61	30, 46, 64, 72	0
23	21	97/98 (98%)	0.78	5 (5%) 27 26	38, 52, 66, 74	0
24	12	70/72 (97%)	0.35	0 100 100	33, 46, 57, 62	0
24	22	70/72 (97%)	0.47	3 (4%) 35 33	53, 63, 69, 75	0
25	13	59/60 (98%)	0.49	0 100 100	23, 35, 54, 66	0
25	23	59/60 (98%)	0.74	6 (10%) 6 6	49, 57, 65, 69	0
26	14	69/71 (97%)	0.23	0 100 100	50, 66, 74, 77	0
26	24	69/71 (97%)	1.05	10 (14%) 2 2	65, 72, 78, 80	0
27	15	59/60 (98%)	0.67	1 (1%) 70 68	21, 32, 47, 58	0
27	25	59/60 (98%)	0.56	1 (1%) 70 68	33, 51, 62, 67	0
28	16	53/54 (98%)	0.47	0 100 100	32, 43, 52, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.48	1 (1%) 66 64	45, 53, 59, 62	0
29	17	48/49 (97%)	0.68	3 (6%) 20 18	21, 27, 44, 55	0
29	27	48/49 (97%)	0.95	5 (10%) 6 6	35, 40, 58, 63	0
30	18	64/65 (98%)	0.55	1 (1%) 72 70	28, 35, 41, 52	0
30	28	64/65 (98%)	1.01	9 (14%) 2 2	42, 51, 55, 59	0
31	19	37/37 (100%)	0.52	0 100 100	27, 38, 48, 51	0
31	29	37/37 (100%)	0.93	2 (5%) 25 24	53, 60, 65, 67	0
32	1a	1488/1521 (97%)	0.15	17 (1%) 80 79	33, 58, 80, 89	0
32	2a	1491/1521 (98%)	0.24	39 (2%) 56 54	46, 67, 81, 93	0
33	1b	231/256 (90%)	0.42	8 (3%) 44 43	55, 66, 74, 78	0
33	2b	231/256 (90%)	0.74	32 (13%) 2 2	61, 72, 77, 82	0
34	1c	206/239 (86%)	0.57	10 (4%) 29 28	50, 61, 71, 77	0
34	2c	206/239 (86%)	1.15	32 (15%) 2 1	62, 71, 75, 81	0
35	1d	208/209 (99%)	0.66	9 (4%) 35 33	48, 60, 68, 72	0
35	2d	208/209 (99%)	0.74	14 (6%) 17 16	51, 63, 69, 75	0
36	1e	148/162 (91%)	0.70	9 (6%) 21 20	47, 57, 66, 67	0
36	2e	148/162 (91%)	0.85	16 (10%) 5 5	57, 65, 71, 75	0
37	1f	100/101 (99%)	0.19	0 100 100	49, 58, 66, 67	0
37	2f	100/101 (99%)	0.22	0 100 100	51, 61, 65, 67	0
38	1g	155/156 (99%)	0.55	9 (5%) 23 22	50, 62, 72, 80	0
38	2g	155/156 (99%)	0.78	23 (14%) 2 2	60, 69, 74, 77	0
39	1h	137/138 (99%)	0.59	5 (3%) 42 42	49, 59, 65, 68	0
39	2h	137/138 (99%)	0.94	21 (15%) 2 1	55, 66, 72, 78	0
40	1i	127/128 (99%)	0.77	13 (10%) 6 6	49, 65, 73, 75	0
40	2i	127/128 (99%)	1.92	54 (42%) 0 0	56, 71, 76, 80	0
41	1j	97/105 (92%)	0.47	4 (4%) 37 36	51, 66, 73, 76	0
41	2j	96/105 (91%)	1.56	27 (28%) 0 0	63, 73, 77, 80	0
42	1k	114/129 (88%)	0.71	8 (7%) 16 15	41, 59, 67, 73	0
42	2k	114/129 (88%)	0.65	6 (5%) 26 25	51, 64, 70, 76	0
43	1l	121/132 (91%)	0.50	0 100 100	40, 48, 58, 64	0
43	2l	121/132 (91%)	1.00	20 (16%) 1 1	47, 58, 66, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.24	2 (1%) 72 70	50, 61, 66, 71	0
44	2m	122/126 (96%)	0.63	9 (7%) 14 13	59, 69, 74, 77	0
45	1n	60/61 (98%)	0.96	8 (13%) 3 3	48, 58, 63, 69	0
45	2n	60/61 (98%)	2.96	38 (63%) 0 0	66, 71, 76, 77	0
46	1o	88/89 (98%)	0.42	1 (1%) 80 79	43, 57, 65, 67	0
46	2o	88/89 (98%)	0.68	4 (4%) 33 31	54, 63, 70, 74	0
47	1p	82/88 (93%)	0.85	7 (8%) 10 10	53, 61, 65, 67	0
47	2p	82/88 (93%)	0.75	7 (8%) 10 10	54, 61, 67, 72	0
48	1q	99/105 (94%)	0.56	6 (6%) 21 20	50, 59, 66, 72	0
48	2q	99/105 (94%)	1.25	21 (21%) 0 0	56, 64, 71, 75	0
49	1r	68/88 (77%)	0.43	3 (4%) 34 33	51, 58, 68, 70	0
49	2r	68/88 (77%)	0.36	2 (2%) 51 50	56, 63, 71, 75	0
50	1s	83/93 (89%)	0.09	0 100 100	53, 62, 67, 71	0
50	2s	83/93 (89%)	1.11	15 (18%) 1 1	64, 71, 76, 80	0
51	1t	96/106 (90%)	0.78	8 (8%) 11 10	52, 62, 69, 73	0
51	2t	96/106 (90%)	0.89	9 (9%) 8 7	55, 63, 72, 76	0
52	1u	23/27 (85%)	1.10	3 (13%) 3 3	54, 58, 65, 66	0
52	2u	23/27 (85%)	1.73	10 (43%) 0 0	65, 69, 71, 75	0
53	1v	13/24 (54%)	1.53	3 (23%) 0 0	45, 48, 77, 86	0
53	2v	13/24 (54%)	2.06	6 (46%) 0 0	56, 64, 85, 87	0
54	1w	66/76 (86%)	0.81	10 (15%) 2 1	25, 73, 83, 87	0
54	2w	64/76 (84%)	1.01	10 (15%) 2 1	44, 78, 85, 88	0
55	1x	71/77 (92%)	0.21	0 100 100	24, 55, 72, 75	0
55	2x	71/77 (92%)	0.31	1 (1%) 75 73	39, 65, 76, 83	0
56	1y	67/76 (88%)	3.30	51 (76%) 0 0	56, 83, 88, 90	0
56	2y	66/76 (86%)	4.33	64 (96%) 0 0	66, 86, 90, 92	0
All	All	20869/21748 (95%)	0.56	1134 (5%) 25 24	19, 57, 77, 94	0

All (1134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	652(C)	G	12.4
1	1A	652(V)	C	11.6

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Mol	Chain	Res	Type	RSRZ
54	2w	71	G	11.2
54	1w	70	G	10.6
56	2y	36	A	9.5
56	1y	1	G	9.4
1	1A	652(U)	G	9.3
1	1A	652(T)	C	9.2
1	2A	652(U)	G	9.1
45	2n	39	LEU	9.0
45	2n	38	GLY	8.6
1	2A	2802	G	8.6
1	1A	653	A	8.6
1	2A	653	A	8.4
23	21	2	SER	8.2
1	2A	652(V)	C	8.1
26	24	49	PHE	7.9
1	1A	2140	C	7.8
56	1y	5	G	7.7
1	1A	2131	G	7.7
1	2A	652(C)	G	7.6
56	1y	34	G	7.6
1	2A	1509	C	7.6
56	1y	35	A	7.6
54	1w	71	G	7.3
40	2i	109	VAL	7.3
45	2n	25	VAL	7.3
38	1g	81	GLY	7.2
1	2A	883	G	7.2
1	2A	2112	G	7.1
56	2y	34	G	7.1
32	2a	1030(A)	G	7.1
54	2w	72	C	7.0
1	2A	2113	U	7.0
1	1A	652(S)	C	7.0
56	2y	15	G	6.9
45	2n	42	ILE	6.9
56	1y	75	C	6.8
26	24	50	VAL	6.8
21	2Z	153	SER	6.7
1	1A	2142	C	6.7
50	2s	50	ALA	6.7
1	1A	652(D)	C	6.7
9	2N	9	VAL	6.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2146	C	6.6
53	1v	12	A	6.6
41	2j	65	LEU	6.5
56	2y	74	C	6.5
54	2w	70	G	6.5
56	2y	57	G	6.5
21	2Z	149	SER	6.5
1	2A	2141	G	6.4
1	2A	2115	G	6.4
1	2A	652(D)	C	6.4
1	2A	2145	C	6.3
56	2y	29	G	6.3
1	1A	2141	G	6.2
56	1y	36	A	6.2
56	2y	65	G	6.2
56	2y	19	G	6.1
1	2A	2140	C	6.1
56	1y	71	G	6.1
45	2n	35	ARG	6.1
34	2c	198	VAL	6.1
41	2j	72	VAL	6.0
1	1A	654	A	6.0
56	2y	62	C	6.0
1	2A	2144	U	6.0
56	2y	66	U	6.0
1	2A	654	A	6.0
56	2y	14	A	5.9
1	2A	652(T)	C	5.9
56	2y	35	A	5.9
56	1y	2	C	5.8
1	2A	2143	C	5.7
3	2D	276	LYS	5.7
1	2A	229	A	5.7
40	2i	65	VAL	5.7
56	1y	74	C	5.6
40	2i	67	GLY	5.6
32	2a	1030(B)	C	5.6
41	2j	74	ILE	5.5
56	2y	5	G	5.5
34	2c	182	ILE	5.5
1	2A	2127	G	5.4
53	2v	24	A	5.4

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Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	5.3
43	2l	28	LYS	5.3
45	2n	34	TYR	5.3
56	1y	65	G	5.3
56	2y	63	G	5.3
1	2A	2155	G	5.2
1	2A	2154	G	5.2
56	2y	26	A	5.2
56	1y	13	C	5.2
1	2A	2110	G	5.2
56	2y	56	C	5.2
56	2y	61	C	5.2
56	2y	75	C	5.2
23	1l	2	SER	5.2
20	2Y	42	VAL	5.2
38	2g	80	VAL	5.2
53	2v	12	A	5.2
56	2y	6	G	5.1
56	2y	21	A	5.1
41	2j	44	VAL	5.1
56	2y	53	G	5.1
1	1A	2130	U	5.0
1	2A	2133	G	5.0
44	2m	123	ALA	5.0
1	2A	2147	G	5.0
34	2c	87	LEU	5.0
52	2u	16	GLY	5.0
1	2A	2803	C	5.0
18	2W	112	GLY	5.0
56	1y	70	G	4.9
1	1A	884	C	4.9
33	2b	121	LEU	4.9
56	2y	1	G	4.9
1	2A	885	C	4.9
51	2t	41	ILE	4.9
1	2A	2793	G	4.9
34	2c	155	GLY	4.9
1	2A	2181	G	4.9
56	2y	28	G	4.9
7	2H	35	VAL	4.9
56	1y	19	G	4.9
1	2A	887	A	4.9

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Mol	Chain	Res	Type	RSRZ
33	2b	34	ALA	4.9
45	2n	40	CYS	4.8
32	2a	1532	U	4.8
1	2A	2128	C	4.8
20	2Y	1	MET	4.8
38	1g	80	VAL	4.8
56	2y	64	A	4.8
56	2y	18	G	4.8
1	1A	2151	G	4.7
1	1A	2181	G	4.7
1	2A	2160	G	4.7
21	2Z	144	LEU	4.7
45	2n	22	THR	4.7
3	2D	2	ALA	4.7
45	2n	37	PHE	4.7
45	2n	26	ARG	4.7
1	2A	884	C	4.7
56	2y	2	C	4.7
45	2n	61	TRP	4.6
56	2y	22	G	4.6
1	2A	2801(A)	A	4.6
1	1A	652(F)	G	4.6
41	2j	96	ILE	4.6
1	1A	1509	C	4.6
1	1A	2145	C	4.6
1	1A	896	A	4.6
56	2y	43	C	4.5
32	2a	1257	U	4.5
1	1A	2159	G	4.5
56	1y	20	U	4.5
1	1A	652(E)	G	4.5
1	2A	882	G	4.5
21	2Z	106	GLY	4.5
45	2n	2	ALA	4.5
1	2A	2138	C	4.5
42	2k	13	GLN	4.5
54	1w	69	G	4.5
1	2A	2142	C	4.5
50	2s	80	TYR	4.5
21	2Z	22	GLY	4.5
40	2i	82	ALA	4.5
38	2g	81	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
9	2N	8	GLN	4.4
7	2H	20	ALA	4.4
26	24	52	THR	4.4
34	2c	60	ALA	4.4
29	27	46	VAL	4.4
43	2l	59	ARG	4.4
1	2A	2182	G	4.4
48	2q	73	VAL	4.4
56	2y	67	C	4.4
21	2Z	155	LEU	4.4
32	1a	1030(C)	G	4.4
33	2b	71	VAL	4.4
1	2A	2174	C	4.4
39	2h	112	LEU	4.4
1	2A	2123	G	4.4
56	1y	38	A	4.3
1	2A	2139	C	4.3
40	2i	63	ILE	4.3
26	24	63	TYR	4.3
40	2i	36	TYR	4.3
1	2A	888	C	4.3
33	2b	17	PHE	4.3
56	2y	47	U	4.3
1	2A	2117	A	4.3
7	2H	36	PRO	4.3
45	2n	44	LEU	4.3
56	2y	71	G	4.3
29	27	47	ARG	4.3
56	2y	33	U	4.3
40	2i	121	ARG	4.3
56	2y	69	G	4.3
53	2v	14	A	4.2
56	1y	73	A	4.2
1	1A	271(K)	U	4.2
48	2q	80	GLY	4.2
7	2H	105	LEU	4.2
56	2y	4	C	4.2
33	2b	215	LEU	4.2
40	2i	9	ARG	4.2
1	1A	2132	U	4.2
1	2A	2804	C	4.2
1	2A	2116	G	4.2

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Mol	Chain	Res	Type	RSRZ
33	2b	165	VAL	4.2
40	2i	14	VAL	4.2
1	2A	2167	U	4.2
32	2a	1030	C	4.2
48	2q	85	VAL	4.2
54	1w	44	G	4.1
38	1g	85	TYR	4.1
38	1g	156	TRP	4.1
1	2A	2161	C	4.1
41	2j	88	LEU	4.1
53	1v	13	A	4.1
38	1g	79	ARG	4.1
56	2y	52	G	4.0
56	2y	45	U	4.0
45	2n	29	ARG	4.0
54	2w	73	A	4.0
26	24	66	SER	4.0
40	2i	86	VAL	4.0
46	2o	60	VAL	4.0
17	2V	71	LEU	4.0
1	1A	2133	G	4.0
1	2A	2166	G	4.0
32	2a	1030(C)	G	4.0
56	1y	24	G	4.0
56	1y	56	C	4.0
56	2y	31	A	4.0
36	2e	12	LEU	4.0
56	2y	44	G	4.0
45	2n	43	CYS	4.0
38	1g	153	HIS	4.0
45	2n	36	PHE	3.9
7	2H	165	ALA	3.9
56	2y	73	A	3.9
34	1c	87	LEU	3.9
36	2e	90	VAL	3.9
33	2b	37	ASN	3.9
20	2Y	55	TYR	3.9
32	2a	1531	A	3.9
1	2A	2168	G	3.9
34	2c	178	LEU	3.9
18	1W	112	GLY	3.9
54	1w	72	C	3.9

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Mol	Chain	Res	Type	RSRZ
45	2n	50	LYS	3.8
32	1a	1257	U	3.8
56	2y	24	G	3.8
1	1A	885	C	3.8
1	1A	2143	C	3.8
1	2A	2129	C	3.8
7	2H	99	VAL	3.8
26	24	51	ASP	3.8
45	2n	53	LEU	3.8
34	2c	13	GLY	3.8
20	2Y	5	MET	3.8
1	2A	897	C	3.8
40	2i	115	GLY	3.8
56	2y	72	C	3.8
7	2H	115	VAL	3.8
40	2i	122	ALA	3.8
1	2A	2111	C	3.8
12	2Q	32	TYR	3.8
32	1a	1030(B)	C	3.8
52	2u	14	TRP	3.8
7	2H	24	VAL	3.8
6	2G	49	ASP	3.8
7	2H	29	PRO	3.8
36	1e	10	MET	3.8
1	1A	1064	C	3.8
1	1A	2111	C	3.8
40	2i	128	ARG	3.8
56	1y	15	G	3.8
56	2y	58	A	3.8
36	2e	125	SER	3.8
44	2m	124	PRO	3.8
41	2j	67	THR	3.7
56	2y	12	U	3.7
56	2y	59	U	3.7
41	2j	66	ARG	3.7
1	2A	2153	G	3.7
43	2l	64	TYR	3.7
50	2s	13	ASP	3.7
56	2y	68	C	3.7
40	2i	90	PRO	3.7
40	2i	8	GLY	3.7
41	2j	47	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	1A	2169	A	3.7
1	2A	896	A	3.7
1	2A	2109	U	3.7
1	1A	2803	C	3.7
3	1D	2	ALA	3.7
56	1y	69	G	3.7
45	1n	7	ILE	3.6
38	1g	82	GLY	3.6
33	2b	232	PRO	3.6
1	1A	2112	G	3.6
32	1a	1030(A)	G	3.6
33	2b	216	SER	3.6
17	2V	72	VAL	3.6
41	2j	15	THR	3.6
1	2A	2148	G	3.6
32	2a	1032	G	3.6
1	1A	2146	C	3.6
7	2H	72	ILE	3.6
48	1q	36	ILE	3.6
1	2A	1026	U	3.6
35	1d	138	TYR	3.6
12	2Q	109	VAL	3.6
38	2g	83	ALA	3.6
56	1y	58	A	3.6
1	1A	2160	G	3.6
16	2U	115	ALA	3.6
33	2b	127	ILE	3.6
56	1y	21	A	3.6
14	2S	58	LEU	3.6
1	1A	2162	G	3.6
1	1A	887	A	3.5
1	1A	897	C	3.5
1	2A	2179	C	3.5
3	2D	38	LYS	3.5
32	2a	1033	G	3.5
7	2H	19	VAL	3.5
29	27	1	MET	3.5
1	1A	2805	G	3.5
1	2A	881	G	3.5
32	2a	1001(A)	G	3.5
32	2a	1031	G	3.5
56	1y	53	G	3.5

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Mol	Chain	Res	Type	RSRZ
56	1y	57	G	3.5
36	2e	84	PHE	3.5
38	1g	4	ARG	3.5
7	2H	16	SER	3.5
15	2T	111	ARG	3.5
43	2l	14	GLY	3.5
38	2g	156	TRP	3.5
29	27	45	ALA	3.5
35	2d	117	ALA	3.5
51	1t	18	GLN	3.5
40	2i	78	LYS	3.5
1	1A	2139	C	3.4
56	1y	3	C	3.4
56	2y	51	U	3.4
40	2i	61	ALA	3.4
50	2s	84	GLY	3.4
1	1A	2152	G	3.4
7	2H	159	GLU	3.4
56	2y	25	C	3.4
32	1a	841	U	3.4
32	1a	1531	A	3.4
34	2c	160	ALA	3.4
45	2n	46	GLU	3.4
19	2X	92	LEU	3.4
34	2c	159	GLY	3.4
38	2g	40	ALA	3.4
1	2A	1041	C	3.4
11	2P	39	LYS	3.4
45	2n	12	ARG	3.4
23	2l	98	LEU	3.4
40	2i	111	ARG	3.4
1	1A	2158	A	3.4
1	2A	2162	G	3.4
50	2s	12	ASP	3.4
56	1y	62	C	3.4
21	2Z	96	VAL	3.4
40	1i	77	ILE	3.4
56	1y	23	A	3.4
32	1a	1029	C	3.4
40	1i	65	VAL	3.4
7	2H	141	VAL	3.3
33	1b	229	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
56	2y	48	C	3.3
34	2c	154	SER	3.3
56	2y	70	G	3.3
56	1y	14	A	3.3
32	1a	204	U	3.3
27	15	60	VAL	3.3
29	27	48	LYS	3.3
39	2h	122	ARG	3.3
43	2l	39	VAL	3.3
45	2n	31	ARG	3.3
43	2l	60	LEU	3.3
40	2i	52	ALA	3.3
40	2i	73	GLN	3.3
40	2i	103	THR	3.3
1	1A	2165	G	3.3
1	1A	2792	G	3.3
1	2A	2792	G	3.3
23	11	98	LEU	3.3
33	2b	29	ALA	3.3
50	2s	79	THR	3.3
1	1A	888	C	3.3
1	1A	2129	C	3.3
1	2A	2119	A	3.3
32	1a	1028	C	3.3
50	2s	30	LEU	3.2
7	2H	121	ILE	3.2
1	1A	886	C	3.2
21	1Z	165	VAL	3.2
40	1i	117	HIS	3.2
38	2g	27	ILE	3.2
50	2s	31	ILE	3.2
54	2w	4	C	3.2
21	1Z	141	VAL	3.2
33	2b	118	LEU	3.2
45	2n	55	GLY	3.2
34	2c	100	ALA	3.2
35	2d	164	ALA	3.2
6	2G	39	ILE	3.2
1	1A	2154	G	3.2
1	2A	2170	A	3.2
32	2a	1287	A	3.2
40	2i	75	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
20	2Y	91	GLU	3.2
40	2i	126	SER	3.2
1	2A	2157	G	3.2
56	2y	30	G	3.2
1	1A	889	C	3.2
19	2X	69	TYR	3.2
40	2i	15	ALA	3.2
1	1A	2113	U	3.2
48	2q	92	ARG	3.2
40	2i	114	TYR	3.2
56	2y	49	C	3.2
1	1A	2117	A	3.2
38	2g	32	ARG	3.2
34	1c	124	ILE	3.2
56	1y	33	U	3.2
45	2n	49	HIS	3.2
34	1c	193	TYR	3.1
41	2j	85	LEU	3.2
1	2A	2104	G	3.1
56	2y	10	G	3.1
33	2b	41	ILE	3.1
1	2A	2106	G	3.1
32	2a	1034	G	3.1
7	2H	18	GLU	3.1
6	2G	29	TRP	3.1
21	2Z	152	ALA	3.1
48	2q	9	VAL	3.1
48	2q	10	VAL	3.1
33	2b	95	GLN	3.1
38	2g	154	TYR	3.1
56	2y	42	C	3.1
1	1A	2182	G	3.1
45	1n	2	ALA	3.1
51	2t	12	ALA	3.1
33	1b	233	SER	3.1
8	2I	13	GLY	3.1
32	2a	1202	G	3.1
1	2A	2189	U	3.1
56	2y	50	U	3.1
43	2l	65	GLU	3.1
1	2A	2183	C	3.1
45	2n	51	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2100	G	3.0
1	2A	2807	G	3.0
56	1y	63	G	3.0
29	17	48	LYS	3.0
16	2U	20	LEU	3.0
53	2v	13	A	3.0
39	2h	134	ILE	3.0
40	2i	33	PHE	3.0
1	1A	2153	G	3.0
19	2X	91	ALA	3.0
36	2e	123	LEU	3.0
40	2i	19	LEU	3.0
26	24	48	ARG	3.0
40	2i	27	THR	3.0
1	2A	2188	C	3.0
4	2E	196	VAL	3.0
42	1k	14	VAL	3.0
41	2j	11	PHE	3.0
48	2q	86	GLU	3.0
1	2A	2156	G	3.0
1	2A	2191	G	3.0
40	2i	13	ALA	3.0
56	1y	30	G	3.0
21	2Z	139	VAL	3.0
36	1e	96	PRO	3.0
47	2p	20	VAL	3.0
56	1y	67	C	3.0
1	1A	1095	A	3.0
41	2j	69	ASN	3.0
1	1A	2144	U	3.0
34	2c	8	ILE	3.0
21	1Z	51	ALA	3.0
51	1t	22	ARG	3.0
11	2P	45	LEU	3.0
35	2d	141	ARG	3.0
33	2b	122	PHE	2.9
18	2W	85	VAL	2.9
40	2i	105	ASP	2.9
36	1e	6	PHE	2.9
32	1a	1036	G	2.9
39	1h	39	LEU	2.9
44	2m	72	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
6	1G	146	TYR	2.9
40	1i	125	TYR	2.9
51	2t	13	LEU	2.9
11	2P	28	GLY	2.9
14	2S	32	LEU	2.9
56	1y	68	C	2.9
1	1A	2168	G	2.9
1	1A	1096	A	2.9
21	2Z	57	ILE	2.9
38	2g	30	ILE	2.9
7	2H	78	GLY	2.9
7	2H	128	PRO	2.9
45	2n	41	ARG	2.9
47	2p	58	TYR	2.9
47	1p	1	MET	2.9
1	2A	2114	A	2.9
48	2q	36	ILE	2.9
19	2X	95	LEU	2.9
40	1i	19	LEU	2.9
35	2d	68	TYR	2.9
39	2h	94	TYR	2.9
54	1w	3	C	2.9
56	2y	3	C	2.9
1	2A	2118	U	2.9
23	2l	13	ILE	2.9
32	1a	1001(A)	G	2.9
34	1c	160	ALA	2.9
40	2i	7	THR	2.9
40	2i	127	LYS	2.9
1	1A	2188	C	2.8
35	2d	180	GLY	2.8
40	2i	108	VAL	2.8
56	1y	48	C	2.8
56	1y	72	C	2.8
1	1A	1508	A	2.8
1	2A	11	G	2.8
50	2s	71	LEU	2.8
53	2v	15	A	2.8
56	2y	7	A	2.8
9	2N	98	VAL	2.8
6	2G	150	ASP	2.8
7	2H	25	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
34	1c	81	GLY	2.8
56	1y	6	G	2.8
34	2c	193	TYR	2.8
36	1e	69	VAL	2.8
22	20	45	PHE	2.8
56	2y	40	C	2.8
35	1d	111	ALA	2.8
46	2o	57	LEU	2.8
43	2l	19	ARG	2.8
45	2n	24	CYS	2.8
1	1A	2115	G	2.8
1	2A	2805	G	2.8
36	1e	51	VAL	2.8
50	2s	41	VAL	2.8
7	2H	106	THR	2.8
40	2i	17	VAL	2.8
52	1u	14	TRP	2.8
42	2k	25	TYR	2.8
1	2A	892	G	2.8
1	2A	2149	G	2.8
21	2Z	93	ASP	2.8
7	2H	98	LEU	2.8
9	2N	1	MET	2.8
40	2i	88	TYR	2.8
1	1A	2155	G	2.8
1	2A	2152	G	2.8
24	22	21	LEU	2.8
56	1y	22	G	2.8
7	2H	27	LYS	2.8
1	1A	2138	C	2.8
54	1w	4	C	2.8
52	2u	22	ARG	2.8
1	1A	2114	A	2.7
11	2P	93	GLY	2.7
33	1b	118	LEU	2.7
1	1A	2148	G	2.7
1	2A	652(E)	G	2.7
1	2A	2159	G	2.7
32	2a	80	G	2.7
54	2w	69	G	2.7
1	1A	2108	C	2.7
56	2y	13	C	2.7

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Mol	Chain	Res	Type	RSRZ
16	2U	2	PRO	2.7
45	2n	33	VAL	2.7
1	2A	2895	U	2.7
41	1j	18	ALA	2.7
48	1q	90	ILE	2.7
52	2u	21	TYR	2.7
48	2q	89	LEU	2.7
56	2y	23	A	2.7
34	2c	4	LYS	2.7
1	2A	2125	G	2.7
32	2a	1249	C	2.7
22	20	12	ASN	2.7
42	2k	76	GLY	2.7
5	2F	42	ALA	2.7
32	2a	204	U	2.7
32	2a	1150	U	2.7
34	2c	157	ILE	2.7
36	2e	58	ALA	2.7
40	2i	110	GLU	2.7
33	2b	211	ILE	2.7
19	2X	66	LEU	2.7
34	2c	23	TYR	2.7
1	1A	2170	A	2.7
1	2A	2169	A	2.7
32	2a	1030(D)	A	2.7
51	2t	38	LYS	2.7
56	2y	76	A	2.7
30	28	20	GLY	2.7
33	1b	136	VAL	2.7
1	1A	2110	G	2.7
1	2A	2190	G	2.7
32	1a	1532	U	2.7
42	1k	64	ALA	2.7
6	1G	139	LEU	2.7
25	23	15	TYR	2.7
33	2b	33	TYR	2.7
3	2D	5	LYS	2.7
1	2A	886	C	2.7
1	2A	894	C	2.7
47	1p	24	ALA	2.7
41	2j	62	HIS	2.7
45	2n	18	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
45	2n	30	ALA	2.7
35	2d	122	ARG	2.7
47	2p	74	LEU	2.7
1	2A	2151	G	2.7
36	2e	29	GLY	2.7
19	2X	1	MET	2.7
7	2H	113	VAL	2.6
32	2a	202	U	2.6
39	2h	39	LEU	2.6
33	2b	92	TYR	2.6
45	2n	14	PRO	2.6
52	2u	23	PRO	2.6
1	1A	2147	G	2.6
33	2b	81	VAL	2.6
34	1c	41	GLY	2.6
35	2d	196	LEU	2.6
36	2e	131	ILE	2.6
41	2j	38	ILE	2.6
56	2y	41	C	2.6
7	2H	125	VAL	2.6
41	2j	20	ALA	2.6
4	2E	130	GLY	2.6
35	1d	110	PHE	2.6
48	1q	27	PHE	2.6
40	2i	66	ARG	2.6
12	2Q	17	LEU	2.6
5	2F	81	PRO	2.6
19	2X	68	ARG	2.6
56	1y	66	U	2.6
1	1A	278	A	2.6
48	2q	39	SER	2.6
20	2Y	30	VAL	2.6
34	2c	92	ALA	2.6
48	2q	27	PHE	2.6
1	2A	652(B)	A	2.6
3	1D	276	LYS	2.6
1	1A	2161	C	2.6
46	2o	61	GLY	2.6
38	2g	5	ARG	2.6
45	2n	45	ARG	2.6
7	2H	34	GLU	2.6
48	2q	22	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
51	2t	99	LEU	2.6
43	2l	46	LYS	2.6
1	2A	2121	G	2.6
32	2a	1036	G	2.6
41	1j	62	HIS	2.6
56	1y	18	G	2.6
30	28	18	ALA	2.5
33	1b	165	VAL	2.5
41	2j	94	VAL	2.5
13	2R	67	LEU	2.5
35	1d	158	ILE	2.5
40	1i	115	GLY	2.5
1	2A	6	A	2.5
1	2A	2126	A	2.5
32	2a	1250	A	2.5
32	1a	1032	G	2.5
44	2m	122	LYS	2.5
41	2j	92	THR	2.5
6	2G	103	LEU	2.5
13	2R	65	LEU	2.5
35	2d	198	VAL	2.5
39	2h	93	VAL	2.5
47	1p	2	VAL	2.5
54	2w	45	U	2.5
33	2b	152	PHE	2.5
40	2i	54	ASP	2.5
48	2q	54	GLY	2.5
21	2Z	170	THR	2.5
30	28	10	ALA	2.5
32	2a	1286	A	2.5
34	2c	61	ALA	2.5
40	2i	87	GLN	2.5
45	2n	48	ALA	2.5
39	2h	101	PRO	2.5
36	2e	32	VAL	2.5
38	2g	6	ARG	2.5
1	1A	1063	G	2.5
1	2A	1040	C	2.5
56	2y	11	C	2.5
21	1Z	164	ALA	2.5
39	2h	58	TYR	2.5
7	2H	30	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
13	2R	111	LEU	2.5
39	2h	133	LEU	2.5
56	2y	38	A	2.5
7	2H	48	GLY	2.5
34	2c	197	GLY	2.5
1	1A	2185	C	2.5
1	2A	2105	C	2.5
41	2j	68	HIS	2.5
1	1A	2157	G	2.5
36	2e	10	MET	2.5
22	20	11	ARG	2.5
34	2c	180	ALA	2.5
39	2h	64	LYS	2.5
43	2l	13	LYS	2.5
35	1d	108	LEU	2.5
42	2k	14	VAL	2.5
43	2l	63	GLY	2.5
1	2A	2175	C	2.5
1	2A	2177	C	2.5
36	2e	20	GLN	2.5
47	2p	9	PHE	2.5
41	2j	91	PRO	2.5
36	2e	130	ASN	2.5
40	2i	125	TYR	2.5
47	1p	59	TRP	2.5
51	1t	62	LEU	2.5
50	2s	35	SER	2.5
1	1A	2135	A	2.5
21	2Z	156	LYS	2.5
32	1a	1030(D)	A	2.5
34	2c	14	ILE	2.5
41	1j	57	LYS	2.5
56	1y	64	A	2.5
33	1b	232	PRO	2.5
36	2e	120	THR	2.5
6	2G	43	LEU	2.4
20	2Y	24	VAL	2.4
44	2m	87	TYR	2.4
44	2m	120	LYS	2.4
48	1q	11	VAL	2.4
54	2w	31	A	2.4
1	2A	898	C	2.4

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Mol	Chain	Res	Type	RSRZ
32	2a	1116	C	2.4
56	1y	49	C	2.4
4	2E	148	GLY	2.4
7	2H	23	ARG	2.4
35	1d	141	ARG	2.4
1	2A	880	G	2.4
32	2a	1023	G	2.4
7	2H	44	VAL	2.4
21	2Z	126	VAL	2.4
34	2c	48	TYR	2.4
40	2i	62	TYR	2.4
7	2H	148	ILE	2.4
52	2u	13	ILE	2.4
40	2i	49	PRO	2.4
4	2E	105	THR	2.4
7	2H	96	ALA	2.4
21	2Z	141	VAL	2.4
43	2l	55	VAL	2.4
48	2q	23	VAL	2.4
1	1A	1176	G	2.4
1	2A	2120	G	2.4
11	2P	51	PHE	2.4
15	2T	110	ILE	2.4
34	2c	5	ILE	2.4
39	2h	86	ILE	2.4
33	2b	48	MET	2.4
41	2j	63	PHE	2.4
45	1n	61	TRP	2.4
45	2n	16	PHE	2.4
19	2X	22	ALA	2.4
20	2Y	65	ALA	2.4
32	1a	1286	A	2.4
38	2g	24	THR	2.4
39	2h	36	LEU	2.4
51	1t	13	LEU	2.4
6	2G	37	VAL	2.4
31	29	26	ILE	2.4
48	2q	42	TYR	2.4
1	1A	2156	G	2.4
32	2a	216	G	2.4
32	2a	1370	G	2.4
48	1q	28	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
56	2y	27	G	2.4
33	2b	16	HIS	2.4
51	1t	95	ALA	2.4
1	2A	889	C	2.4
33	1b	61	LEU	2.4
33	2b	233	SER	2.4
29	17	46	VAL	2.4
1	1A	1060	U	2.4
1	2A	2180	U	2.4
34	2c	184	TYR	2.4
39	2h	111	ILE	2.4
40	2i	5	TYR	2.4
23	21	68	PRO	2.4
1	1A	2166	G	2.4
34	2c	22	TRP	2.4
52	2u	6	ARG	2.4
38	2g	12	LEU	2.4
56	1y	7	A	2.4
56	1y	12	U	2.4
56	1y	51	U	2.4
39	2h	83	ILE	2.4
5	2F	113	ALA	2.4
36	1e	21	ALA	2.4
40	1i	119	ALA	2.4
46	2o	68	ARG	2.4
21	1Z	166	SER	2.4
1	2A	2101	G	2.3
32	2a	1220	G	2.3
56	1y	29	G	2.3
11	2P	44	GLY	2.3
30	28	7	HIS	2.3
54	2w	14	A	2.3
21	2Z	148	ASP	2.3
45	2n	13	THR	2.3
4	2E	106	GLY	2.3
7	2H	166	GLY	2.3
14	2S	54	LEU	2.3
19	2X	67	GLY	2.3
34	2c	96	GLY	2.3
20	2Y	45	VAL	2.3
31	29	16	VAL	2.3
43	2l	82	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	2A	1113	U	2.3
35	2d	134	ASP	2.3
5	2F	82	ILE	2.3
32	1a	1447	A	2.3
35	2d	70	ILE	2.3
43	2l	61	THR	2.3
15	1T	38	ASN	2.3
29	17	47	ARG	2.3
7	2H	79	VAL	2.3
39	2h	9	MET	2.3
1	1A	2174	C	2.3
1	2A	2569	G	2.3
6	2G	88	ILE	2.3
32	1a	1031	G	2.3
51	1t	9	ASN	2.3
12	2Q	86	GLY	2.3
39	2h	2	LEU	2.3
10	2O	52	VAL	2.3
41	2j	34	VAL	2.3
7	2H	145	ALA	2.3
9	2N	10	GLU	2.3
1	1A	229	A	2.3
32	2a	1002	G	2.3
32	2a	1027	C	2.3
32	2a	1226	C	2.3
41	2j	10	GLY	2.3
40	2i	4	TYR	2.3
52	2u	17	THR	2.3
20	2Y	90	LEU	2.3
42	1k	78	GLN	2.3
49	1r	85	LEU	2.3
45	1n	18	VAL	2.3
1	1A	1963	U	2.3
44	2m	64	TRP	2.3
16	2U	17	ILE	2.3
5	2F	80	ALA	2.3
40	1i	15	ALA	2.3
40	1i	126	SER	2.3
51	1t	32	ALA	2.3
35	2d	160	GLN	2.3
48	2q	7	THR	2.3
1	1A	2804	C	2.3

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Mol	Chain	Res	Type	RSRZ
32	2a	1029	C	2.3
35	1d	20	TYR	2.3
21	2Z	151	HIS	2.3
39	1h	112	LEU	2.3
53	2v	23	A	2.3
6	2G	182	LYS	2.3
33	2b	201	ILE	2.3
35	1d	164	ALA	2.3
1	2A	2896	C	2.3
34	2c	91	LEU	2.3
41	2j	71	LEU	2.3
56	1y	4	C	2.3
7	2H	95	ARG	2.2
42	1k	126	ARG	2.2
43	2l	48	PRO	2.2
48	2q	100	LYS	2.2
54	2w	5	G	2.2
56	1y	44	G	2.2
7	2H	52	VAL	2.2
34	2c	28	GLN	2.2
36	2e	17	ALA	2.2
38	2g	25	ALA	2.2
34	1c	52	LEU	2.2
41	1j	46	ARG	2.2
48	1q	31	LEU	2.2
30	28	64	TYR	2.2
54	1w	67	C	2.2
12	2Q	33	GLY	2.2
39	2h	131	GLY	2.2
32	2a	1358	U	2.2
38	2g	31	MET	2.2
7	2H	167	GLU	2.2
32	2a	1224	G	2.2
33	2b	207	ALA	2.2
33	2b	223	ILE	2.2
30	28	60	LEU	2.2
21	2Z	159	PRO	2.2
8	2I	43	ASN	2.2
7	2H	100	GLY	2.2
12	2Q	102	VAL	2.2
1	2A	2122	U	2.2
16	1U	69	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
40	2i	70	LYS	2.2
40	2i	71	SER	2.2
17	2V	70	ILE	2.2
33	2b	19	HIS	2.2
35	2d	158	ILE	2.2
39	2h	124	ALA	2.2
40	1i	121	ARG	2.2
40	2i	81	ILE	2.2
30	28	48	PHE	2.2
42	2k	87	THR	2.2
45	1n	13	THR	2.2
32	2a	1061	G	2.2
32	2a	1154	G	2.2
6	2G	3	LEU	2.2
6	2G	62	LEU	2.2
9	2N	69	GLN	2.2
21	2Z	50	GLN	2.2
30	18	60	LEU	2.2
21	2Z	147	GLY	2.2
1	2A	895	U	2.2
9	2N	46	VAL	2.2
25	23	56	VAL	2.2
36	2e	33	VAL	2.2
43	2l	15	ARG	2.2
56	1y	60	U	2.2
4	2E	132	HIS	2.2
50	2s	14	HIS	2.2
3	2D	144	ALA	2.2
38	2g	121	ALA	2.2
40	1i	45	ALA	2.2
40	2i	31	GLN	2.2
21	2Z	140	ASP	2.2
30	28	9	GLY	2.2
41	2j	90	LEU	2.2
14	2S	92	TYR	2.2
3	2D	51	VAL	2.2
55	2x	47	U	2.2
38	2g	39	ALA	2.2
21	2Z	171	ILE	2.2
41	2j	73	ASP	2.2
40	2i	80	GLY	2.2
49	1r	31	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
50	2s	15	LEU	2.2
51	2t	72	LEU	2.2
6	2G	136	ARG	2.2
11	2P	50	ARG	2.2
38	2g	4	ARG	2.2
40	2i	93	ARG	2.2
42	1k	25	TYR	2.2
56	1y	28	G	2.2
12	2Q	113	GLN	2.2
33	2b	74	LYS	2.2
47	1p	62	VAL	2.2
34	2c	149	ALA	2.2
38	2g	147	ALA	2.2
1	2A	2103	C	2.2
1	2A	2108	C	2.2
19	2X	94	GLY	2.2
23	2l	44	PRO	2.2
25	23	29	ARG	2.2
38	2g	41	ARG	2.2
42	2k	125	PHE	2.2
52	2u	10	ARG	2.2
53	1v	14	A	2.2
45	1n	32	SER	2.2
15	2T	66	VAL	2.1
34	2c	18	TRP	2.1
47	1p	7	ALA	2.1
7	2H	51	ARG	2.1
17	2V	92	THR	2.1
36	2e	13	ILE	2.1
38	1g	34	GLY	2.1
40	2i	51	ARG	2.1
39	1h	38	ILE	2.1
48	2q	33	GLY	2.1
38	2g	11	GLN	2.1
46	1o	69	TYR	2.1
1	1A	2109	U	2.1
9	2N	5	VAL	2.1
12	2Q	114	ALA	2.1
33	2b	93	VAL	2.1
34	1c	189	ALA	2.1
38	2g	82	GLY	2.1
44	2m	42	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
47	1p	48	TRP	2.1
7	2H	123	PHE	2.1
16	2U	109	LEU	2.1
22	20	62	LEU	2.1
30	28	61	LEU	2.1
56	1y	42	C	2.1
12	2Q	6	ARG	2.1
40	2i	35	GLU	2.1
9	2N	105	GLY	2.1
42	1k	76	GLY	2.1
42	1k	88	GLY	2.1
1	1A	1094	U	2.1
6	2G	73	ALA	2.1
20	2Y	13	VAL	2.1
39	1h	93	VAL	2.1
43	2l	18	VAL	2.1
21	2Z	167	PRO	2.1
40	2i	77	ILE	2.1
48	2q	59	ILE	2.1
51	1t	45	GLN	2.1
6	2G	106	LEU	2.1
8	2I	44	LEU	2.1
25	23	23	LEU	2.1
39	1h	133	LEU	2.1
1	2A	2319	G	2.1
11	2P	15	ARG	2.1
34	1c	190	ARG	2.1
52	2u	5	ASP	2.1
20	2Y	25	GLY	2.1
1	1A	1077	A	2.1
1	2A	652(A)	A	2.1
1	2A	2310	A	2.1
1	1A	2189	U	2.1
9	2N	102	ALA	2.1
18	2W	93	ALA	2.1
47	2p	7	ALA	2.1
11	2P	91	PHE	2.1
35	2d	11	LEU	2.1
33	1b	75	LYS	2.1
43	2l	29	GLY	2.1
25	23	12	PRO	2.1
32	2a	1035	A	2.1

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Mol	Chain	Res	Type	RSRZ
33	2b	136	VAL	2.1
33	2b	229	VAL	2.1
36	1e	138	ALA	2.1
36	1e	128	PRO	2.1
38	2g	9	VAL	2.1
49	1r	24	ALA	2.1
52	1u	18	TYR	2.1
7	2H	65	HIS	2.1
7	2H	88	LEU	2.1
24	22	60	LEU	2.1
36	1e	28	PHE	2.1
51	2t	73	HIS	2.1
43	2l	49	ASN	2.1
12	1Q	15	GLY	2.1
39	2h	130	GLY	2.1
32	2a	1114	C	2.1
34	2c	189	ALA	2.1
45	2n	23	ARG	2.1
49	2r	24	ALA	2.1
34	1c	86	VAL	2.1
49	2r	22	VAL	2.1
48	2q	90	ILE	2.1
3	2D	155	LEU	2.1
12	2Q	65	PHE	2.1
43	2l	32	PHE	2.1
42	1k	42	TRP	2.1
27	25	28	PRO	2.0
45	2n	54	PRO	2.0
1	2A	2897	U	2.0
20	2Y	72	VAL	2.0
28	26	5	VAL	2.0
35	1d	112	VAL	2.0
54	1w	20	U	2.0
32	2a	1117	G	2.0
34	2c	124	ILE	2.0
6	2G	120	LEU	2.0
26	24	42	PHE	2.0
39	2h	15	ASN	2.0
47	2p	60	LEU	2.0
51	2t	91	LEU	2.0
54	1w	73	A	2.0
45	2n	58	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
18	2W	92	ARG	2.0
44	2m	102	ARG	2.0
44	1m	123	ALA	2.0
1	1A	2164	C	2.0
1	2A	2172	U	2.0
21	2Z	169	GLU	2.0
40	1i	14	VAL	2.0
50	2s	19	VAL	2.0
14	2S	3	ARG	2.0
21	2Z	8	TYR	2.0
24	22	24	LEU	2.0
25	23	45	GLY	2.0
26	24	32	TYR	2.0
39	2h	71	GLY	2.0
40	2i	30	GLY	2.0
45	2n	47	LEU	2.0
52	1u	11	GLY	2.0
1	1A	2171	A	2.0
1	2A	1508	A	2.0
8	2I	85	GLU	2.0
26	24	36	CYS	2.0
45	1n	48	ALA	2.0
51	2t	77	ALA	2.0
7	2H	37	VAL	2.0
19	2X	71	GLY	2.0
21	1Z	149	SER	2.0
45	1n	56	VAL	2.0
56	1y	47	U	2.0
35	2d	73	ARG	2.0
40	1i	8	GLY	2.0
47	2p	55	ARG	2.0
50	2s	37	ARG	2.0
3	2D	37	LEU	2.0
21	2Z	91	LEU	2.0
48	2q	71	PHE	2.0
7	2H	47	GLU	2.0
1	1A	2807	G	2.0
33	2b	133	LYS	2.0
8	2I	1	MET	2.0
41	2j	39	PRO	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
56	4SU	2y	8	20/21	0.70	0.32	85,90,100,110	0
56	PSU	1y	55	20/21	0.71	0.37	81,84,96,104	0
56	7MG	1y	46	24/25	0.71	0.25	74,84,96,103	0
56	MIA	2y	37	22/30	0.72	0.48	72,83,86,92	0
56	PSU	2y	32	20/21	0.73	0.52	77,84,91,95	0
56	5MU	2y	54	21/22	0.73	0.45	77,85,91,108	0
56	5MU	1y	54	21/22	0.74	0.30	78,80,87,94	0
56	PSU	2y	55	20/21	0.76	0.39	67,85,89,96	0
56	4SU	1y	8	20/21	0.77	0.29	82,86,93,99	0
54	7MG	2w	46	24/25	0.78	0.21	69,79,92,108	0
56	7MG	2y	46	24/25	0.78	0.32	78,86,90,106	0
56	MIA	1y	37	22/30	0.79	0.35	72,77,83,92	0
54	7MG	1w	46	24/25	0.79	0.18	65,76,91,106	0
54	4SU	2w	8	20/21	0.80	0.16	74,80,90,93	0
56	PSU	2y	39	20/21	0.83	0.38	78,83,91,95	0
56	PSU	1y	32	20/21	0.84	0.33	70,78,85,94	0
56	PSU	1y	39	20/21	0.84	0.38	74,82,85,86	0
54	PSU	1w	55	20/21	0.88	0.21	53,61,68,69	0
54	PSU	2w	55	20/21	0.88	0.16	64,71,80,81	0
54	4SU	1w	8	20/21	0.89	0.18	69,76,83,84	0
32	2MG	2a	1207	24/25	0.90	0.19	66,70,73,75	0
54	PSU	2w	32	20/21	0.90	0.25	61,69,76,81	0
32	5MC	2a	967	21/22	0.90	0.19	54,63,68,70	0
43	0TD	1l	92	10/11	0.90	0.20	38,45,48,62	0
55	4SU	2x	8	20/21	0.90	0.15	61,65,72,73	0
43	0TD	2l	92	10/11	0.90	0.20	49,56,61,72	0
55	5MU	2x	54	21/22	0.91	0.26	67,71,76,79	0
54	5MU	2w	54	21/22	0.92	0.16	49,65,70,73	0
32	PSU	2a	516	20/21	0.92	0.15	55,63,67,69	0
55	PSU	1x	55	20/21	0.92	0.18	51,55,65,68	0
1	5MU	2A	1915	21/22	0.93	0.17	51,58,62,64	0
32	M2G	2a	966	25/26	0.93	0.20	54,60,72,75	0
55	PSU	2x	55	20/21	0.93	0.16	58,67,70,74	0
54	PSU	1w	32	20/21	0.93	0.17	49,58,63,64	0
54	PSU	2w	39	20/21	0.93	0.26	60,67,72,74	0
1	5MC	2A	1962	21/22	0.94	0.17	37,46,56,61	0
32	PSU	1a	516	20/21	0.94	0.17	41,47,51,52	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	0.94	0.18	44,54,59,66	0
32	7MG	2a	527	24/25	0.94	0.19	53,58,70,76	0
32	MA6	2a	1518	24/25	0.94	0.22	45,54,59,61	0
55	4SU	1x	8	20/21	0.94	0.18	52,58,63,66	0
54	MIA	2w	37	25/30	0.94	0.21	53,65,69,75	0
32	4OC	2a	1402	22/23	0.95	0.17	46,55,58,61	0
32	5MC	2a	1404	21/22	0.95	0.20	47,55,60,69	0
55	31H	2x	76	32/33	0.95	0.21	35,43,50,55	0
1	PSU	2A	1917	20/21	0.95	0.16	45,55,60,62	0
32	MA6	2a	1519	24/25	0.95	0.24	45,55,59,61	0
32	5MC	2a	1407	21/22	0.95	0.18	48,53,57,64	0
1	2MU	2A	2552	21/23	0.95	0.21	35,43,49,53	0
1	4OC	2A	1920	21/23	0.95	0.19	51,56,58,60	0
55	5MC	2x	32	21/22	0.95	0.21	57,62,69,74	0
1	PSU	2A	1911	20/21	0.95	0.17	49,53,60,62	0
1	5MU	1A	1915	21/22	0.95	0.20	35,48,55,60	0
32	5MC	2a	1400	21/22	0.95	0.24	53,59,67,70	0
32	5MC	1a	967	21/22	0.95	0.20	38,50,55,57	0
32	UR3	2a	1498	21/22	0.96	0.23	49,52,58,59	0
55	5MC	1x	32	21/22	0.96	0.19	40,45,51,56	0
32	5MC	1a	1400	21/22	0.96	0.17	39,47,50,54	0
1	PSU	2A	2605	20/21	0.96	0.18	28,37,42,43	0
32	2MG	1a	1207	24/25	0.96	0.16	44,56,63,68	0
32	MA6	1a	1519	24/25	0.96	0.23	35,39,46,48	0
54	F3N	2w	76	33/34	0.96	0.24	29,39,44,46	0
32	M2G	1a	966	25/26	0.96	0.19	44,50,56,59	0
54	PSU	1w	39	20/21	0.96	0.20	45,52,58,62	0
55	31H	1x	76	32/33	0.96	0.22	19,26,36,36	10
55	5MU	1x	54	21/22	0.96	0.17	52,60,64,66	0
1	MA6	2A	2058	24/25	0.97	0.23	30,39,45,45	0
1	OMG	2A	2251	24/25	0.97	0.20	29,36,43,46	0
32	4OC	1a	1402	22/23	0.97	0.22	37,42,47,55	0
32	5MC	1a	1404	21/22	0.97	0.17	33,41,46,47	0
54	MIA	1w	37	29/30	0.97	0.20	36,45,59,63	0
1	5MC	2A	1942	21/22	0.97	0.16	43,50,54,63	0
32	MA6	1a	1518	24/25	0.97	0.22	32,42,46,46	0
1	5MC	1A	1942	21/22	0.97	0.20	27,38,44,52	0
1	5MC	1A	1962	21/22	0.97	0.18	20,32,35,39	0
1	5MU	2A	1939	21/22	0.97	0.19	29,37,41,44	0
32	5MC	1a	1407	21/22	0.97	0.19	31,41,44,46	0
32	UR3	1a	1498	21/22	0.97	0.22	36,42,47,48	0
32	7MG	1a	527	24/25	0.97	0.19	37,44,49,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	PSU	1A	2605	20/21	0.98	0.20	23,27,30,32	0
1	PSU	1A	1917	20/21	0.98	0.19	27,43,47,48	0
1	OMG	1A	2251	24/25	0.98	0.21	20,27,31,34	0
1	PSU	1A	1911	20/21	0.98	0.20	36,43,51,51	0
1	2MU	1A	2552	21/23	0.98	0.21	19,27,29,38	0
1	2MA	2A	2503	23/24	0.98	0.20	30,35,39,41	0
1	5MU	1A	1939	21/22	0.98	0.21	18,27,34,38	0
54	F3N	1w	76	33/34	0.98	0.20	17,22,26,27	0
1	4OC	1A	1920	21/23	0.98	0.20	29,40,44,45	0
1	2MA	1A	2503	23/24	0.98	0.24	15,23,28,30	0
1	MA6	1A	2058	24/25	0.98	0.22	15,22,29,39	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1734	1/1	-0.07	0.45	88,88,88,88	0
57	MG	2a	1749	1/1	-0.05	0.25	92,92,92,92	0
57	MG	1A	4010	1/1	0.08	0.18	74,74,74,74	0
57	MG	1A	3955	1/1	0.17	0.17	54,54,54,54	0
57	MG	18	106	1/1	0.20	0.23	60,60,60,60	0
57	MG	2A	3865	1/1	0.27	0.13	62,62,62,62	0
57	MG	1A	4082	1/1	0.29	0.49	75,75,75,75	0
57	MG	1A	4049	1/1	0.31	0.19	67,67,67,67	0
57	MG	2B	218	1/1	0.35	0.43	81,81,81,81	0
57	MG	2a	1780	1/1	0.36	0.33	79,79,79,79	0
57	MG	2A	3802	1/1	0.38	0.29	73,73,73,73	0
57	MG	2a	1739	1/1	0.38	0.15	62,62,62,62	0
57	MG	1a	1818	1/1	0.42	0.29	69,69,69,69	0
57	MG	1A	4066	1/1	0.42	0.20	55,55,55,55	0
57	MG	2a	1744	1/1	0.43	0.59	79,79,79,79	0
57	MG	1A	4065	1/1	0.44	0.15	47,47,47,47	0
57	MG	2A	3606	1/1	0.45	0.11	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	3991	1/1	0.46	0.38	67,67,67,67	0
57	MG	1A	3996	1/1	0.46	0.39	70,70,70,70	0
57	MG	2a	1776	1/1	0.47	0.26	85,85,85,85	0
57	MG	1A	4000	1/1	0.47	0.09	64,64,64,64	0
57	MG	2A	3856	1/1	0.47	0.12	58,58,58,58	0
57	MG	2a	1681	1/1	0.47	0.14	64,64,64,64	0
57	MG	1A	4105	1/1	0.48	0.34	71,71,71,71	0
57	MG	1a	1778	1/1	0.48	0.38	69,69,69,69	0
57	MG	2A	3823	1/1	0.48	0.11	69,69,69,69	0
57	MG	2A	3810	1/1	0.48	0.22	71,71,71,71	0
57	MG	1A	3994	1/1	0.49	0.12	67,67,67,67	0
57	MG	1A	3965	1/1	0.49	0.15	76,76,76,76	0
57	MG	1A	3933	1/1	0.50	0.20	67,67,67,67	0
57	MG	1A	4084	1/1	0.51	0.13	55,55,55,55	0
57	MG	2G	201	1/1	0.51	0.11	61,61,61,61	0
57	MG	2a	1664	1/1	0.52	0.33	78,78,78,78	0
57	MG	2a	1807	1/1	0.52	0.16	55,55,55,55	0
57	MG	2A	3355	1/1	0.52	0.15	79,79,79,79	0
57	MG	2A	3790	1/1	0.52	0.12	76,76,76,76	0
57	MG	2a	1803	1/1	0.53	0.31	65,65,65,65	0
57	MG	1a	1782	1/1	0.53	0.14	57,57,57,57	0
57	MG	1a	1785	1/1	0.53	0.13	63,63,63,63	0
57	MG	1A	4042	1/1	0.53	0.11	67,67,67,67	0
57	MG	1A	4093	1/1	0.54	0.37	58,58,58,58	0
57	MG	1A	3936	1/1	0.55	0.13	35,35,35,35	0
57	MG	2a	1660	1/1	0.56	0.15	78,78,78,78	0
57	MG	2A	3816	1/1	0.56	0.13	61,61,61,61	0
57	MG	1A	3562	1/1	0.56	0.14	63,63,63,63	0
57	MG	2A	3891	1/1	0.56	0.17	55,55,55,55	0
57	MG	2a	1743	1/1	0.56	0.25	66,66,66,66	0
57	MG	1B	226	1/1	0.57	0.20	71,71,71,71	0
57	MG	28	103	1/1	0.57	0.09	68,68,68,68	0
57	MG	1A	3890	1/1	0.57	0.12	44,44,44,44	0
57	MG	1A	3952	1/1	0.57	0.15	49,49,49,49	0
57	MG	1a	1764	1/1	0.58	0.24	66,66,66,66	0
57	MG	2A	3822	1/1	0.58	0.16	60,60,60,60	0
57	MG	2a	1764	1/1	0.58	0.08	75,75,75,75	0
57	MG	2a	1687	1/1	0.58	0.19	65,65,65,65	0
57	MG	2A	3101	1/1	0.59	0.22	71,71,71,71	0
57	MG	1A	3968	1/1	0.59	0.12	48,48,48,48	0
57	MG	2A	3578	1/1	0.59	0.17	67,67,67,67	0
57	MG	1B	225	1/1	0.59	0.23	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	2A	3107	1/1	0.59	0.20	53,53,53,53	0
57	MG	1y	103	1/1	0.59	0.21	83,83,83,83	0
57	MG	2A	3589	1/1	0.60	0.33	66,66,66,66	0
57	MG	2A	3299	1/1	0.60	0.16	69,69,69,69	0
57	MG	1a	1773	1/1	0.60	0.09	70,70,70,70	0
57	MG	1A	3098	1/1	0.61	0.20	63,63,63,63	0
57	MG	1A	4081	1/1	0.61	0.10	44,44,44,44	0
57	MG	1A	3988	1/1	0.61	0.13	61,61,61,61	0
57	MG	2A	3868	1/1	0.62	0.18	66,66,66,66	0
57	MG	2A	3331	1/1	0.62	0.38	69,69,69,69	0
57	MG	2A	3841	1/1	0.62	0.16	50,50,50,50	0
57	MG	2A	3476	1/1	0.62	0.20	53,53,53,53	0
57	MG	2A	3544	1/1	0.62	0.13	53,53,53,53	0
57	MG	1a	1699	1/1	0.62	0.21	69,69,69,69	0
57	MG	1w	108	1/1	0.63	0.20	73,73,73,73	0
57	MG	1a	1803	1/1	0.63	0.14	72,72,72,72	0
57	MG	1G	204	1/1	0.64	0.18	60,60,60,60	0
57	MG	2A	3008	1/1	0.64	0.21	58,58,58,58	0
57	MG	2a	1609	1/1	0.64	0.13	75,75,75,75	0
57	MG	1A	3316	1/1	0.64	0.23	57,57,57,57	0
57	MG	1A	4026	1/1	0.64	0.18	60,60,60,60	0
57	MG	1a	1817	1/1	0.65	0.11	66,66,66,66	0
57	MG	2A	3863	1/1	0.65	0.55	77,77,77,77	0
57	MG	2A	3801	1/1	0.65	0.09	56,56,56,56	0
57	MG	2a	1737	1/1	0.65	0.10	57,57,57,57	0
57	MG	2A	3796	1/1	0.65	0.20	67,67,67,67	0
57	MG	2A	3314	1/1	0.66	0.20	57,57,57,57	0
57	MG	1A	3967	1/1	0.66	0.18	72,72,72,72	0
57	MG	1A	4112	1/1	0.66	0.12	33,33,33,33	0
57	MG	2A	3847	1/1	0.66	0.09	61,61,61,61	0
57	MG	2a	1829	1/1	0.66	0.15	63,63,63,63	0
57	MG	2A	3677	1/1	0.66	0.22	66,66,66,66	0
57	MG	2A	3111	1/1	0.66	0.10	67,67,67,67	0
57	MG	2A	3673	1/1	0.66	0.17	54,54,54,54	0
57	MG	1A	3059	1/1	0.67	0.22	48,48,48,48	0
57	MG	1A	3518	1/1	0.67	0.16	49,49,49,49	0
57	MG	2a	1618	1/1	0.67	0.18	68,68,68,68	0
57	MG	2a	1759	1/1	0.67	0.10	60,60,60,60	0
57	MG	2A	3813	1/1	0.67	0.17	77,77,77,77	0
57	MG	2A	3401	1/1	0.68	0.17	53,53,53,53	0
57	MG	1A	4035	1/1	0.68	0.09	36,36,36,36	0
57	MG	1d	301	1/1	0.68	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	3258	1/1	0.68	0.20	68,68,68,68	0
57	MG	1A	4121	1/1	0.68	0.23	57,57,57,57	0
57	MG	1A	3932	1/1	0.68	0.22	69,69,69,69	0
57	MG	2A	3507	1/1	0.68	0.15	66,66,66,66	0
57	MG	2A	3352	1/1	0.69	0.33	67,67,67,67	0
57	MG	1A	3934	1/1	0.69	0.10	58,58,58,58	0
57	MG	2a	1763	1/1	0.69	0.11	72,72,72,72	0
57	MG	2A	3339	1/1	0.69	0.53	67,67,67,67	0
57	MG	1A	3646	1/1	0.69	0.17	52,52,52,52	0
57	MG	1A	3857	1/1	0.69	0.13	58,58,58,58	0
57	MG	1A	3978	1/1	0.69	0.30	56,56,56,56	0
57	MG	1A	3974	1/1	0.69	0.11	41,41,41,41	0
57	MG	2A	3805	1/1	0.69	0.12	56,56,56,56	0
57	MG	2A	3402	1/1	0.69	0.33	61,61,61,61	0
57	MG	1A	3292	1/1	0.70	0.22	53,53,53,53	0
57	MG	1A	4028	1/1	0.70	0.11	69,69,69,69	0
57	MG	2a	1752	1/1	0.70	0.11	66,66,66,66	0
57	MG	2A	3853	1/1	0.70	0.14	45,45,45,45	0
57	MG	2a	1728	1/1	0.70	0.18	52,52,52,52	0
57	MG	2a	1772	1/1	0.70	0.17	66,66,66,66	0
57	MG	2A	3288	1/1	0.70	0.16	66,66,66,66	0
57	MG	1a	1772	1/1	0.70	0.12	58,58,58,58	0
57	MG	1A	3077	1/1	0.70	0.18	57,57,57,57	0
57	MG	1a	1624	1/1	0.71	0.18	58,58,58,58	0
57	MG	2B	212	1/1	0.71	0.25	74,74,74,74	0
57	MG	2A	3731	1/1	0.71	0.11	64,64,64,64	0
57	MG	2A	3654	1/1	0.71	0.12	75,75,75,75	0
57	MG	2A	3090	1/1	0.71	0.11	61,61,61,61	0
57	MG	2A	3752	1/1	0.71	0.13	51,51,51,51	0
57	MG	2a	1605	1/1	0.71	0.16	62,62,62,62	0
57	MG	1A	3810	1/1	0.71	0.15	71,71,71,71	0
57	MG	2A	3211	1/1	0.71	0.19	59,59,59,59	0
57	MG	1A	3461	1/1	0.72	0.20	61,61,61,61	0
57	MG	2A	3704	1/1	0.72	0.07	54,54,54,54	0
57	MG	2A	3533	1/1	0.72	0.13	51,51,51,51	0
57	MG	1a	1796	1/1	0.72	0.12	44,44,44,44	0
57	MG	2A	3383	1/1	0.72	0.35	65,65,65,65	0
57	MG	2a	1765	1/1	0.72	0.18	75,75,75,75	0
57	MG	1A	4048	1/1	0.72	0.20	66,66,66,66	0
57	MG	2A	3773	1/1	0.72	0.60	51,51,51,51	0
57	MG	1A	4033	1/1	0.72	0.25	50,50,50,50	0
57	MG	1A	3265	1/1	0.72	0.11	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	3864	1/1	0.72	0.15	52,52,52,52	0
57	MG	1A	4046	1/1	0.73	0.26	44,44,44,44	0
57	MG	1A	4044	1/1	0.73	0.13	74,74,74,74	0
57	MG	1A	3790	1/1	0.73	0.16	55,55,55,55	0
57	MG	2a	1615	1/1	0.73	0.19	59,59,59,59	0
57	MG	2W	202	1/1	0.73	0.43	47,47,47,47	0
57	MG	1A	3533	1/1	0.73	0.19	55,55,55,55	0
57	MG	1A	3328	1/1	0.73	0.13	43,43,43,43	0
57	MG	2a	1710	1/1	0.73	0.14	60,60,60,60	0
57	MG	1A	3615	1/1	0.73	0.23	36,36,36,36	0
57	MG	2A	3824	1/1	0.73	0.12	58,58,58,58	0
57	MG	1A	3964	1/1	0.74	0.09	59,59,59,59	0
57	MG	1A	4056	1/1	0.74	0.22	50,50,50,50	0
57	MG	2a	1620	1/1	0.74	0.23	65,65,65,65	0
57	MG	1A	3628	1/1	0.74	0.15	68,68,68,68	0
57	MG	2A	3605	1/1	0.74	0.12	72,72,72,72	0
57	MG	2A	3364	1/1	0.74	0.40	70,70,70,70	0
57	MG	2a	1838	1/1	0.74	0.08	78,78,78,78	0
57	MG	2A	3798	1/1	0.74	0.16	56,56,56,56	0
57	MG	2A	3664	1/1	0.74	0.14	59,59,59,59	0
57	MG	2V	201	1/1	0.74	0.34	66,66,66,66	0
57	MG	2A	3309	1/1	0.74	0.21	58,58,58,58	0
57	MG	2A	3228	1/1	0.74	0.21	63,63,63,63	0
57	MG	1A	4069	1/1	0.75	0.10	47,47,47,47	0
57	MG	2A	3285	1/1	0.75	0.13	64,64,64,64	0
57	MG	2A	3349	1/1	0.75	0.31	72,72,72,72	0
57	MG	1A	3855	1/1	0.75	0.21	69,69,69,69	0
57	MG	1a	1628	1/1	0.75	0.20	58,58,58,58	0
57	MG	1A	3992	1/1	0.75	0.18	46,46,46,46	0
57	MG	1a	1788	1/1	0.75	0.34	67,67,67,67	0
57	MG	1A	3820	1/1	0.75	0.20	61,61,61,61	0
57	MG	2A	3721	1/1	0.75	0.13	52,52,52,52	0
57	MG	2A	3455	1/1	0.75	0.20	63,63,63,63	0
57	MG	2r	101	1/1	0.75	0.12	61,61,61,61	0
57	MG	2X	101	1/1	0.75	0.19	65,65,65,65	0
57	MG	2a	1833	1/1	0.75	0.12	68,68,68,68	0
57	MG	2A	3833	1/1	0.75	0.28	74,74,74,74	0
57	MG	2a	1727	1/1	0.75	0.17	71,71,71,71	0
57	MG	1a	1804	1/1	0.75	0.10	52,52,52,52	0
57	MG	2a	1775	1/1	0.75	0.13	66,66,66,66	0
57	MG	2a	1724	1/1	0.75	0.18	70,70,70,70	0
57	MG	2A	3174	1/1	0.75	0.17	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	4057	1/1	0.75	0.16	61,61,61,61	0
57	MG	2j	202	1/1	0.75	0.16	69,69,69,69	0
57	MG	2A	3379	1/1	0.75	0.14	67,67,67,67	0
57	MG	2A	3417	1/1	0.75	0.22	71,71,71,71	0
57	MG	2A	3749	1/1	0.75	0.58	67,67,67,67	0
57	MG	2A	3367	1/1	0.75	0.24	63,63,63,63	0
57	MG	2A	3400	1/1	0.75	0.16	63,63,63,63	0
57	MG	1A	3963	1/1	0.76	0.22	65,65,65,65	0
57	MG	2A	3525	1/1	0.76	0.09	39,39,39,39	0
57	MG	1A	4075	1/1	0.76	0.11	52,52,52,52	0
57	MG	1A	3776	1/1	0.76	0.21	38,38,38,38	0
57	MG	2A	3220	1/1	0.76	0.20	45,45,45,45	0
57	MG	2A	3854	1/1	0.76	0.10	49,49,49,49	0
57	MG	1A	3852	1/1	0.76	0.10	50,50,50,50	0
57	MG	1A	4030	1/1	0.76	0.27	42,42,42,42	0
57	MG	2A	3323	1/1	0.76	0.29	61,61,61,61	0
57	MG	1A	3579	1/1	0.76	0.26	46,46,46,46	0
57	MG	1a	1752	1/1	0.76	0.12	58,58,58,58	0
57	MG	2A	3835	1/1	0.76	0.17	44,44,44,44	0
57	MG	2A	3017	1/1	0.76	0.12	46,46,46,46	0
57	MG	2A	3764	1/1	0.76	0.17	66,66,66,66	0
57	MG	1A	3875	1/1	0.76	0.12	51,51,51,51	0
57	MG	2j	201	1/1	0.76	0.14	65,65,65,65	0
57	MG	1A	3126	1/1	0.76	0.16	58,58,58,58	0
57	MG	2a	1760	1/1	0.76	0.10	69,69,69,69	0
57	MG	1A	3604	1/1	0.76	0.21	53,53,53,53	0
57	MG	2A	3690	1/1	0.76	0.13	52,52,52,52	0
57	MG	2A	3565	1/1	0.77	0.12	44,44,44,44	0
57	MG	2a	1670	1/1	0.77	0.15	68,68,68,68	0
57	MG	2A	3209	1/1	0.77	0.14	43,43,43,43	0
57	MG	2A	3278	1/1	0.77	0.12	71,71,71,71	0
57	MG	1A	3715	1/1	0.77	0.20	43,43,43,43	0
57	MG	2A	3612	1/1	0.77	0.12	35,35,35,35	0
57	MG	1A	4004	1/1	0.77	0.12	39,39,39,39	0
57	MG	2A	3443	1/1	0.77	0.17	59,59,59,59	0
57	MG	2A	3809	1/1	0.77	0.22	53,53,53,53	0
57	MG	2a	1801	1/1	0.77	0.14	67,67,67,67	0
57	MG	1A	3050	1/1	0.77	0.23	46,46,46,46	0
57	MG	2A	3348	1/1	0.77	0.18	67,67,67,67	0
57	MG	2a	1738	1/1	0.77	0.13	79,79,79,79	0
57	MG	2A	3830	1/1	0.77	0.13	57,57,57,57	0
57	MG	2A	3784	1/1	0.77	0.09	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	1w	103	1/1	0.77	0.12	52,52,52,52	0
57	MG	1A	3631	1/1	0.77	0.14	30,30,30,30	0
57	MG	1A	4007	1/1	0.77	0.16	37,37,37,37	0
57	MG	2a	1746	1/1	0.77	0.14	58,58,58,58	0
57	MG	1a	1668	1/1	0.77	0.19	51,51,51,51	0
57	MG	2A	3869	1/1	0.77	0.11	60,60,60,60	0
57	MG	1A	4060	1/1	0.77	0.15	46,46,46,46	0
57	MG	2B	202	1/1	0.77	0.19	58,58,58,58	0
57	MG	1a	1791	1/1	0.77	0.11	67,67,67,67	0
57	MG	2A	3696	1/1	0.77	0.10	60,60,60,60	0
57	MG	2A	3739	1/1	0.77	0.09	65,65,65,65	0
57	MG	2a	1641	1/1	0.77	0.19	64,64,64,64	0
57	MG	2A	3409	1/1	0.78	0.19	54,54,54,54	0
57	MG	1A	3551	1/1	0.78	0.18	56,56,56,56	0
57	MG	2A	3028	1/1	0.78	0.22	51,51,51,51	0
57	MG	2A	3832	1/1	0.78	0.08	46,46,46,46	0
57	MG	2B	204	1/1	0.78	0.14	72,72,72,72	0
57	MG	2A	3357	1/1	0.78	0.25	56,56,56,56	0
57	MG	2A	3343	1/1	0.78	0.16	59,59,59,59	0
57	MG	1A	3421	1/1	0.78	0.26	53,53,53,53	0
57	MG	1A	3609	1/1	0.78	0.11	45,45,45,45	0
57	MG	1A	3959	1/1	0.78	0.12	67,67,67,67	0
57	MG	2a	1799	1/1	0.78	0.18	59,59,59,59	0
57	MG	2A	3669	1/1	0.78	0.25	75,75,75,75	0
57	MG	1A	3931	1/1	0.78	0.12	63,63,63,63	0
57	MG	2a	1825	1/1	0.78	0.25	76,76,76,76	0
57	MG	2a	1740	1/1	0.78	0.13	78,78,78,78	0
57	MG	2y	105	1/1	0.78	0.25	94,94,94,94	0
57	MG	2A	3235	1/1	0.78	0.52	64,64,64,64	0
57	MG	2A	3509	1/1	0.78	0.18	53,53,53,53	0
57	MG	2A	3873	1/1	0.78	0.14	44,44,44,44	0
57	MG	2A	3495	1/1	0.78	0.40	69,69,69,69	0
57	MG	2A	3180	1/1	0.78	0.16	59,59,59,59	0
57	MG	1A	4011	1/1	0.78	0.20	49,49,49,49	0
57	MG	1a	1779	1/1	0.78	0.11	71,71,71,71	0
57	MG	1A	3291	1/1	0.78	0.22	41,41,41,41	0
57	MG	2A	3623	1/1	0.78	0.17	64,64,64,64	0
57	MG	1a	1766	1/1	0.78	0.18	52,52,52,52	0
57	MG	1a	1611	1/1	0.79	0.12	59,59,59,59	0
57	MG	2a	1773	1/1	0.79	0.11	55,55,55,55	0
57	MG	1A	3961	1/1	0.79	0.09	39,39,39,39	0
57	MG	1a	1797	1/1	0.79	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3022	1/1	0.79	0.11	69,69,69,69	0
57	MG	2A	3639	1/1	0.79	0.16	50,50,50,50	0
57	MG	2d	302	1/1	0.79	0.10	61,61,61,61	0
57	MG	2A	3265	1/1	0.79	0.18	65,65,65,65	0
57	MG	1A	3749	1/1	0.79	0.13	53,53,53,53	0
57	MG	2A	3564	1/1	0.79	0.08	35,35,35,35	0
57	MG	1A	3359	1/1	0.79	0.15	56,56,56,56	0
57	MG	1A	4001	1/1	0.79	0.23	64,64,64,64	0
57	MG	2A	3827	1/1	0.79	0.22	58,58,58,58	0
57	MG	2A	3191	1/1	0.79	0.12	68,68,68,68	0
57	MG	2A	3353	1/1	0.79	0.22	63,63,63,63	0
57	MG	1A	3971	1/1	0.79	0.14	48,48,48,48	0
57	MG	2A	3703	1/1	0.79	0.16	52,52,52,52	0
57	MG	2A	3819	1/1	0.79	0.09	51,51,51,51	0
57	MG	2A	3376	1/1	0.79	0.21	56,56,56,56	0
57	MG	1A	4051	1/1	0.79	0.10	70,70,70,70	0
57	MG	1b	302	1/1	0.79	0.10	59,59,59,59	0
57	MG	2A	3193	1/1	0.79	0.21	60,60,60,60	0
57	MG	1A	4096	1/1	0.79	0.12	48,48,48,48	0
57	MG	2A	3808	1/1	0.79	0.11	53,53,53,53	0
57	MG	1A	3205	1/1	0.79	0.24	50,50,50,50	0
57	MG	2A	3807	1/1	0.79	0.18	58,58,58,58	0
57	MG	1x	108	1/1	0.79	0.16	59,59,59,59	0
57	MG	2A	3775	1/1	0.79	0.12	66,66,66,66	0
57	MG	1A	4013	1/1	0.79	0.26	58,58,58,58	0
57	MG	1a	1736	1/1	0.79	0.09	45,45,45,45	0
57	MG	2a	1830	1/1	0.79	0.34	69,69,69,69	0
57	MG	1A	3522	1/1	0.79	0.17	65,65,65,65	0
57	MG	1a	1784	1/1	0.79	0.16	65,65,65,65	0
57	MG	2A	3260	1/1	0.79	0.39	54,54,54,54	0
57	MG	2A	3184	1/1	0.79	0.17	49,49,49,49	0
57	MG	2A	3719	1/1	0.79	0.09	53,53,53,53	0
57	MG	2A	3720	1/1	0.80	0.07	45,45,45,45	0
57	MG	2A	3530	1/1	0.80	0.41	71,71,71,71	0
57	MG	2A	3829	1/1	0.80	0.09	61,61,61,61	0
57	MG	2a	1693	1/1	0.80	0.09	57,57,57,57	0
57	MG	2A	3413	1/1	0.80	0.15	65,65,65,65	0
57	MG	2A	3453	1/1	0.80	0.15	61,61,61,61	0
57	MG	1A	3689	1/1	0.80	0.14	27,27,27,27	0
57	MG	1A	3647	1/1	0.80	0.16	44,44,44,44	0
57	MG	2A	3336	1/1	0.80	0.12	61,61,61,61	0
57	MG	2A	3377	1/1	0.80	0.36	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	2w	106	1/1	0.80	0.49	52,52,52,52	0
57	MG	1E	307	1/1	0.80	0.45	55,55,55,55	0
57	MG	2A	3517	1/1	0.80	0.09	54,54,54,54	0
57	MG	1A	4043	1/1	0.80	0.05	54,54,54,54	0
57	MG	2A	3106	1/1	0.80	0.16	64,64,64,64	0
57	MG	1A	3948	1/1	0.80	0.06	64,64,64,64	0
57	MG	2g	201	1/1	0.80	0.13	65,65,65,65	0
57	MG	2A	3344	1/1	0.80	0.16	60,60,60,60	0
57	MG	2A	3577	1/1	0.80	0.15	67,67,67,67	0
57	MG	2A	3592	1/1	0.80	0.13	42,42,42,42	0
57	MG	1Q	206	1/1	0.80	0.13	61,61,61,61	0
57	MG	1A	3353	1/1	0.80	0.32	70,70,70,70	0
57	MG	2A	3147	1/1	0.81	0.20	49,49,49,49	0
57	MG	2A	3770	1/1	0.81	0.20	62,62,62,62	0
57	MG	1A	3211	1/1	0.81	0.14	62,62,62,62	0
57	MG	1l	105	1/1	0.81	0.14	47,47,47,47	0
57	MG	1A	3808	1/1	0.81	0.14	59,59,59,59	0
57	MG	1A	3913	1/1	0.81	0.19	42,42,42,42	0
57	MG	2N	201	1/1	0.81	0.15	71,71,71,71	0
57	MG	2A	3198	1/1	0.81	0.19	60,60,60,60	0
57	MG	1A	3672	1/1	0.81	0.16	40,40,40,40	0
57	MG	1A	3311	1/1	0.81	0.14	56,56,56,56	0
57	MG	2A	3566	1/1	0.81	0.11	42,42,42,42	0
57	MG	1A	4039	1/1	0.81	0.12	45,45,45,45	0
57	MG	2y	106	1/1	0.81	0.13	67,67,67,67	0
57	MG	2B	216	1/1	0.81	0.12	60,60,60,60	0
57	MG	2A	3743	1/1	0.81	0.13	48,48,48,48	0
57	MG	2A	3717	1/1	0.81	0.30	51,51,51,51	0
57	MG	1a	1799	1/1	0.81	0.08	57,57,57,57	0
57	MG	1A	3733	1/1	0.81	0.13	53,53,53,53	0
57	MG	1A	3848	1/1	0.81	0.08	37,37,37,37	0
57	MG	2A	3290	1/1	0.81	0.36	67,67,67,67	0
57	MG	1A	3929	1/1	0.81	0.13	55,55,55,55	0
57	MG	2A	3876	1/1	0.81	0.10	49,49,49,49	0
57	MG	2a	1750	1/1	0.81	0.24	64,64,64,64	0
57	MG	2A	3756	1/1	0.81	0.13	48,48,48,48	0
57	MG	2a	1702	1/1	0.81	0.19	59,59,59,59	0
57	MG	1A	3657	1/1	0.81	0.11	66,66,66,66	0
57	MG	1a	1814	1/1	0.81	0.10	56,56,56,56	0
57	MG	13	104	1/1	0.81	0.33	55,55,55,55	0
57	MG	2A	3310	1/1	0.81	0.26	56,56,56,56	0
57	MG	2A	3758	1/1	0.81	0.17	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	2a	1621	1/1	0.81	0.11	58,58,58,58	0
57	MG	1A	4074	1/1	0.81	0.44	53,53,53,53	0
57	MG	2a	1642	1/1	0.81	0.10	64,64,64,64	0
57	MG	1A	3607	1/1	0.81	0.18	60,60,60,60	0
57	MG	1A	3417	1/1	0.82	0.19	45,45,45,45	0
57	MG	2a	1735	1/1	0.82	0.09	65,65,65,65	0
57	MG	2a	1611	1/1	0.82	0.15	65,65,65,65	0
57	MG	2A	3240	1/1	0.82	0.18	47,47,47,47	0
57	MG	2A	3442	1/1	0.82	0.33	70,70,70,70	0
57	MG	1A	3570	1/1	0.82	0.27	71,71,71,71	0
57	MG	1A	3816	1/1	0.82	0.19	45,45,45,45	0
57	MG	1a	1793	1/1	0.82	0.10	53,53,53,53	0
57	MG	1A	3336	1/1	0.82	0.18	57,57,57,57	0
57	MG	2A	3741	1/1	0.82	0.18	49,49,49,49	0
57	MG	1A	3920	1/1	0.82	0.15	66,66,66,66	0
57	MG	1A	3937	1/1	0.82	0.14	56,56,56,56	0
57	MG	2D	304	1/1	0.82	0.15	59,59,59,59	0
57	MG	2A	3890	1/1	0.82	0.13	46,46,46,46	0
57	MG	2a	1771	1/1	0.82	0.13	59,59,59,59	0
57	MG	2A	3296	1/1	0.82	0.13	69,69,69,69	0
57	MG	2A	3387	1/1	0.82	0.15	60,60,60,60	0
57	MG	1v	101	1/1	0.82	0.12	67,67,67,67	0
57	MG	2A	3710	1/1	0.82	0.14	62,62,62,62	0
57	MG	2a	1778	1/1	0.82	0.10	64,64,64,64	0
57	MG	1A	3798	1/1	0.82	0.18	75,75,75,75	0
57	MG	2A	3414	1/1	0.82	0.10	64,64,64,64	0
57	MG	2A	3298	1/1	0.82	0.09	58,58,58,58	0
57	MG	1A	3453	1/1	0.82	0.20	45,45,45,45	0
57	MG	1a	1794	1/1	0.82	0.17	58,58,58,58	0
57	MG	1m	3002	1/1	0.82	0.10	63,63,63,63	0
57	MG	2A	3751	1/1	0.82	0.16	67,67,67,67	0
57	MG	1A	3954	1/1	0.82	0.10	55,55,55,55	0
57	MG	2A	3256	1/1	0.82	0.25	62,62,62,62	0
57	MG	1A	3960	1/1	0.82	0.09	49,49,49,49	0
57	MG	1G	203	1/1	0.82	0.12	60,60,60,60	0
57	MG	2A	3791	1/1	0.82	0.28	72,72,72,72	0
57	MG	1a	1716	1/1	0.82	0.18	38,38,38,38	0
57	MG	1a	1768	1/1	0.82	0.12	65,65,65,65	0
57	MG	1a	1601	1/1	0.82	0.13	54,54,54,54	0
57	MG	2w	102	1/1	0.82	0.10	73,73,73,73	0
57	MG	2a	1662	1/1	0.82	0.20	50,50,50,50	0
57	MG	2A	3534	1/1	0.82	0.15	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	1a	1812	1/1	0.82	0.12	60,60,60,60	0
57	MG	1x	103	1/1	0.82	0.31	59,59,59,59	0
57	MG	1A	3332	1/1	0.82	0.24	60,60,60,60	0
57	MG	2A	3857	1/1	0.82	0.15	43,43,43,43	0
57	MG	2A	3170	1/1	0.82	0.24	64,64,64,64	0
57	MG	2A	3836	1/1	0.83	0.09	53,53,53,53	0
57	MG	1A	3329	1/1	0.83	0.17	43,43,43,43	0
57	MG	2A	3279	1/1	0.83	0.15	58,58,58,58	0
57	MG	1A	3189	1/1	0.83	0.19	54,54,54,54	0
57	MG	2A	3846	1/1	0.83	0.14	40,40,40,40	0
57	MG	1B	227	1/1	0.83	0.18	59,59,59,59	0
57	MG	1A	3914	1/1	0.83	0.31	33,33,33,33	0
57	MG	2a	1698	1/1	0.83	0.10	59,59,59,59	0
57	MG	1a	1636	1/1	0.83	0.15	46,46,46,46	0
57	MG	1A	3242	1/1	0.83	0.22	59,59,59,59	0
57	MG	2A	3618	1/1	0.83	0.11	61,61,61,61	0
57	MG	2A	3164	1/1	0.83	0.12	60,60,60,60	0
57	MG	1a	1749	1/1	0.83	0.15	48,48,48,48	0
57	MG	2A	3748	1/1	0.83	0.15	57,57,57,57	0
57	MG	1E	310	1/1	0.83	0.16	58,58,58,58	0
57	MG	2a	1767	1/1	0.83	0.10	58,58,58,58	0
57	MG	2a	1684	1/1	0.83	0.12	56,56,56,56	0
57	MG	2A	3257	1/1	0.83	0.22	59,59,59,59	0
57	MG	1A	3499	1/1	0.83	0.17	52,52,52,52	0
57	MG	1A	3539	1/1	0.83	0.17	53,53,53,53	0
57	MG	2A	3325	1/1	0.83	0.18	52,52,52,52	0
57	MG	2a	1822	1/1	0.83	0.18	65,65,65,65	0
57	MG	1A	4097	1/1	0.83	0.09	36,36,36,36	0
57	MG	2A	3699	1/1	0.83	0.27	83,83,83,83	0
57	MG	1A	3759	1/1	0.83	0.16	66,66,66,66	0
57	MG	1A	4040	1/1	0.83	0.35	59,59,59,59	0
57	MG	2A	3811	1/1	0.83	0.30	55,55,55,55	0
57	MG	1A	3430	1/1	0.83	0.50	56,56,56,56	0
57	MG	1A	3115	1/1	0.83	0.26	46,46,46,46	0
57	MG	2A	3295	1/1	0.83	0.54	66,66,66,66	0
57	MG	2a	1613	1/1	0.83	0.14	53,53,53,53	0
57	MG	1A	3678	1/1	0.83	0.14	46,46,46,46	0
57	MG	2a	1639	1/1	0.83	0.17	53,53,53,53	0
57	MG	2A	3599	1/1	0.83	0.15	34,34,34,34	0
57	MG	2A	3645	1/1	0.83	0.70	66,66,66,66	0
57	MG	1a	1678	1/1	0.83	0.32	55,55,55,55	0
57	MG	2a	1713	1/1	0.83	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	ZN	24	501	1/1	0.83	0.07	108,108,108,108	0
57	MG	2A	3551	1/1	0.83	0.17	55,55,55,55	0
57	MG	2A	3115	1/1	0.83	0.23	65,65,65,65	0
57	MG	2A	3858	1/1	0.83	0.15	33,33,33,33	0
57	MG	1A	3884	1/1	0.83	0.35	58,58,58,58	0
57	MG	2A	3239	1/1	0.83	0.34	40,40,40,40	0
57	MG	1a	1787	1/1	0.83	0.11	59,59,59,59	0
57	MG	1A	3972	1/1	0.83	0.09	58,58,58,58	0
57	MG	2A	3735	1/1	0.83	0.21	56,56,56,56	0
57	MG	1x	101	1/1	0.83	0.14	22,22,22,22	0
57	MG	1A	3935	1/1	0.83	0.12	26,26,26,26	0
57	MG	2A	3615	1/1	0.83	0.13	40,40,40,40	0
57	MG	1a	1810	1/1	0.83	0.13	57,57,57,57	0
57	MG	2A	3655	1/1	0.83	0.28	52,52,52,52	0
57	MG	2A	3814	1/1	0.83	0.19	73,73,73,73	0
57	MG	1A	3370	1/1	0.83	0.20	67,67,67,67	0
57	MG	1A	3789	1/1	0.83	0.10	54,54,54,54	0
57	MG	2A	3372	1/1	0.83	0.19	60,60,60,60	0
57	MG	2A	3667	1/1	0.83	0.10	48,48,48,48	0
57	MG	2A	3882	1/1	0.83	0.19	64,64,64,64	0
57	MG	2A	3515	1/1	0.84	0.08	57,57,57,57	0
57	MG	1a	1705	1/1	0.84	0.16	60,60,60,60	0
57	MG	1A	3308	1/1	0.84	0.23	51,51,51,51	0
57	MG	2A	3085	1/1	0.84	0.12	57,57,57,57	0
57	MG	2A	3047	1/1	0.84	0.19	57,57,57,57	0
57	MG	2a	1705	1/1	0.84	0.10	61,61,61,61	0
57	MG	2A	3435	1/1	0.84	0.19	57,57,57,57	0
57	MG	1A	3853	1/1	0.84	0.18	47,47,47,47	0
57	MG	1A	3856	1/1	0.84	0.12	53,53,53,53	0
57	MG	1A	3854	1/1	0.84	0.15	57,57,57,57	0
57	MG	2A	3695	1/1	0.84	0.17	75,75,75,75	0
57	MG	2A	3073	1/1	0.84	0.08	50,50,50,50	0
57	MG	2A	3179	1/1	0.84	0.09	47,47,47,47	0
57	MG	2a	1646	1/1	0.84	0.12	63,63,63,63	0
57	MG	2A	3563	1/1	0.84	0.12	39,39,39,39	0
57	MG	1a	1709	1/1	0.84	0.30	54,54,54,54	0
57	MG	1A	3688	1/1	0.84	0.17	43,43,43,43	0
57	MG	1x	106	1/1	0.84	0.11	61,61,61,61	0
57	MG	1a	1603	1/1	0.84	0.12	56,56,56,56	0
57	MG	2A	3817	1/1	0.84	0.38	65,65,65,65	0
57	MG	2A	3465	1/1	0.84	0.20	49,49,49,49	0
57	MG	1a	1735	1/1	0.84	0.09	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	1A	3813	1/1	0.84	0.06	49,49,49,49	0
57	MG	2A	3718	1/1	0.84	0.15	49,49,49,49	0
57	MG	1a	1808	1/1	0.84	0.07	64,64,64,64	0
57	MG	1A	4055	1/1	0.84	0.12	44,44,44,44	0
57	MG	1a	1623	1/1	0.84	0.28	55,55,55,55	0
57	MG	2E	304	1/1	0.84	0.14	37,37,37,37	0
57	MG	2A	3797	1/1	0.84	0.08	58,58,58,58	0
57	MG	12	102	1/1	0.84	0.24	46,46,46,46	0
57	MG	1A	3294	1/1	0.84	0.18	50,50,50,50	0
57	MG	1A	3606	1/1	0.84	0.20	58,58,58,58	0
57	MG	1A	3393	1/1	0.84	0.16	51,51,51,51	0
57	MG	1A	3671	1/1	0.84	0.13	46,46,46,46	0
57	MG	1A	3170	1/1	0.84	0.14	41,41,41,41	0
57	MG	2x	104	1/1	0.84	0.16	56,56,56,56	0
57	MG	1A	4018	1/1	0.84	0.13	42,42,42,42	0
57	MG	18	103	1/1	0.84	0.36	50,50,50,50	0
57	MG	1A	3313	1/1	0.84	0.22	54,54,54,54	0
57	MG	1A	3082	1/1	0.84	0.37	29,29,29,29	0
57	MG	1A	3124	1/1	0.84	0.32	50,50,50,50	0
57	MG	2a	1602	1/1	0.84	0.41	77,77,77,77	0
57	MG	1a	1674	1/1	0.84	0.19	56,56,56,56	0
57	MG	1A	3338	1/1	0.84	0.16	47,47,47,47	0
57	MG	1A	3269	1/1	0.84	0.35	48,48,48,48	0
57	MG	1A	3162	1/1	0.84	0.23	36,36,36,36	0
57	MG	2A	3678	1/1	0.84	0.17	52,52,52,52	0
57	MG	1A	3500	1/1	0.84	0.21	54,54,54,54	0
57	MG	1A	4012	1/1	0.84	0.35	51,51,51,51	0
57	MG	2B	217	1/1	0.84	0.37	77,77,77,77	0
57	MG	1A	3705	1/1	0.84	0.17	33,33,33,33	0
57	MG	2A	3560	1/1	0.85	0.12	40,40,40,40	0
57	MG	1a	1748	1/1	0.85	0.13	68,68,68,68	0
57	MG	2a	1682	1/1	0.85	0.15	62,62,62,62	0
57	MG	2A	3553	1/1	0.85	0.10	48,48,48,48	0
57	MG	2A	3305	1/1	0.85	0.24	62,62,62,62	0
57	MG	1A	3470	1/1	0.85	0.28	51,51,51,51	0
57	MG	1A	4111	1/1	0.85	0.20	24,24,24,24	0
57	MG	1A	3665	1/1	0.85	0.14	54,54,54,54	0
57	MG	1a	1634	1/1	0.85	0.33	57,57,57,57	0
57	MG	2y	104	1/1	0.85	0.22	67,67,67,67	0
57	MG	1l	201	1/1	0.85	0.15	60,60,60,60	0
57	MG	1A	4009	1/1	0.85	0.06	73,73,73,73	0
57	MG	2A	3307	1/1	0.85	0.11	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	3033	1/1	0.85	0.11	47,47,47,47	0
57	MG	1a	1657	1/1	0.85	0.27	56,56,56,56	0
57	MG	2A	3571	1/1	0.85	0.16	43,43,43,43	0
57	MG	1A	3750	1/1	0.85	0.18	28,28,28,28	0
57	MG	2A	3795	1/1	0.85	0.46	68,68,68,68	0
57	MG	2A	3087	1/1	0.85	0.13	63,63,63,63	0
57	MG	2a	1770	1/1	0.85	0.06	72,72,72,72	0
57	MG	2A	3294	1/1	0.85	0.10	57,57,57,57	0
57	MG	2A	3397	1/1	0.85	0.14	68,68,68,68	0
57	MG	2A	3131	1/1	0.85	0.11	47,47,47,47	0
57	MG	2a	1748	1/1	0.85	0.09	59,59,59,59	0
57	MG	1a	1809	1/1	0.85	0.20	65,65,65,65	0
57	MG	2A	3322	1/1	0.85	0.21	58,58,58,58	0
57	MG	2A	3036	1/1	0.85	0.28	47,47,47,47	0
57	MG	1A	3027	1/1	0.85	0.07	68,68,68,68	0
57	MG	10	107	1/1	0.85	0.19	59,59,59,59	0
57	MG	2A	3067	1/1	0.85	0.17	49,49,49,49	0
57	MG	2a	1607	1/1	0.85	0.12	56,56,56,56	0
57	MG	1a	1680	1/1	0.85	0.12	44,44,44,44	0
57	MG	1A	4072	1/1	0.85	0.20	38,38,38,38	0
57	MG	1A	3320	1/1	0.85	0.17	27,27,27,27	0
57	MG	1A	3685	1/1	0.85	0.15	24,24,24,24	0
57	MG	1A	3091	1/1	0.85	0.09	68,68,68,68	0
57	MG	1A	3698	1/1	0.85	0.19	28,28,28,28	0
57	MG	2A	3072	1/1	0.85	0.13	41,41,41,41	0
57	MG	10	102	1/1	0.85	0.25	46,46,46,46	0
57	MG	2E	305	1/1	0.85	0.16	62,62,62,62	0
57	MG	2a	1626	1/1	0.85	0.42	51,51,51,51	0
57	MG	1A	4027	1/1	0.85	0.17	61,61,61,61	0
57	MG	2A	3014	1/1	0.85	0.11	41,41,41,41	0
57	MG	2A	3386	1/1	0.85	0.10	57,57,57,57	0
57	MG	1A	3714	1/1	0.85	0.20	32,32,32,32	0
57	MG	2A	3693	1/1	0.85	0.08	58,58,58,58	0
57	MG	2A	3683	1/1	0.85	0.14	62,62,62,62	0
57	MG	2A	3005	1/1	0.85	0.26	52,52,52,52	0
57	MG	2A	3557	1/1	0.85	0.21	45,45,45,45	0
57	MG	1B	232	1/1	0.85	0.15	67,67,67,67	0
57	MG	1A	3087	1/1	0.85	0.25	35,35,35,35	0
57	MG	1A	3287	1/1	0.85	0.23	48,48,48,48	0
57	MG	1A	3494	1/1	0.85	0.19	48,48,48,48	0
57	MG	2A	3213	1/1	0.85	0.15	45,45,45,45	0
57	MG	1a	1646	1/1	0.85	0.12	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	2x	105	1/1	0.85	0.15	52,52,52,52	0
57	MG	2A	3229	1/1	0.85	0.19	60,60,60,60	0
57	MG	2a	1655	1/1	0.85	0.20	58,58,58,58	0
57	MG	1A	3257	1/1	0.85	0.26	42,42,42,42	0
57	MG	1a	1702	1/1	0.85	0.21	55,55,55,55	0
57	MG	2A	3886	1/1	0.85	0.22	50,50,50,50	0
57	MG	2A	3711	1/1	0.85	0.14	44,44,44,44	0
57	MG	1A	4058	1/1	0.85	0.32	42,42,42,42	0
57	MG	1A	4054	1/1	0.85	0.09	50,50,50,50	0
57	MG	1E	308	1/1	0.85	0.14	27,27,27,27	0
57	MG	2A	3080	1/1	0.86	0.15	57,57,57,57	0
57	MG	2A	3552	1/1	0.86	0.12	43,43,43,43	0
57	MG	1A	3337	1/1	0.86	0.24	55,55,55,55	0
57	MG	2a	1653	1/1	0.86	0.17	62,62,62,62	0
57	MG	2D	307	1/1	0.86	0.28	52,52,52,52	0
57	MG	1A	3548	1/1	0.86	0.23	57,57,57,57	0
57	MG	1a	1742	1/1	0.86	0.14	55,55,55,55	0
57	MG	2A	3630	1/1	0.86	0.12	58,58,58,58	0
57	MG	2A	3754	1/1	0.86	0.14	52,52,52,52	0
57	MG	1A	4002	1/1	0.86	0.12	47,47,47,47	0
57	MG	1A	4036	1/1	0.86	0.19	40,40,40,40	0
57	MG	2a	1731	1/1	0.86	0.14	62,62,62,62	0
57	MG	2A	3464	1/1	0.86	0.22	52,52,52,52	0
57	MG	1R	204	1/1	0.86	0.31	44,44,44,44	0
57	MG	2a	1827	1/1	0.86	0.15	57,57,57,57	0
57	MG	2A	3511	1/1	0.86	0.15	61,61,61,61	0
57	MG	1A	3550	1/1	0.86	0.17	55,55,55,55	0
57	MG	2A	3327	1/1	0.86	0.12	55,55,55,55	0
57	MG	2T	201	1/1	0.86	0.12	58,58,58,58	0
57	MG	2A	3477	1/1	0.86	0.60	57,57,57,57	0
57	MG	2A	3568	1/1	0.86	0.13	63,63,63,63	0
57	MG	1A	4094	1/1	0.86	0.10	35,35,35,35	0
57	MG	1A	3491	1/1	0.86	0.19	47,47,47,47	0
57	MG	2A	3335	1/1	0.86	0.21	60,60,60,60	0
57	MG	2a	1612	1/1	0.86	0.29	53,53,53,53	0
57	MG	2A	3318	1/1	0.86	0.20	43,43,43,43	0
57	MG	1A	4122	1/1	0.86	0.33	65,65,65,65	0
57	MG	1A	3224	1/1	0.86	0.22	34,34,34,34	0
57	MG	2A	3448	1/1	0.86	0.11	56,56,56,56	0
57	MG	2A	3550	1/1	0.86	0.22	36,36,36,36	0
57	MG	2w	104	1/1	0.86	0.10	60,60,60,60	0
57	MG	1A	3428	1/1	0.86	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3766	1/1	0.86	0.10	50,50,50,50	0
57	MG	2A	3167	1/1	0.86	0.10	49,49,49,49	0
57	MG	1S	203	1/1	0.86	0.12	62,62,62,62	0
57	MG	1A	3369	1/1	0.86	0.14	45,45,45,45	0
57	MG	1O	201	1/1	0.86	0.26	59,59,59,59	0
57	MG	2A	3463	1/1	0.86	0.14	42,42,42,42	0
57	MG	1A	3879	1/1	0.86	0.10	36,36,36,36	0
57	MG	1A	3368	1/1	0.86	0.15	32,32,32,32	0
57	MG	2A	3671	1/1	0.86	0.15	62,62,62,62	0
57	MG	2A	3716	1/1	0.86	0.28	65,65,65,65	0
57	MG	1A	3756	1/1	0.86	0.15	44,44,44,44	0
57	MG	2a	1806	1/1	0.86	0.12	69,69,69,69	0
57	MG	1A	3406	1/1	0.86	0.15	35,35,35,35	0
57	MG	2A	3062	1/1	0.86	0.12	58,58,58,58	0
57	MG	2A	3834	1/1	0.86	0.10	47,47,47,47	0
57	MG	1A	3869	1/1	0.86	0.12	45,45,45,45	0
57	MG	1A	3433	1/1	0.86	0.20	41,41,41,41	0
57	MG	1A	3333	1/1	0.86	0.23	43,43,43,43	0
57	MG	1A	3674	1/1	0.86	0.12	38,38,38,38	0
57	MG	1A	3981	1/1	0.86	0.14	42,42,42,42	0
57	MG	1A	3700	1/1	0.86	0.17	29,29,29,29	0
57	MG	1A	4061	1/1	0.86	0.21	51,51,51,51	0
57	MG	1A	3905	1/1	0.86	0.12	50,50,50,50	0
57	MG	1A	3095	1/1	0.86	0.17	42,42,42,42	0
57	MG	2B	208	1/1	0.86	0.15	59,59,59,59	0
57	MG	1A	3792	1/1	0.86	0.07	67,67,67,67	0
57	MG	1a	1676	1/1	0.86	0.24	65,65,65,65	0
57	MG	2A	3723	1/1	0.86	0.11	40,40,40,40	0
57	MG	2A	3074	1/1	0.86	0.20	59,59,59,59	0
57	MG	10	106	1/1	0.86	0.09	47,47,47,47	0
57	MG	2a	1661	1/1	0.86	0.48	60,60,60,60	0
57	MG	2a	1717	1/1	0.86	0.23	50,50,50,50	0
57	MG	1A	3728	1/1	0.86	0.22	44,44,44,44	0
57	MG	1A	4095	1/1	0.86	0.23	53,53,53,53	0
57	MG	1a	1604	1/1	0.86	0.14	57,57,57,57	0
57	MG	1a	1630	1/1	0.87	0.18	47,47,47,47	0
57	MG	1B	219	1/1	0.87	0.23	57,57,57,57	0
57	MG	1y	102	1/1	0.87	0.26	73,73,73,73	0
57	MG	2A	3384	1/1	0.87	0.17	53,53,53,53	0
57	MG	10	108	1/1	0.87	0.12	42,42,42,42	0
57	MG	2A	3554	1/1	0.87	0.19	37,37,37,37	0
57	MG	1a	1781	1/1	0.87	0.18	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	3221	1/1	0.87	0.12	50,50,50,50	0
57	MG	2A	3320	1/1	0.87	0.20	49,49,49,49	0
57	MG	1a	1720	1/1	0.87	0.34	57,57,57,57	0
57	MG	2a	1630	1/1	0.87	0.21	59,59,59,59	0
57	MG	2a	1699	1/1	0.87	0.27	65,65,65,65	0
57	MG	2Z	301	1/1	0.87	0.17	70,70,70,70	0
57	MG	1A	3324	1/1	0.87	0.21	34,34,34,34	0
57	MG	2B	203	1/1	0.87	0.23	66,66,66,66	0
57	MG	2A	3040	1/1	0.87	0.14	48,48,48,48	0
57	MG	2a	1815	1/1	0.87	0.16	58,58,58,58	0
57	MG	2A	3133	1/1	0.87	0.14	66,66,66,66	0
57	MG	1A	3141	1/1	0.87	0.14	43,43,43,43	0
57	MG	2A	3138	1/1	0.87	0.21	46,46,46,46	0
57	MG	1A	3448	1/1	0.87	0.12	52,52,52,52	0
57	MG	1A	3661	1/1	0.87	0.22	40,40,40,40	0
59	ZN	2Y	501	1/1	0.87	0.07	99,99,99,99	0
57	MG	1A	3475	1/1	0.87	0.19	41,41,41,41	0
57	MG	1A	3384	1/1	0.87	0.23	54,54,54,54	0
57	MG	2a	1712	1/1	0.87	0.15	67,67,67,67	0
57	MG	1A	3677	1/1	0.87	0.18	23,23,23,23	0
57	MG	1A	3834	1/1	0.87	0.16	36,36,36,36	0
57	MG	1A	3939	1/1	0.87	0.10	52,52,52,52	0
57	MG	2a	1795	1/1	0.87	0.18	62,62,62,62	0
57	MG	2A	3326	1/1	0.87	0.22	55,55,55,55	0
57	MG	2x	103	1/1	0.87	0.13	56,56,56,56	0
57	MG	1A	3440	1/1	0.87	0.24	51,51,51,51	0
57	MG	1A	3074	1/1	0.87	0.17	53,53,53,53	0
57	MG	2A	3709	1/1	0.87	0.08	59,59,59,59	0
57	MG	2A	3650	1/1	0.87	0.13	54,54,54,54	0
57	MG	2A	3369	1/1	0.87	0.12	53,53,53,53	0
57	MG	1A	3692	1/1	0.87	0.16	40,40,40,40	0
57	MG	2v	103	1/1	0.87	0.23	63,63,63,63	0
57	MG	1a	1765	1/1	0.87	0.14	65,65,65,65	0
57	MG	2A	3818	1/1	0.87	0.13	63,63,63,63	0
57	MG	2v	101	1/1	0.87	0.22	59,59,59,59	0
57	MG	2a	1732	1/1	0.87	0.21	62,62,62,62	0
57	MG	1A	3938	1/1	0.87	0.13	54,54,54,54	0
57	MG	2B	209	1/1	0.87	0.12	61,61,61,61	0
57	MG	2A	3803	1/1	0.87	0.09	60,60,60,60	0
57	MG	2A	3821	1/1	0.87	0.10	66,66,66,66	0
57	MG	2A	3230	1/1	0.87	0.40	39,39,39,39	0
57	MG	1A	3335	1/1	0.87	0.35	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	2A	3236	1/1	0.87	0.19	50,50,50,50	0
57	MG	1a	1712	1/1	0.87	0.13	49,49,49,49	0
57	MG	2a	1715	1/1	0.87	0.17	61,61,61,61	0
57	MG	2A	3371	1/1	0.87	0.13	51,51,51,51	0
57	MG	1l	101	1/1	0.87	0.35	38,38,38,38	0
57	MG	2A	3273	1/1	0.87	0.14	46,46,46,46	0
57	MG	2A	3227	1/1	0.87	0.14	55,55,55,55	0
57	MG	2A	3539	1/1	0.87	0.16	43,43,43,43	0
57	MG	1A	3975	1/1	0.87	0.10	49,49,49,49	0
57	MG	2A	3633	1/1	0.87	0.28	54,54,54,54	0
57	MG	2A	3217	1/1	0.87	0.18	57,57,57,57	0
57	MG	2F	303	1/1	0.87	0.15	59,59,59,59	0
57	MG	1A	3161	1/1	0.87	0.10	49,49,49,49	0
57	MG	2A	3804	1/1	0.87	0.23	67,67,67,67	0
57	MG	2A	3485	1/1	0.87	0.35	59,59,59,59	0
57	MG	2A	3274	1/1	0.88	0.29	57,57,57,57	0
57	MG	2t	201	1/1	0.88	0.18	54,54,54,54	0
57	MG	1A	3796	1/1	0.88	0.13	38,38,38,38	0
57	MG	1A	3054	1/1	0.88	0.11	39,39,39,39	0
57	MG	1x	104	1/1	0.88	0.17	64,64,64,64	0
57	MG	1A	3090	1/1	0.88	0.22	26,26,26,26	0
57	MG	2a	1672	1/1	0.88	0.16	52,52,52,52	0
57	MG	1a	1629	1/1	0.88	0.32	52,52,52,52	0
57	MG	2a	1834	1/1	0.88	0.09	65,65,65,65	0
57	MG	1A	3492	1/1	0.88	0.22	34,34,34,34	0
57	MG	2a	1726	1/1	0.88	0.16	57,57,57,57	0
57	MG	1A	3763	1/1	0.88	0.12	32,32,32,32	0
57	MG	2A	3451	1/1	0.88	0.14	58,58,58,58	0
57	MG	1a	1730	1/1	0.88	0.28	49,49,49,49	0
57	MG	1A	3888	1/1	0.88	0.09	44,44,44,44	0
57	MG	1A	3590	1/1	0.88	0.28	43,43,43,43	0
57	MG	2a	1741	1/1	0.88	0.17	72,72,72,72	0
57	MG	2A	3661	1/1	0.88	0.10	53,53,53,53	0
57	MG	1A	3745	1/1	0.88	0.10	39,39,39,39	0
57	MG	1A	3233	1/1	0.88	0.37	37,37,37,37	0
57	MG	1A	3520	1/1	0.88	0.16	47,47,47,47	0
57	MG	2A	3753	1/1	0.88	0.14	64,64,64,64	0
57	MG	2A	3241	1/1	0.88	0.13	45,45,45,45	0
57	MG	1A	4050	1/1	0.88	0.12	49,49,49,49	0
57	MG	2a	1674	1/1	0.88	0.10	59,59,59,59	0
57	MG	1A	3017	1/1	0.88	0.18	59,59,59,59	0
57	MG	1A	4041	1/1	0.88	0.34	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	3553	1/1	0.88	0.12	46,46,46,46	0
57	MG	2A	3137	1/1	0.88	0.17	57,57,57,57	0
57	MG	1A	3340	1/1	0.88	0.14	52,52,52,52	0
57	MG	2A	3003	1/1	0.88	0.28	52,52,52,52	0
57	MG	1A	3206	1/1	0.88	0.14	59,59,59,59	0
57	MG	2a	1721	1/1	0.88	0.07	73,73,73,73	0
57	MG	1A	3140	1/1	0.88	0.19	56,56,56,56	0
57	MG	2A	3060	1/1	0.88	0.15	50,50,50,50	0
57	MG	1A	3910	1/1	0.88	0.18	46,46,46,46	0
57	MG	2A	3449	1/1	0.88	0.29	59,59,59,59	0
57	MG	2a	1636	1/1	0.88	0.18	72,72,72,72	0
57	MG	1A	4087	1/1	0.88	0.26	59,59,59,59	0
57	MG	1a	1727	1/1	0.88	0.26	64,64,64,64	0
57	MG	2A	3105	1/1	0.88	0.08	67,67,67,67	0
57	MG	2A	3433	1/1	0.88	0.15	55,55,55,55	0
57	MG	2B	210	1/1	0.88	0.11	65,65,65,65	0
57	MG	2a	1837	1/1	0.88	0.13	61,61,61,61	0
57	MG	1A	3357	1/1	0.88	0.17	54,54,54,54	0
57	MG	1A	3088	1/1	0.88	0.23	54,54,54,54	0
57	MG	1A	3563	1/1	0.88	0.25	58,58,58,58	0
57	MG	1a	1602	1/1	0.88	0.13	49,49,49,49	0
57	MG	1A	3836	1/1	0.88	0.13	52,52,52,52	0
57	MG	2A	3505	1/1	0.88	0.20	37,37,37,37	0
57	MG	1A	3105	1/1	0.88	0.33	30,30,30,30	0
57	MG	1A	3767	1/1	0.88	0.18	17,17,17,17	0
57	MG	1A	3360	1/1	0.88	0.14	50,50,50,50	0
57	MG	1a	1654	1/1	0.88	0.15	65,65,65,65	0
57	MG	2A	3215	1/1	0.88	0.14	63,63,63,63	0
57	MG	1A	3580	1/1	0.88	0.20	35,35,35,35	0
57	MG	1A	3216	1/1	0.88	0.18	40,40,40,40	0
57	MG	1A	3634	1/1	0.88	0.19	64,64,64,64	0
57	MG	1A	3383	1/1	0.88	0.22	42,42,42,42	0
57	MG	2A	3392	1/1	0.88	0.18	48,48,48,48	0
57	MG	1A	3376	1/1	0.88	0.16	39,39,39,39	0
57	MG	1A	3900	1/1	0.88	0.11	30,30,30,30	0
57	MG	1A	3593	1/1	0.88	0.23	50,50,50,50	0
57	MG	1a	1805	1/1	0.88	0.10	40,40,40,40	0
57	MG	1A	3582	1/1	0.88	0.21	41,41,41,41	0
57	MG	1A	3894	1/1	0.88	0.17	34,34,34,34	0
57	MG	2A	3360	1/1	0.88	0.16	61,61,61,61	0
57	MG	2A	3210	1/1	0.88	0.15	48,48,48,48	0
57	MG	2A	3321	1/1	0.88	0.18	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	3613	1/1	0.88	0.14	52,52,52,52	0
57	MG	2A	3437	1/1	0.88	0.14	39,39,39,39	0
57	MG	1A	3029	1/1	0.88	0.17	29,29,29,29	0
57	MG	1A	3982	1/1	0.88	0.15	25,25,25,25	0
57	MG	1A	3779	1/1	0.88	0.12	23,23,23,23	0
57	MG	1a	1800	1/1	0.88	0.09	59,59,59,59	0
57	MG	2A	3859	1/1	0.88	0.06	59,59,59,59	0
57	MG	2A	3224	1/1	0.88	0.17	57,57,57,57	0
57	MG	2a	1747	1/1	0.88	0.09	66,66,66,66	0
57	MG	2A	3255	1/1	0.88	0.12	60,60,60,60	0
57	MG	1A	3222	1/1	0.88	0.20	37,37,37,37	0
57	MG	2A	3195	1/1	0.88	0.10	56,56,56,56	0
57	MG	2a	1604	1/1	0.88	0.23	58,58,58,58	0
57	MG	1Y	201	1/1	0.88	0.16	40,40,40,40	0
57	MG	2A	3466	1/1	0.88	0.19	57,57,57,57	0
57	MG	1A	3228	1/1	0.88	0.14	42,42,42,42	0
57	MG	2A	3629	1/1	0.88	0.14	34,34,34,34	0
57	MG	2a	1601	1/1	0.88	0.14	61,61,61,61	0
57	MG	1F	303	1/1	0.88	0.15	37,37,37,37	0
57	MG	1B	207	1/1	0.88	0.21	51,51,51,51	0
57	MG	1A	4008	1/1	0.88	0.13	33,33,33,33	0
57	MG	1A	3881	1/1	0.88	0.19	46,46,46,46	0
57	MG	2a	1659	1/1	0.88	0.15	72,72,72,72	0
57	MG	1A	3410	1/1	0.88	0.14	57,57,57,57	0
57	MG	1A	3457	1/1	0.88	0.19	56,56,56,56	0
57	MG	1A	3505	1/1	0.88	0.11	56,56,56,56	0
57	MG	2A	3676	1/1	0.88	0.10	53,53,53,53	0
57	MG	2A	3287	1/1	0.88	0.19	64,64,64,64	0
57	MG	2A	3884	1/1	0.88	0.16	49,49,49,49	0
57	MG	1A	3006	1/1	0.88	0.34	52,52,52,52	0
57	MG	2A	3150	1/1	0.88	0.20	65,65,65,65	0
57	MG	2A	3738	1/1	0.88	0.13	43,43,43,43	0
57	MG	2A	3316	1/1	0.88	0.19	65,65,65,65	0
57	MG	1A	3516	1/1	0.88	0.18	56,56,56,56	0
57	MG	1A	3437	1/1	0.88	0.14	60,60,60,60	0
57	MG	1a	1708	1/1	0.89	0.17	61,61,61,61	0
57	MG	2A	3497	1/1	0.89	0.08	62,62,62,62	0
57	MG	2A	3385	1/1	0.89	0.13	40,40,40,40	0
57	MG	2A	3341	1/1	0.89	0.12	60,60,60,60	0
57	MG	2A	3862	1/1	0.89	0.06	52,52,52,52	0
57	MG	1x	112	1/1	0.89	0.16	46,46,46,46	0
57	MG	2A	3593	1/1	0.89	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	1a	1722	1/1	0.89	0.14	62,62,62,62	0
57	MG	2F	302	1/1	0.89	0.17	45,45,45,45	0
57	MG	2A	3282	1/1	0.89	0.15	47,47,47,47	0
57	MG	1A	3758	1/1	0.89	0.18	36,36,36,36	0
57	MG	2A	3032	1/1	0.89	0.12	45,45,45,45	0
57	MG	1A	3821	1/1	0.89	0.14	51,51,51,51	0
57	MG	15	107	1/1	0.89	0.09	53,53,53,53	0
57	MG	2A	3177	1/1	0.89	0.25	48,48,48,48	0
57	MG	2a	1716	1/1	0.89	0.15	57,57,57,57	0
57	MG	2A	3088	1/1	0.89	0.13	55,55,55,55	0
57	MG	1A	3849	1/1	0.89	0.22	57,57,57,57	0
57	MG	2A	3831	1/1	0.89	0.23	63,63,63,63	0
57	MG	1a	1777	1/1	0.89	0.08	60,60,60,60	0
57	MG	1w	106	1/1	0.89	0.21	60,60,60,60	0
57	MG	2a	1824	1/1	0.89	0.19	54,54,54,54	0
57	MG	1A	3772	1/1	0.89	0.20	26,26,26,26	0
57	MG	1a	1614	1/1	0.89	0.15	53,53,53,53	0
57	MG	1a	1763	1/1	0.89	0.14	42,42,42,42	0
57	MG	1A	3860	1/1	0.89	0.14	41,41,41,41	0
57	MG	25	105	1/1	0.89	0.13	48,48,48,48	0
57	MG	2A	3394	1/1	0.89	0.21	53,53,53,53	0
57	MG	1a	1726	1/1	0.89	0.23	57,57,57,57	0
57	MG	2A	3124	1/1	0.89	0.26	72,72,72,72	0
57	MG	2a	1808	1/1	0.89	0.14	62,62,62,62	0
57	MG	2A	3380	1/1	0.89	0.16	66,66,66,66	0
57	MG	1A	3469	1/1	0.89	0.13	58,58,58,58	0
57	MG	2A	3541	1/1	0.89	0.14	43,43,43,43	0
57	MG	1A	4032	1/1	0.89	0.12	28,28,28,28	0
57	MG	1A	4064	1/1	0.89	0.06	54,54,54,54	0
57	MG	1B	234	1/1	0.89	0.21	31,31,31,31	0
57	MG	1A	3458	1/1	0.89	0.12	38,38,38,38	0
57	MG	1A	3408	1/1	0.89	0.17	51,51,51,51	0
57	MG	2a	1624	1/1	0.89	0.19	51,51,51,51	0
57	MG	1A	3902	1/1	0.89	0.16	33,33,33,33	0
57	MG	2a	1616	1/1	0.89	0.15	51,51,51,51	0
57	MG	2A	3182	1/1	0.89	0.13	46,46,46,46	0
57	MG	2A	3403	1/1	0.89	0.10	66,66,66,66	0
57	MG	1A	3601	1/1	0.89	0.17	56,56,56,56	0
57	MG	1a	1648	1/1	0.89	0.20	46,46,46,46	0
57	MG	1A	3479	1/1	0.89	0.20	36,36,36,36	0
57	MG	1B	220	1/1	0.89	0.14	47,47,47,47	0
57	MG	2A	3631	1/1	0.89	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3805	1/1	0.89	0.19	26,26,26,26	0
57	MG	1a	1737	1/1	0.89	0.17	36,36,36,36	0
57	MG	2a	1671	1/1	0.89	0.12	57,57,57,57	0
57	MG	2A	3125	1/1	0.89	0.18	49,49,49,49	0
57	MG	1A	3619	1/1	0.89	0.17	46,46,46,46	0
57	MG	1A	3149	1/1	0.89	0.20	40,40,40,40	0
57	MG	1A	4102	1/1	0.89	0.07	59,59,59,59	0
57	MG	2A	3057	1/1	0.89	0.20	51,51,51,51	0
57	MG	1A	3186	1/1	0.89	0.46	33,33,33,33	0
57	MG	2A	3574	1/1	0.89	0.14	39,39,39,39	0
57	MG	1A	3399	1/1	0.89	0.19	34,34,34,34	0
57	MG	1A	3734	1/1	0.89	0.19	64,64,64,64	0
57	MG	1a	1645	1/1	0.89	0.13	65,65,65,65	0
57	MG	1A	3483	1/1	0.89	0.15	50,50,50,50	0
57	MG	1A	3356	1/1	0.89	0.21	43,43,43,43	0
57	MG	2A	3186	1/1	0.89	0.15	54,54,54,54	0
57	MG	1A	3918	1/1	0.89	0.14	48,48,48,48	0
57	MG	1B	203	1/1	0.89	0.20	43,43,43,43	0
57	MG	2A	3142	1/1	0.89	0.12	56,56,56,56	0
57	MG	2A	3340	1/1	0.89	0.17	55,55,55,55	0
57	MG	1A	4047	1/1	0.89	0.08	37,37,37,37	0
57	MG	2A	3472	1/1	0.89	0.59	55,55,55,55	0
57	MG	2A	3286	1/1	0.89	0.13	48,48,48,48	0
57	MG	1A	3436	1/1	0.89	0.13	60,60,60,60	0
57	MG	2A	3548	1/1	0.89	0.11	32,32,32,32	0
57	MG	1a	1687	1/1	0.89	0.32	54,54,54,54	0
57	MG	1A	3526	1/1	0.89	0.18	53,53,53,53	0
57	MG	2A	3439	1/1	0.89	0.19	56,56,56,56	0
57	MG	2A	3501	1/1	0.89	0.11	47,47,47,47	0
57	MG	1A	3402	1/1	0.89	0.24	42,42,42,42	0
57	MG	2A	3187	1/1	0.89	0.15	48,48,48,48	0
57	MG	1a	1711	1/1	0.89	0.23	60,60,60,60	0
57	MG	1A	3521	1/1	0.89	0.19	52,52,52,52	0
57	MG	2A	3828	1/1	0.89	0.06	51,51,51,51	0
57	MG	1A	3774	1/1	0.89	0.12	29,29,29,29	0
57	MG	2A	3851	1/1	0.89	0.09	59,59,59,59	0
57	MG	2a	1788	1/1	0.89	0.09	63,63,63,63	0
57	MG	2A	3653	1/1	0.89	0.11	55,55,55,55	0
57	MG	1A	3741	1/1	0.89	0.25	68,68,68,68	0
57	MG	1a	1744	1/1	0.89	0.12	67,67,67,67	0
57	MG	2a	1668	1/1	0.89	0.12	62,62,62,62	0
57	MG	2A	3503	1/1	0.89	0.10	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	3640	1/1	0.89	0.18	39,39,39,39	0
57	MG	1A	3231	1/1	0.89	0.15	55,55,55,55	0
57	MG	1A	3720	1/1	0.89	0.11	42,42,42,42	0
57	MG	1V	209	1/1	0.89	0.16	70,70,70,70	0
57	MG	2A	3611	1/1	0.89	0.08	36,36,36,36	0
57	MG	1A	3441	1/1	0.89	0.21	37,37,37,37	0
57	MG	10	101	1/1	0.89	0.15	39,39,39,39	0
57	MG	1A	4118	1/1	0.90	0.24	64,64,64,64	0
57	MG	2A	3041	1/1	0.90	0.13	44,44,44,44	0
57	MG	2a	1817	1/1	0.90	0.12	62,62,62,62	0
57	MG	2A	3861	1/1	0.90	0.08	57,57,57,57	0
57	MG	1A	3171	1/1	0.90	0.15	32,32,32,32	0
57	MG	2Q	204	1/1	0.90	0.17	54,54,54,54	0
57	MG	1A	4115	1/1	0.90	0.20	53,53,53,53	0
57	MG	1A	3285	1/1	0.90	0.44	45,45,45,45	0
57	MG	2a	1692	1/1	0.90	0.11	60,60,60,60	0
57	MG	2A	3702	1/1	0.90	0.13	64,64,64,64	0
57	MG	2A	3199	1/1	0.90	0.20	54,54,54,54	0
57	MG	1A	3252	1/1	0.90	0.13	56,56,56,56	0
57	MG	1A	3246	1/1	0.90	0.14	32,32,32,32	0
57	MG	2A	3782	1/1	0.90	0.18	52,52,52,52	0
57	MG	1A	3148	1/1	0.90	0.17	32,32,32,32	0
57	MG	1A	3452	1/1	0.90	0.15	44,44,44,44	0
57	MG	1a	1738	1/1	0.90	0.17	41,41,41,41	0
57	MG	2A	3447	1/1	0.90	0.17	59,59,59,59	0
57	MG	2A	3370	1/1	0.90	0.20	60,60,60,60	0
57	MG	1A	3735	1/1	0.90	0.12	48,48,48,48	0
57	MG	1f	201	1/1	0.90	0.26	39,39,39,39	0
57	MG	26	101	1/1	0.90	0.16	52,52,52,52	0
57	MG	2A	3291	1/1	0.90	0.14	52,52,52,52	0
57	MG	2A	3275	1/1	0.90	0.14	51,51,51,51	0
57	MG	2A	3166	1/1	0.90	0.29	64,64,64,64	0
57	MG	2A	3610	1/1	0.90	0.13	60,60,60,60	0
57	MG	1A	3478	1/1	0.90	0.16	40,40,40,40	0
57	MG	2a	1809	1/1	0.90	0.12	59,59,59,59	0
57	MG	2a	1798	1/1	0.90	0.13	69,69,69,69	0
57	MG	2a	1819	1/1	0.90	0.10	58,58,58,58	0
57	MG	1A	3377	1/1	0.90	0.16	49,49,49,49	0
57	MG	1A	4079	1/1	0.90	0.16	50,50,50,50	0
57	MG	2a	1619	1/1	0.90	0.19	65,65,65,65	0
57	MG	1A	3795	1/1	0.90	0.08	46,46,46,46	0
57	MG	1A	3260	1/1	0.90	0.13	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	1A	4067	1/1	0.90	0.18	30,30,30,30	0
57	MG	2A	3855	1/1	0.90	0.13	37,37,37,37	0
57	MG	1a	1760	1/1	0.90	0.14	60,60,60,60	0
57	MG	1a	1751	1/1	0.90	0.09	45,45,45,45	0
57	MG	1W	202	1/1	0.90	0.29	42,42,42,42	0
57	MG	2A	3324	1/1	0.90	0.11	68,68,68,68	0
57	MG	1A	3873	1/1	0.90	0.20	53,53,53,53	0
57	MG	2A	3608	1/1	0.90	0.17	50,50,50,50	0
57	MG	2a	1796	1/1	0.90	0.07	54,54,54,54	0
57	MG	2A	3046	1/1	0.90	0.15	42,42,42,42	0
57	MG	2A	3188	1/1	0.90	0.24	52,52,52,52	0
57	MG	2A	3742	1/1	0.90	0.07	59,59,59,59	0
57	MG	1A	4085	1/1	0.90	0.24	62,62,62,62	0
57	MG	2A	3837	1/1	0.90	0.15	45,45,45,45	0
57	MG	1A	3712	1/1	0.90	0.11	45,45,45,45	0
57	MG	1A	3203	1/1	0.90	0.14	55,55,55,55	0
57	MG	2A	3297	1/1	0.90	0.12	66,66,66,66	0
57	MG	1a	1776	1/1	0.90	0.13	56,56,56,56	0
57	MG	2A	3328	1/1	0.90	0.31	66,66,66,66	0
57	MG	2A	3649	1/1	0.90	0.12	39,39,39,39	0
57	MG	2A	3799	1/1	0.90	0.17	71,71,71,71	0
57	MG	1X	107	1/1	0.90	0.10	40,40,40,40	0
57	MG	2A	3153	1/1	0.90	0.17	60,60,60,60	0
57	MG	2A	3054	1/1	0.90	0.12	54,54,54,54	0
57	MG	1A	3577	1/1	0.90	0.17	35,35,35,35	0
57	MG	2a	1787	1/1	0.90	0.11	50,50,50,50	0
57	MG	1A	3559	1/1	0.90	0.14	33,33,33,33	0
57	MG	1a	1650	1/1	0.90	0.19	61,61,61,61	0
57	MG	1A	3989	1/1	0.90	0.07	61,61,61,61	0
57	MG	1A	3513	1/1	0.90	0.42	33,33,33,33	0
57	MG	2a	1745	1/1	0.90	0.15	60,60,60,60	0
57	MG	1A	3731	1/1	0.90	0.13	60,60,60,60	0
57	MG	1F	307	1/1	0.90	0.21	44,44,44,44	0
57	MG	1a	1767	1/1	0.90	0.11	45,45,45,45	0
57	MG	1A	3904	1/1	0.90	0.20	67,67,67,67	0
57	MG	1A	3015	1/1	0.90	0.21	34,34,34,34	0
57	MG	1A	3947	1/1	0.90	0.20	52,52,52,52	0
57	MG	2A	3254	1/1	0.90	0.10	55,55,55,55	0
57	MG	2A	3500	1/1	0.90	0.07	53,53,53,53	0
57	MG	2A	3197	1/1	0.90	0.23	50,50,50,50	0
57	MG	1A	3155	1/1	0.90	0.10	48,48,48,48	0
57	MG	1A	3040	1/1	0.90	0.23	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	1A	3702	1/1	0.90	0.22	20,20,20,20	0
57	MG	1a	1691	1/1	0.90	0.17	64,64,64,64	0
57	MG	2A	3470	1/1	0.90	0.28	59,59,59,59	0
57	MG	2A	3729	1/1	0.90	0.07	39,39,39,39	0
57	MG	2A	3872	1/1	0.90	0.53	59,59,59,59	0
57	MG	2A	3712	1/1	0.90	0.14	35,35,35,35	0
57	MG	2a	1623	1/1	0.90	0.14	66,66,66,66	0
57	MG	1A	3598	1/1	0.90	0.12	54,54,54,54	0
57	MG	1a	1672	1/1	0.90	0.19	52,52,52,52	0
57	MG	1Q	204	1/1	0.90	0.15	60,60,60,60	0
57	MG	2A	3482	1/1	0.90	0.11	50,50,50,50	0
57	MG	2a	1627	1/1	0.90	0.52	57,57,57,57	0
57	MG	2A	3102	1/1	0.90	0.10	48,48,48,48	0
57	MG	1A	3498	1/1	0.90	0.19	39,39,39,39	0
57	MG	1P	204	1/1	0.90	0.16	37,37,37,37	0
57	MG	1A	4021	1/1	0.90	0.15	39,39,39,39	0
57	MG	2A	3128	1/1	0.90	0.24	52,52,52,52	0
57	MG	2a	1723	1/1	0.90	0.11	69,69,69,69	0
57	MG	1A	3390	1/1	0.90	0.28	44,44,44,44	0
57	MG	2A	3066	1/1	0.90	0.11	53,53,53,53	0
57	MG	2A	3559	1/1	0.90	0.14	47,47,47,47	0
57	MG	1A	3181	1/1	0.90	0.12	59,59,59,59	0
57	MG	2A	3096	1/1	0.90	0.17	53,53,53,53	0
57	MG	2A	3781	1/1	0.90	0.15	67,67,67,67	0
57	MG	2x	102	1/1	0.90	0.17	67,67,67,67	0
57	MG	1A	3638	1/1	0.90	0.09	37,37,37,37	0
57	MG	2A	3496	1/1	0.90	0.08	59,59,59,59	0
57	MG	1A	3200	1/1	0.90	0.14	44,44,44,44	0
57	MG	1A	3993	1/1	0.90	0.09	67,67,67,67	0
57	MG	1A	4089	1/1	0.90	0.14	35,35,35,35	0
57	MG	1A	4016	1/1	0.90	0.07	51,51,51,51	0
57	MG	2A	3815	1/1	0.90	0.25	56,56,56,56	0
57	MG	1a	1696	1/1	0.90	0.23	41,41,41,41	0
57	MG	2P	201	1/1	0.90	0.14	56,56,56,56	0
57	MG	1A	3326	1/1	0.90	0.15	48,48,48,48	0
57	MG	1A	4059	1/1	0.90	0.13	24,24,24,24	0
57	MG	1A	3573	1/1	0.90	0.23	49,49,49,49	0
57	MG	2A	3777	1/1	0.90	0.13	55,55,55,55	0
57	MG	2A	3366	1/1	0.90	0.37	59,59,59,59	0
57	MG	2A	3407	1/1	0.90	0.10	53,53,53,53	0
57	MG	2A	3345	1/1	0.90	0.10	64,64,64,64	0
57	MG	1A	3534	1/1	0.90	0.20	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	3826	1/1	0.90	0.12	43,43,43,43	0
57	MG	2A	3584	1/1	0.90	0.13	53,53,53,53	0
57	MG	1A	3391	1/1	0.90	0.15	32,32,32,32	0
57	MG	2A	3242	1/1	0.90	0.13	50,50,50,50	0
57	MG	2a	1754	1/1	0.90	0.12	64,64,64,64	0
57	MG	1A	3600	1/1	0.90	0.12	70,70,70,70	0
57	MG	1A	3323	1/1	0.90	0.26	49,49,49,49	0
57	MG	2a	1756	1/1	0.90	0.19	55,55,55,55	0
57	MG	2A	3269	1/1	0.90	0.14	47,47,47,47	0
57	MG	1A	3414	1/1	0.90	0.12	49,49,49,49	0
57	MG	2A	3422	1/1	0.90	0.10	61,61,61,61	0
57	MG	2a	1706	1/1	0.90	0.07	60,60,60,60	0
57	MG	1A	3824	1/1	0.90	0.14	56,56,56,56	0
57	MG	1A	3183	1/1	0.90	0.18	40,40,40,40	0
57	MG	1A	3683	1/1	0.90	0.19	24,24,24,24	0
57	MG	2A	3098	1/1	0.90	0.18	36,36,36,36	0
57	MG	1A	3589	1/1	0.91	0.17	41,41,41,41	0
57	MG	2A	3276	1/1	0.91	0.16	56,56,56,56	0
57	MG	1A	3704	1/1	0.91	0.12	42,42,42,42	0
57	MG	2A	3418	1/1	0.91	0.13	52,52,52,52	0
57	MG	2A	3767	1/1	0.91	0.19	55,55,55,55	0
57	MG	1A	3119	1/1	0.91	0.18	30,30,30,30	0
57	MG	1a	1713	1/1	0.91	0.12	59,59,59,59	0
57	MG	2A	3252	1/1	0.91	0.13	58,58,58,58	0
57	MG	2A	3408	1/1	0.91	0.07	65,65,65,65	0
57	MG	1A	3775	1/1	0.91	0.19	37,37,37,37	0
57	MG	1A	3722	1/1	0.91	0.22	58,58,58,58	0
57	MG	1A	3544	1/1	0.91	0.12	56,56,56,56	0
57	MG	2A	3643	1/1	0.91	0.15	43,43,43,43	0
57	MG	2A	3084	1/1	0.91	0.08	52,52,52,52	0
57	MG	1A	3352	1/1	0.91	0.15	40,40,40,40	0
57	MG	1a	1662	1/1	0.91	0.19	45,45,45,45	0
57	MG	1A	3220	1/1	0.91	0.10	31,31,31,31	0
57	MG	2A	3521	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3760	1/1	0.91	0.12	49,49,49,49	0
57	MG	1a	1658	1/1	0.91	0.22	54,54,54,54	0
57	MG	1A	3109	1/1	0.91	0.16	30,30,30,30	0
57	MG	2a	1797	1/1	0.91	0.12	61,61,61,61	0
57	MG	1A	3420	1/1	0.91	0.10	41,41,41,41	0
57	MG	1W	203	1/1	0.91	0.16	39,39,39,39	0
57	MG	1R	203	1/1	0.91	0.15	26,26,26,26	0
57	MG	2a	1725	1/1	0.91	0.11	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	2y	103	1/1	0.91	0.14	64,64,64,64	0
57	MG	2a	1704	1/1	0.91	0.12	56,56,56,56	0
57	MG	1A	3984	1/1	0.91	0.11	38,38,38,38	0
57	MG	2a	1707	1/1	0.91	0.08	62,62,62,62	0
57	MG	1A	3026	1/1	0.91	0.21	42,42,42,42	0
57	MG	2A	3023	1/1	0.91	0.12	57,57,57,57	0
57	MG	1A	3327	1/1	0.91	0.23	48,48,48,48	0
57	MG	1N	202	1/1	0.91	0.15	41,41,41,41	0
57	MG	2a	1617	1/1	0.91	0.13	55,55,55,55	0
57	MG	1A	3474	1/1	0.91	0.27	54,54,54,54	0
57	MG	1a	1693	1/1	0.91	0.14	60,60,60,60	0
57	MG	2w	108	1/1	0.91	0.19	47,47,47,47	0
57	MG	1A	3467	1/1	0.91	0.10	48,48,48,48	0
57	MG	1A	3675	1/1	0.91	0.15	31,31,31,31	0
57	MG	1A	4024	1/1	0.91	0.18	32,32,32,32	0
57	MG	1A	3290	1/1	0.91	0.27	27,27,27,27	0
57	MG	1A	3255	1/1	0.91	0.16	34,34,34,34	0
57	MG	2A	3687	1/1	0.91	0.09	64,64,64,64	0
57	MG	2A	3575	1/1	0.91	0.13	40,40,40,40	0
57	MG	1A	3310	1/1	0.91	0.17	54,54,54,54	0
57	MG	1A	3746	1/1	0.91	0.11	44,44,44,44	0
57	MG	2A	3312	1/1	0.91	0.14	49,49,49,49	0
57	MG	1A	3663	1/1	0.91	0.20	39,39,39,39	0
57	MG	2A	3545	1/1	0.91	0.10	39,39,39,39	0
57	MG	2A	3617	1/1	0.91	0.43	51,51,51,51	0
57	MG	1a	1758	1/1	0.91	0.10	39,39,39,39	0
57	MG	2A	3259	1/1	0.91	0.15	52,52,52,52	0
57	MG	1A	3179	1/1	0.91	0.16	47,47,47,47	0
57	MG	1A	3710	1/1	0.91	0.14	28,28,28,28	0
57	MG	2w	103	1/1	0.91	0.16	69,69,69,69	0
57	MG	1a	1780	1/1	0.91	0.12	66,66,66,66	0
57	MG	2B	201	1/1	0.91	0.21	66,66,66,66	0
57	MG	2A	3745	1/1	0.91	0.13	60,60,60,60	0
57	MG	1A	3655	1/1	0.91	0.16	31,31,31,31	0
57	MG	1a	1813	1/1	0.91	0.08	52,52,52,52	0
57	MG	2A	3416	1/1	0.91	0.21	42,42,42,42	0
57	MG	1A	3005	1/1	0.91	0.13	37,37,37,37	0
57	MG	2x	101	1/1	0.91	0.18	51,51,51,51	0
57	MG	1A	3651	1/1	0.91	0.26	59,59,59,59	0
57	MG	1A	4005	1/1	0.91	0.24	36,36,36,36	0
57	MG	2a	1755	1/1	0.91	0.07	45,45,45,45	0
57	MG	1A	3523	1/1	0.91	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	1a	1703	1/1	0.91	0.11	51,51,51,51	0
57	MG	1A	3361	1/1	0.91	0.19	50,50,50,50	0
57	MG	1A	3633	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3086	1/1	0.91	0.14	44,44,44,44	0
57	MG	1A	3112	1/1	0.91	0.12	35,35,35,35	0
57	MG	1a	1815	1/1	0.91	0.09	48,48,48,48	0
57	MG	2a	1606	1/1	0.91	0.14	53,53,53,53	0
57	MG	2A	3613	1/1	0.91	0.13	48,48,48,48	0
57	MG	1a	1807	1/1	0.91	0.09	53,53,53,53	0
57	MG	2A	3555	1/1	0.91	0.10	50,50,50,50	0
57	MG	1a	1774	1/1	0.91	0.06	78,78,78,78	0
57	MG	1a	1625	1/1	0.91	0.25	55,55,55,55	0
57	MG	2A	3556	1/1	0.91	0.14	31,31,31,31	0
57	MG	2A	3423	1/1	0.91	0.19	57,57,57,57	0
57	MG	1a	1643	1/1	0.91	0.15	59,59,59,59	0
57	MG	2A	3468	1/1	0.91	0.12	54,54,54,54	0
57	MG	1A	3139	1/1	0.91	0.17	40,40,40,40	0
57	MG	1A	3511	1/1	0.91	0.23	55,55,55,55	0
57	MG	2A	3281	1/1	0.91	0.13	55,55,55,55	0
57	MG	2A	3146	1/1	0.91	0.14	55,55,55,55	0
57	MG	2A	3641	1/1	0.91	0.17	42,42,42,42	0
57	MG	2A	3410	1/1	0.91	0.11	65,65,65,65	0
57	MG	2a	1603	1/1	0.91	0.10	62,62,62,62	0
57	MG	1A	3472	1/1	0.91	0.23	61,61,61,61	0
57	MG	1A	3035	1/1	0.91	0.07	42,42,42,42	0
57	MG	2A	3438	1/1	0.91	0.13	42,42,42,42	0
57	MG	2A	3666	1/1	0.91	0.08	53,53,53,53	0
57	MG	1X	103	1/1	0.91	0.18	36,36,36,36	0
57	MG	2A	3030	1/1	0.91	0.18	56,56,56,56	0
57	MG	1a	1683	1/1	0.91	0.23	51,51,51,51	0
57	MG	2A	3622	1/1	0.91	0.16	34,34,34,34	0
57	MG	1A	3785	1/1	0.91	0.12	42,42,42,42	0
57	MG	2A	3037	1/1	0.91	0.14	43,43,43,43	0
57	MG	2A	3475	1/1	0.91	0.15	59,59,59,59	0
57	MG	1A	4090	1/1	0.91	0.31	65,65,65,65	0
57	MG	1A	3218	1/1	0.91	0.18	37,37,37,37	0
57	MG	1V	204	1/1	0.91	0.17	36,36,36,36	0
57	MG	2Q	202	1/1	0.91	0.22	54,54,54,54	0
57	MG	2A	3684	1/1	0.91	0.28	60,60,60,60	0
57	MG	1l	104	1/1	0.91	0.20	40,40,40,40	0
57	MG	2a	1631	1/1	0.91	0.19	66,66,66,66	0
57	MG	2A	3251	1/1	0.91	0.22	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	1A	3701	1/1	0.91	0.14	52,52,52,52	0
57	MG	1I	201	1/1	0.91	0.12	50,50,50,50	0
57	MG	1A	3396	1/1	0.91	0.23	40,40,40,40	0
57	MG	2Q	205	1/1	0.91	0.21	42,42,42,42	0
57	MG	2a	1793	1/1	0.91	0.20	47,47,47,47	0
57	MG	1A	3970	1/1	0.91	0.12	49,49,49,49	0
57	MG	1B	228	1/1	0.91	0.09	67,67,67,67	0
57	MG	2A	3620	1/1	0.91	0.15	69,69,69,69	0
57	MG	2A	3467	1/1	0.91	0.28	49,49,49,49	0
57	MG	2A	3219	1/1	0.91	0.25	59,59,59,59	0
57	MG	1A	3636	1/1	0.91	0.14	52,52,52,52	0
57	MG	1A	3861	1/1	0.91	0.17	63,63,63,63	0
57	MG	1A	3463	1/1	0.91	0.14	53,53,53,53	0
57	MG	1a	1649	1/1	0.91	0.20	58,58,58,58	0
57	MG	1A	3549	1/1	0.91	0.24	42,42,42,42	0
57	MG	1U	203	1/1	0.91	0.14	47,47,47,47	0
57	MG	1a	1816	1/1	0.91	0.11	38,38,38,38	0
57	MG	1A	3103	1/1	0.91	0.13	20,20,20,20	0
57	MG	2A	3118	1/1	0.91	0.16	47,47,47,47	0
57	MG	2A	3850	1/1	0.91	0.06	54,54,54,54	0
57	MG	2A	3330	1/1	0.91	0.09	49,49,49,49	0
57	MG	1A	3451	1/1	0.91	0.17	69,69,69,69	0
57	MG	2A	3109	1/1	0.91	0.19	47,47,47,47	0
57	MG	1A	3690	1/1	0.91	0.23	69,69,69,69	0
57	MG	1A	3819	1/1	0.91	0.22	39,39,39,39	0
57	MG	1a	1701	1/1	0.91	0.18	51,51,51,51	0
57	MG	2A	3528	1/1	0.91	0.12	59,59,59,59	0
57	MG	27	101	1/1	0.91	0.22	49,49,49,49	0
57	MG	1A	3016	1/1	0.91	0.27	53,53,53,53	0
57	MG	1A	3295	1/1	0.91	0.18	44,44,44,44	0
57	MG	1A	3866	1/1	0.91	0.11	49,49,49,49	0
57	MG	2A	3081	1/1	0.91	0.22	41,41,41,41	0
57	MG	2a	1665	1/1	0.91	0.08	61,61,61,61	0
57	MG	1A	3906	1/1	0.91	0.25	35,35,35,35	0
57	MG	2U	201	1/1	0.91	0.18	54,54,54,54	0
57	MG	1x	110	1/1	0.91	0.23	63,63,63,63	0
57	MG	1D	311	1/1	0.91	0.13	46,46,46,46	0
57	MG	2a	1652	1/1	0.91	0.14	63,63,63,63	0
57	MG	1A	3909	1/1	0.91	0.07	48,48,48,48	0
57	MG	1a	1605	1/1	0.91	0.30	56,56,56,56	0
57	MG	1A	3567	1/1	0.91	0.13	48,48,48,48	0
57	MG	2a	1835	1/1	0.91	0.29	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	1A	3566	1/1	0.91	0.17	43,43,43,43	0
57	MG	2A	3319	1/1	0.91	0.31	42,42,42,42	0
57	MG	2A	3736	1/1	0.91	0.14	45,45,45,45	0
57	MG	2A	3347	1/1	0.91	0.11	49,49,49,49	0
57	MG	2A	3432	1/1	0.91	0.23	42,42,42,42	0
57	MG	2A	3844	1/1	0.91	0.10	41,41,41,41	0
57	MG	1A	3564	1/1	0.91	0.24	42,42,42,42	0
57	MG	1A	3755	1/1	0.91	0.12	55,55,55,55	0
57	MG	2A	3866	1/1	0.91	0.11	54,54,54,54	0
57	MG	2A	3308	1/1	0.91	0.14	62,62,62,62	0
57	MG	2A	3637	1/1	0.91	0.06	47,47,47,47	0
57	MG	1A	3068	1/1	0.91	0.17	43,43,43,43	0
57	MG	1A	3135	1/1	0.91	0.13	38,38,38,38	0
57	MG	2A	3450	1/1	0.91	0.24	49,49,49,49	0
57	MG	2A	3373	1/1	0.91	0.20	64,64,64,64	0
57	MG	1x	107	1/1	0.91	0.21	44,44,44,44	0
57	MG	2A	3018	1/1	0.91	0.30	38,38,38,38	0
57	MG	1A	3067	1/1	0.91	0.14	29,29,29,29	0
57	MG	2A	3430	1/1	0.91	0.34	54,54,54,54	0
57	MG	2a	1649	1/1	0.91	0.19	63,63,63,63	0
57	MG	1A	3687	1/1	0.91	0.17	50,50,50,50	0
57	MG	1a	1761	1/1	0.92	0.09	50,50,50,50	0
57	MG	2A	3136	1/1	0.92	0.09	42,42,42,42	0
57	MG	1a	1661	1/1	0.92	0.10	56,56,56,56	0
57	MG	1A	3481	1/1	0.92	0.18	56,56,56,56	0
57	MG	2A	3052	1/1	0.92	0.14	55,55,55,55	0
57	MG	1A	3102	1/1	0.92	0.14	37,37,37,37	0
57	MG	2a	1719	1/1	0.92	0.12	74,74,74,74	0
57	MG	2a	1686	1/1	0.92	0.11	56,56,56,56	0
57	MG	1a	1719	1/1	0.92	0.19	44,44,44,44	0
57	MG	2A	3116	1/1	0.92	0.27	58,58,58,58	0
57	MG	2A	3454	1/1	0.92	0.09	48,48,48,48	0
57	MG	2A	3421	1/1	0.92	0.26	47,47,47,47	0
57	MG	1A	3809	1/1	0.92	0.06	44,44,44,44	0
57	MG	1A	3985	1/1	0.92	0.23	49,49,49,49	0
57	MG	2A	3043	1/1	0.92	0.14	55,55,55,55	0
57	MG	2A	3715	1/1	0.92	0.15	43,43,43,43	0
57	MG	1A	3429	1/1	0.92	0.13	39,39,39,39	0
57	MG	2A	3201	1/1	0.92	0.10	50,50,50,50	0
57	MG	1A	3101	1/1	0.92	0.15	52,52,52,52	0
57	MG	1A	3116	1/1	0.92	0.16	34,34,34,34	0
57	MG	2A	3024	1/1	0.92	0.26	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3382	1/1	0.92	0.14	45,45,45,45	0
57	MG	1A	3748	1/1	0.92	0.53	68,68,68,68	0
57	MG	2V	203	1/1	0.92	0.11	65,65,65,65	0
57	MG	1A	3754	1/1	0.92	0.23	58,58,58,58	0
57	MG	1a	1663	1/1	0.92	0.19	62,62,62,62	0
57	MG	2A	3444	1/1	0.92	0.12	54,54,54,54	0
57	MG	1A	3765	1/1	0.92	0.15	49,49,49,49	0
57	MG	1A	3519	1/1	0.92	0.19	52,52,52,52	0
57	MG	2A	3301	1/1	0.92	0.09	45,45,45,45	0
57	MG	1A	3768	1/1	0.92	0.18	51,51,51,51	0
57	MG	2A	3707	1/1	0.92	0.08	68,68,68,68	0
57	MG	2A	3728	1/1	0.92	0.11	53,53,53,53	0
57	MG	1A	3927	1/1	0.92	0.14	30,30,30,30	0
57	MG	2A	3572	1/1	0.92	0.13	42,42,42,42	0
57	MG	1A	3150	1/1	0.92	0.12	38,38,38,38	0
57	MG	2A	3194	1/1	0.92	0.20	57,57,57,57	0
57	MG	1A	3998	1/1	0.92	0.36	55,55,55,55	0
57	MG	2A	3685	1/1	0.92	0.08	50,50,50,50	0
57	MG	2A	3069	1/1	0.92	0.12	29,29,29,29	0
57	MG	2A	3598	1/1	0.92	0.18	55,55,55,55	0
57	MG	1A	3169	1/1	0.92	0.15	45,45,45,45	0
57	MG	1w	101	1/1	0.92	0.09	47,47,47,47	0
57	MG	2A	3365	1/1	0.92	0.11	57,57,57,57	0
57	MG	2A	3419	1/1	0.92	0.08	69,69,69,69	0
57	MG	2A	3302	1/1	0.92	0.18	50,50,50,50	0
57	MG	2A	3169	1/1	0.92	0.16	42,42,42,42	0
57	MG	2A	3686	1/1	0.92	0.11	59,59,59,59	0
57	MG	1A	3729	1/1	0.92	0.20	33,33,33,33	0
57	MG	1A	3916	1/1	0.92	0.10	43,43,43,43	0
57	MG	2a	1800	1/1	0.92	0.12	47,47,47,47	0
57	MG	1Z	302	1/1	0.92	0.18	55,55,55,55	0
57	MG	2A	3800	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3240	1/1	0.92	0.13	44,44,44,44	0
57	MG	1A	3752	1/1	0.92	0.19	26,26,26,26	0
57	MG	1a	1750	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3546	1/1	0.92	0.08	44,44,44,44	0
57	MG	2A	3680	1/1	0.92	0.11	61,61,61,61	0
57	MG	1A	3949	1/1	0.92	0.13	30,30,30,30	0
57	MG	2A	3155	1/1	0.92	0.15	51,51,51,51	0
57	MG	1A	3956	1/1	0.92	0.08	39,39,39,39	0
57	MG	1A	3343	1/1	0.92	0.29	47,47,47,47	0
57	MG	2A	3398	1/1	0.92	0.07	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	1A	3761	1/1	0.92	0.13	42,42,42,42	0
57	MG	2A	3774	1/1	0.92	0.23	48,48,48,48	0
57	MG	1A	3709	1/1	0.92	0.19	33,33,33,33	0
57	MG	1A	3832	1/1	0.92	0.14	30,30,30,30	0
57	MG	1a	1681	1/1	0.92	0.17	45,45,45,45	0
57	MG	18	105	1/1	0.92	0.27	45,45,45,45	0
57	MG	2A	3248	1/1	0.92	0.12	51,51,51,51	0
57	MG	2a	1666	1/1	0.92	0.12	55,55,55,55	0
57	MG	2A	3100	1/1	0.92	0.21	56,56,56,56	0
57	MG	1A	3043	1/1	0.92	0.15	27,27,27,27	0
57	MG	1A	3497	1/1	0.92	0.10	41,41,41,41	0
57	MG	1A	3979	1/1	0.92	0.14	47,47,47,47	0
57	MG	1a	1801	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3556	1/1	0.92	0.20	42,42,42,42	0
57	MG	1A	3603	1/1	0.92	0.25	37,37,37,37	0
57	MG	1O	204	1/1	0.92	0.15	47,47,47,47	0
57	MG	2A	3391	1/1	0.92	0.17	58,58,58,58	0
57	MG	1A	3892	1/1	0.92	0.25	31,31,31,31	0
57	MG	1A	3846	1/1	0.92	0.09	62,62,62,62	0
57	MG	1A	3443	1/1	0.92	0.15	38,38,38,38	0
57	MG	2A	3411	1/1	0.92	0.15	48,48,48,48	0
57	MG	1A	3309	1/1	0.92	0.24	54,54,54,54	0
57	MG	1B	213	1/1	0.92	0.13	34,34,34,34	0
57	MG	1a	1789	1/1	0.92	0.19	48,48,48,48	0
57	MG	1A	4077	1/1	0.92	0.13	41,41,41,41	0
57	MG	1A	3847	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3518	1/1	0.92	0.13	37,37,37,37	0
57	MG	2A	3104	1/1	0.92	0.17	45,45,45,45	0
57	MG	2A	3714	1/1	0.92	0.10	35,35,35,35	0
57	MG	1A	3742	1/1	0.92	0.14	51,51,51,51	0
57	MG	1A	3851	1/1	0.92	0.13	48,48,48,48	0
57	MG	2A	3487	1/1	0.92	0.21	43,43,43,43	0
57	MG	2A	3006	1/1	0.92	0.23	53,53,53,53	0
57	MG	2A	3342	1/1	0.92	0.14	46,46,46,46	0
57	MG	1a	1771	1/1	0.92	0.14	70,70,70,70	0
57	MG	2A	3737	1/1	0.92	0.06	54,54,54,54	0
57	MG	2W	201	1/1	0.92	0.15	60,60,60,60	0
57	MG	2a	1783	1/1	0.92	0.11	65,65,65,65	0
57	MG	1A	3345	1/1	0.92	0.17	36,36,36,36	0
57	MG	1D	307	1/1	0.92	0.12	52,52,52,52	0
57	MG	1A	3943	1/1	0.92	0.12	36,36,36,36	0
57	MG	2a	1685	1/1	0.92	0.14	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	3679	1/1	0.92	0.11	63,63,63,63	0
57	MG	23	103	1/1	0.92	0.13	52,52,52,52	0
57	MG	1A	4017	1/1	0.92	0.09	43,43,43,43	0
57	MG	1A	3977	1/1	0.92	0.20	54,54,54,54	0
57	MG	2A	3378	1/1	0.92	0.14	56,56,56,56	0
57	MG	1A	3466	1/1	0.92	0.15	53,53,53,53	0
57	MG	1A	3744	1/1	0.92	0.19	52,52,52,52	0
57	MG	1a	1706	1/1	0.92	0.27	52,52,52,52	0
57	MG	1A	4078	1/1	0.92	0.12	44,44,44,44	0
57	MG	2A	3393	1/1	0.92	0.11	52,52,52,52	0
57	MG	2q	202	1/1	0.92	0.12	62,62,62,62	0
57	MG	1A	3394	1/1	0.92	0.34	48,48,48,48	0
57	MG	1a	1741	1/1	0.92	0.08	61,61,61,61	0
57	MG	2F	306	1/1	0.92	0.11	56,56,56,56	0
57	MG	1a	1659	1/1	0.92	0.17	63,63,63,63	0
57	MG	2A	3233	1/1	0.92	0.13	53,53,53,53	0
57	MG	2A	3558	1/1	0.92	0.19	61,61,61,61	0
57	MG	1P	203	1/1	0.92	0.31	34,34,34,34	0
57	MG	1A	3514	1/1	0.92	0.17	25,25,25,25	0
59	ZN	1Y	204	1/1	0.92	0.10	70,70,70,70	0
57	MG	1A	3899	1/1	0.92	0.20	30,30,30,30	0
57	MG	2A	3860	1/1	0.92	0.07	60,60,60,60	0
57	MG	1A	3296	1/1	0.92	0.11	29,29,29,29	0
57	MG	2A	3165	1/1	0.92	0.16	40,40,40,40	0
57	MG	2A	3134	1/1	0.92	0.18	42,42,42,42	0
57	MG	2A	3601	1/1	0.92	0.20	41,41,41,41	0
57	MG	2A	3424	1/1	0.92	0.28	54,54,54,54	0
57	MG	1A	3721	1/1	0.92	0.06	57,57,57,57	0
57	MG	2A	3483	1/1	0.92	0.17	52,52,52,52	0
57	MG	1A	3844	1/1	0.92	0.15	52,52,52,52	0
57	MG	1A	3999	1/1	0.92	0.12	58,58,58,58	0
57	MG	1A	3266	1/1	0.92	0.21	47,47,47,47	0
57	MG	1A	3592	1/1	0.92	0.14	40,40,40,40	0
57	MG	2A	3284	1/1	0.92	0.15	57,57,57,57	0
57	MG	1B	204	1/1	0.92	0.32	53,53,53,53	0
57	MG	1l	202	1/1	0.92	0.13	67,67,67,67	0
57	MG	2l	203	1/1	0.92	0.09	53,53,53,53	0
57	MG	1A	3504	1/1	0.92	0.17	41,41,41,41	0
57	MG	2A	3272	1/1	0.92	0.22	47,47,47,47	0
57	MG	2A	3428	1/1	0.92	0.24	34,34,34,34	0
57	MG	1R	201	1/1	0.92	0.21	45,45,45,45	0
57	MG	1a	1783	1/1	0.92	0.22	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	1A	3680	1/1	0.92	0.14	25,25,25,25	0
57	MG	1A	3239	1/1	0.92	0.25	36,36,36,36	0
57	MG	2B	219	1/1	0.92	0.23	64,64,64,64	0
57	MG	2A	3691	1/1	0.92	0.15	50,50,50,50	0
57	MG	1A	3843	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3241	1/1	0.92	0.20	39,39,39,39	0
57	MG	1A	4086	1/1	0.92	0.12	42,42,42,42	0
57	MG	2a	1711	1/1	0.92	0.11	68,68,68,68	0
57	MG	2A	3045	1/1	0.92	0.10	56,56,56,56	0
57	MG	1B	201	1/1	0.92	0.17	46,46,46,46	0
57	MG	2A	3434	1/1	0.92	0.20	52,52,52,52	0
57	MG	1T	202	1/1	0.92	0.23	53,53,53,53	0
57	MG	1a	1746	1/1	0.92	0.12	43,43,43,43	0
57	MG	1A	3204	1/1	0.92	0.11	31,31,31,31	0
57	MG	2A	3065	1/1	0.92	0.17	53,53,53,53	0
57	MG	1A	3640	1/1	0.92	0.11	25,25,25,25	0
57	MG	1A	3351	1/1	0.92	0.20	45,45,45,45	0
57	MG	1A	3024	1/1	0.92	0.24	50,50,50,50	0
57	MG	2A	3056	1/1	0.92	0.19	49,49,49,49	0
57	MG	13	101	1/1	0.93	0.18	35,35,35,35	0
57	MG	2a	1804	1/1	0.93	0.07	67,67,67,67	0
57	MG	2w	109	1/1	0.93	0.19	62,62,62,62	0
57	MG	1A	4083	1/1	0.93	0.15	15,15,15,15	0
57	MG	1A	3253	1/1	0.93	0.21	64,64,64,64	0
57	MG	2A	3015	1/1	0.93	0.23	46,46,46,46	0
57	MG	1A	3930	1/1	0.93	0.12	39,39,39,39	0
57	MG	1a	1652	1/1	0.93	0.15	39,39,39,39	0
57	MG	2A	3582	1/1	0.93	0.12	54,54,54,54	0
57	MG	2B	207	1/1	0.93	0.19	53,53,53,53	0
57	MG	1a	1621	1/1	0.93	0.22	53,53,53,53	0
57	MG	1A	3190	1/1	0.93	0.27	34,34,34,34	0
57	MG	2A	3375	1/1	0.93	0.07	66,66,66,66	0
57	MG	1A	3597	1/1	0.93	0.14	32,32,32,32	0
57	MG	1A	3618	1/1	0.93	0.12	31,31,31,31	0
57	MG	2A	3730	1/1	0.93	0.09	47,47,47,47	0
57	MG	2A	3474	1/1	0.93	0.16	36,36,36,36	0
57	MG	2A	3144	1/1	0.93	0.15	40,40,40,40	0
57	MG	2a	1625	1/1	0.93	0.12	57,57,57,57	0
57	MG	1A	3822	1/1	0.93	0.18	67,67,67,67	0
57	MG	1a	1638	1/1	0.93	0.23	49,49,49,49	0
57	MG	1A	3542	1/1	0.93	0.27	23,23,23,23	0
57	MG	2a	1632	1/1	0.93	0.16	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	1673	1/1	0.93	0.14	51,51,51,51	0
57	MG	1A	3111	1/1	0.93	0.23	39,39,39,39	0
57	MG	2A	3358	1/1	0.93	0.27	57,57,57,57	0
57	MG	1A	3405	1/1	0.93	0.23	45,45,45,45	0
57	MG	2a	1695	1/1	0.93	0.31	54,54,54,54	0
57	MG	2A	3071	1/1	0.93	0.12	38,38,38,38	0
57	MG	2A	3513	1/1	0.93	0.12	43,43,43,43	0
57	MG	2a	1667	1/1	0.93	0.15	63,63,63,63	0
57	MG	2f	201	1/1	0.93	0.20	38,38,38,38	0
57	MG	2A	3011	1/1	0.93	0.15	38,38,38,38	0
57	MG	1A	3069	1/1	0.93	0.17	32,32,32,32	0
57	MG	2A	3245	1/1	0.93	0.16	43,43,43,43	0
57	MG	1B	230	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	4116	1/1	0.93	0.21	42,42,42,42	0
57	MG	2A	3888	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3268	1/1	0.93	0.18	44,44,44,44	0
57	MG	1A	3788	1/1	0.93	0.15	36,36,36,36	0
57	MG	2A	3887	1/1	0.93	0.16	44,44,44,44	0
57	MG	1A	3764	1/1	0.93	0.20	59,59,59,59	0
57	MG	1A	3127	1/1	0.93	0.14	33,33,33,33	0
57	MG	1A	3986	1/1	0.93	0.14	45,45,45,45	0
57	MG	1B	208	1/1	0.93	0.16	45,45,45,45	0
57	MG	1A	3667	1/1	0.93	0.19	25,25,25,25	0
57	MG	1A	3585	1/1	0.93	0.15	32,32,32,32	0
57	MG	1A	3258	1/1	0.93	0.12	49,49,49,49	0
57	MG	1a	1677	1/1	0.93	0.19	52,52,52,52	0
57	MG	1a	1622	1/1	0.93	0.13	44,44,44,44	0
57	MG	2A	3202	1/1	0.93	0.20	62,62,62,62	0
57	MG	2l	201	1/1	0.93	0.18	56,56,56,56	0
57	MG	2A	3270	1/1	0.93	0.17	48,48,48,48	0
57	MG	2a	1753	1/1	0.93	0.15	60,60,60,60	0
57	MG	2A	3788	1/1	0.93	0.14	54,54,54,54	0
57	MG	1A	3925	1/1	0.93	0.18	26,26,26,26	0
57	MG	1A	3273	1/1	0.93	0.12	52,52,52,52	0
57	MG	1A	3682	1/1	0.93	0.13	23,23,23,23	0
57	MG	2A	3143	1/1	0.93	0.18	45,45,45,45	0
57	MG	2a	1761	1/1	0.93	0.19	57,57,57,57	0
57	MG	2A	3185	1/1	0.93	0.14	35,35,35,35	0
57	MG	1A	3401	1/1	0.93	0.24	45,45,45,45	0
57	MG	2A	3820	1/1	0.93	0.08	56,56,56,56	0
57	MG	2A	3354	1/1	0.93	0.20	55,55,55,55	0
57	MG	2A	3651	1/1	0.93	0.21	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	3161	1/1	0.93	0.13	62,62,62,62	0
57	MG	25	103	1/1	0.93	0.12	50,50,50,50	0
57	MG	1x	115	1/1	0.93	0.09	47,47,47,47	0
57	MG	2A	3253	1/1	0.93	0.08	59,59,59,59	0
57	MG	2a	1678	1/1	0.93	0.14	36,36,36,36	0
57	MG	1A	4003	1/1	0.93	0.27	23,23,23,23	0
57	MG	2A	3762	1/1	0.93	0.09	56,56,56,56	0
57	MG	1N	205	1/1	0.93	0.24	43,43,43,43	0
57	MG	1A	3740	1/1	0.93	0.16	24,24,24,24	0
57	MG	2A	3765	1/1	0.93	0.10	49,49,49,49	0
57	MG	2a	1709	1/1	0.93	0.18	53,53,53,53	0
57	MG	1A	3385	1/1	0.93	0.25	41,41,41,41	0
57	MG	1A	4029	1/1	0.93	0.16	45,45,45,45	0
57	MG	2A	3338	1/1	0.93	0.12	52,52,52,52	0
57	MG	2A	3280	1/1	0.93	0.29	56,56,56,56	0
57	MG	2A	3097	1/1	0.93	0.18	47,47,47,47	0
57	MG	1a	1697	1/1	0.93	0.21	59,59,59,59	0
57	MG	2A	3334	1/1	0.93	0.21	42,42,42,42	0
57	MG	2A	3311	1/1	0.93	0.13	48,48,48,48	0
57	MG	2B	214	1/1	0.93	0.14	62,62,62,62	0
57	MG	1A	3317	1/1	0.93	0.27	57,57,57,57	0
57	MG	2A	3792	1/1	0.93	0.10	37,37,37,37	0
57	MG	2A	3783	1/1	0.93	0.11	41,41,41,41	0
57	MG	2a	1718	1/1	0.93	0.17	56,56,56,56	0
57	MG	2A	3225	1/1	0.93	0.14	44,44,44,44	0
57	MG	1P	201	1/1	0.93	0.11	26,26,26,26	0
57	MG	2a	1785	1/1	0.93	0.07	55,55,55,55	0
57	MG	1A	4052	1/1	0.93	0.13	40,40,40,40	0
57	MG	1A	3136	1/1	0.93	0.08	44,44,44,44	0
57	MG	1B	233	1/1	0.93	0.14	37,37,37,37	0
57	MG	1A	3125	1/1	0.93	0.25	31,31,31,31	0
57	MG	1A	3908	1/1	0.93	0.17	33,33,33,33	0
57	MG	2a	1729	1/1	0.93	0.17	59,59,59,59	0
57	MG	1A	3901	1/1	0.93	0.18	26,26,26,26	0
57	MG	1A	3880	1/1	0.93	0.24	40,40,40,40	0
57	MG	1A	4103	1/1	0.93	0.14	42,42,42,42	0
57	MG	1A	3411	1/1	0.93	0.10	38,38,38,38	0
57	MG	2A	3064	1/1	0.93	0.07	56,56,56,56	0
57	MG	2A	3706	1/1	0.93	0.14	31,31,31,31	0
57	MG	1A	3462	1/1	0.93	0.24	49,49,49,49	0
57	MG	1A	3917	1/1	0.93	0.16	42,42,42,42	0
57	MG	2A	3232	1/1	0.93	0.11	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	3245	1/1	0.93	0.20	53,53,53,53	0
57	MG	2A	3725	1/1	0.93	0.09	59,59,59,59	0
57	MG	1A	3305	1/1	0.93	0.32	52,52,52,52	0
57	MG	1a	1802	1/1	0.93	0.12	54,54,54,54	0
57	MG	1a	1695	1/1	0.93	0.18	52,52,52,52	0
57	MG	1A	3990	1/1	0.93	0.10	48,48,48,48	0
57	MG	2A	3053	1/1	0.93	0.17	55,55,55,55	0
57	MG	1A	3983	1/1	0.93	0.13	42,42,42,42	0
57	MG	1A	4015	1/1	0.93	0.17	52,52,52,52	0
57	MG	1F	301	1/1	0.93	0.19	33,33,33,33	0
57	MG	2E	302	1/1	0.93	0.10	36,36,36,36	0
57	MG	1Z	301	1/1	0.93	0.24	51,51,51,51	0
57	MG	1A	3194	1/1	0.93	0.17	36,36,36,36	0
57	MG	1A	3620	1/1	0.93	0.11	34,34,34,34	0
57	MG	2A	3493	1/1	0.93	0.08	53,53,53,53	0
57	MG	1y	101	1/1	0.93	0.11	60,60,60,60	0
57	MG	2a	1811	1/1	0.93	0.08	64,64,64,64	0
57	MG	2R	202	1/1	0.93	0.18	53,53,53,53	0
57	MG	1A	3299	1/1	0.93	0.40	34,34,34,34	0
57	MG	1A	3456	1/1	0.93	0.18	42,42,42,42	0
57	MG	2A	3768	1/1	0.93	0.10	62,62,62,62	0
57	MG	1a	1655	1/1	0.93	0.17	51,51,51,51	0
57	MG	1B	205	1/1	0.93	0.12	47,47,47,47	0
57	MG	1A	3367	1/1	0.93	0.10	33,33,33,33	0
57	MG	2A	3238	1/1	0.93	0.42	55,55,55,55	0
57	MG	2a	1831	1/1	0.93	0.14	66,66,66,66	0
57	MG	2A	3508	1/1	0.93	0.08	38,38,38,38	0
57	MG	1A	3444	1/1	0.93	0.32	35,35,35,35	0
57	MG	1a	1641	1/1	0.93	0.22	59,59,59,59	0
57	MG	1a	1769	1/1	0.93	0.19	62,62,62,62	0
57	MG	2A	3001	1/1	0.93	0.17	42,42,42,42	0
57	MG	2A	3089	1/1	0.93	0.09	45,45,45,45	0
57	MG	2a	1651	1/1	0.93	0.20	47,47,47,47	0
57	MG	1A	3022	1/1	0.93	0.11	44,44,44,44	0
57	MG	1A	3815	1/1	0.93	0.23	29,29,29,29	0
57	MG	1A	3536	1/1	0.93	0.18	57,57,57,57	0
57	MG	2a	1610	1/1	0.93	0.12	59,59,59,59	0
57	MG	1A	3446	1/1	0.93	0.14	54,54,54,54	0
57	MG	1a	1633	1/1	0.93	0.21	50,50,50,50	0
57	MG	1A	3063	1/1	0.93	0.25	45,45,45,45	0
57	MG	1A	4014	1/1	0.93	0.12	29,29,29,29	0
57	MG	17	104	1/1	0.93	0.17	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	3694	1/1	0.93	0.20	52,52,52,52	0
57	MG	2A	3761	1/1	0.93	0.15	56,56,56,56	0
57	MG	28	101	1/1	0.93	0.24	45,45,45,45	0
57	MG	2A	3244	1/1	0.93	0.14	51,51,51,51	0
57	MG	2A	3778	1/1	0.93	0.25	52,52,52,52	0
57	MG	2A	3313	1/1	0.93	0.08	57,57,57,57	0
57	MG	2A	3531	1/1	0.93	0.22	67,67,67,67	0
57	MG	2A	3590	1/1	0.93	0.16	59,59,59,59	0
57	MG	2A	3445	1/1	0.93	0.26	49,49,49,49	0
57	MG	1A	3381	1/1	0.93	0.17	46,46,46,46	0
57	MG	2A	3426	1/1	0.93	0.23	57,57,57,57	0
57	MG	1A	3044	1/1	0.93	0.15	33,33,33,33	0
57	MG	1A	3878	1/1	0.93	0.32	37,37,37,37	0
57	MG	2a	1694	1/1	0.93	0.10	53,53,53,53	0
57	MG	1A	3248	1/1	0.93	0.15	52,52,52,52	0
57	MG	1A	3415	1/1	0.93	0.14	65,65,65,65	0
57	MG	1A	4119	1/1	0.93	0.19	44,44,44,44	0
57	MG	1A	3178	1/1	0.93	0.37	32,32,32,32	0
57	MG	1A	3247	1/1	0.93	0.11	64,64,64,64	0
57	MG	1O	203	1/1	0.93	0.14	52,52,52,52	0
57	MG	1A	4031	1/1	0.93	0.21	24,24,24,24	0
57	MG	2A	3151	1/1	0.93	0.10	41,41,41,41	0
57	MG	2A	3587	1/1	0.93	0.12	63,63,63,63	0
57	MG	1b	301	1/1	0.93	0.15	68,68,68,68	0
57	MG	1w	102	1/1	0.93	0.17	67,67,67,67	0
57	MG	1a	1626	1/1	0.93	0.19	53,53,53,53	0
57	MG	2A	3689	1/1	0.93	0.10	54,54,54,54	0
57	MG	2A	3849	1/1	0.93	0.10	53,53,53,53	0
57	MG	1A	4110	1/1	0.93	0.16	50,50,50,50	0
57	MG	2E	303	1/1	0.93	0.17	44,44,44,44	0
57	MG	1A	3066	1/1	0.93	0.31	54,54,54,54	0
57	MG	2a	1614	1/1	0.93	0.17	53,53,53,53	0
57	MG	1A	3842	1/1	0.93	0.12	40,40,40,40	0
57	MG	1A	3487	1/1	0.93	0.20	55,55,55,55	0
57	MG	2A	3825	1/1	0.93	0.11	60,60,60,60	0
57	MG	14	101	1/1	0.93	0.24	54,54,54,54	0
57	MG	1A	3145	1/1	0.93	0.18	34,34,34,34	0
57	MG	1A	3418	1/1	0.93	0.15	48,48,48,48	0
57	MG	1B	210	1/1	0.93	0.07	48,48,48,48	0
57	MG	1a	1640	1/1	0.93	0.15	55,55,55,55	0
57	MG	2A	3779	1/1	0.93	0.15	42,42,42,42	0
57	MG	1A	3480	1/1	0.93	0.12	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	3957	1/1	0.93	0.17	28,28,28,28	0
57	MG	2A	3123	1/1	0.93	0.14	33,33,33,33	0
57	MG	1A	3395	1/1	0.93	0.14	55,55,55,55	0
57	MG	2a	1677	1/1	0.93	0.20	51,51,51,51	0
57	MG	2a	1730	1/1	0.93	0.13	53,53,53,53	0
57	MG	1a	1710	1/1	0.93	0.12	53,53,53,53	0
57	MG	2A	3300	1/1	0.93	0.11	59,59,59,59	0
57	MG	2A	3113	1/1	0.93	0.12	57,57,57,57	0
57	MG	2A	3681	1/1	0.93	0.13	43,43,43,43	0
57	MG	2a	1637	1/1	0.93	0.18	39,39,39,39	0
57	MG	1A	3793	1/1	0.93	0.09	46,46,46,46	0
57	MG	2A	3616	1/1	0.93	0.10	40,40,40,40	0
57	MG	2a	1669	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3358	1/1	0.93	0.31	37,37,37,37	0
57	MG	2A	3004	1/1	0.93	0.14	54,54,54,54	0
57	MG	2A	3527	1/1	0.94	0.34	54,54,54,54	0
57	MG	1A	3250	1/1	0.94	0.18	38,38,38,38	0
57	MG	1A	3896	1/1	0.94	0.12	34,34,34,34	0
57	MG	2A	3459	1/1	0.94	0.17	40,40,40,40	0
57	MG	2A	3140	1/1	0.94	0.13	59,59,59,59	0
57	MG	2a	1812	1/1	0.94	0.11	66,66,66,66	0
57	MG	1A	3919	1/1	0.94	0.16	36,36,36,36	0
57	MG	2A	3160	1/1	0.94	0.13	48,48,48,48	0
57	MG	1A	3193	1/1	0.94	0.10	48,48,48,48	0
57	MG	1A	3288	1/1	0.94	0.13	59,59,59,59	0
57	MG	2A	3688	1/1	0.94	0.12	47,47,47,47	0
57	MG	1A	3773	1/1	0.94	0.16	29,29,29,29	0
57	MG	25	101	1/1	0.94	0.31	44,44,44,44	0
57	MG	1A	3624	1/1	0.94	0.16	34,34,34,34	0
57	MG	2q	201	1/1	0.94	0.23	61,61,61,61	0
57	MG	1A	4045	1/1	0.94	0.27	75,75,75,75	0
57	MG	2A	3793	1/1	0.94	0.14	46,46,46,46	0
57	MG	1A	3699	1/1	0.94	0.15	25,25,25,25	0
57	MG	2A	3602	1/1	0.94	0.19	60,60,60,60	0
57	MG	2A	3747	1/1	0.94	0.14	65,65,65,65	0
57	MG	2A	3573	1/1	0.94	0.14	41,41,41,41	0
57	MG	1A	3073	1/1	0.94	0.13	24,24,24,24	0
57	MG	1A	3802	1/1	0.94	0.19	24,24,24,24	0
57	MG	1A	3594	1/1	0.94	0.20	50,50,50,50	0
57	MG	1A	3460	1/1	0.94	0.26	55,55,55,55	0
57	MG	1A	3770	1/1	0.94	0.18	24,24,24,24	0
57	MG	1A	3584	1/1	0.94	0.19	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3569	1/1	0.94	0.10	37,37,37,37	0
57	MG	1A	3321	1/1	0.94	0.15	35,35,35,35	0
57	MG	2A	3567	1/1	0.94	0.11	58,58,58,58	0
57	MG	2a	1676	1/1	0.94	0.14	47,47,47,47	0
57	MG	1A	3495	1/1	0.94	0.18	26,26,26,26	0
57	MG	1A	3602	1/1	0.94	0.20	36,36,36,36	0
57	MG	16	101	1/1	0.94	0.31	54,54,54,54	0
57	MG	2A	3091	1/1	0.94	0.17	68,68,68,68	0
57	MG	2A	3203	1/1	0.94	0.28	56,56,56,56	0
57	MG	1A	3121	1/1	0.94	0.24	29,29,29,29	0
57	MG	2A	3579	1/1	0.94	0.14	31,31,31,31	0
57	MG	2A	3878	1/1	0.94	0.22	50,50,50,50	0
57	MG	2A	3461	1/1	0.94	0.23	56,56,56,56	0
57	MG	1A	3486	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3425	1/1	0.94	0.14	48,48,48,48	0
57	MG	1A	3325	1/1	0.94	0.17	28,28,28,28	0
57	MG	1A	3144	1/1	0.94	0.13	35,35,35,35	0
57	MG	1A	3626	1/1	0.94	0.18	34,34,34,34	0
57	MG	2A	3306	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3826	1/1	0.94	0.11	39,39,39,39	0
57	MG	1A	3924	1/1	0.94	0.14	27,27,27,27	0
57	MG	2A	3499	1/1	0.94	0.13	55,55,55,55	0
57	MG	1A	3777	1/1	0.94	0.27	30,30,30,30	0
57	MG	1A	3110	1/1	0.94	0.13	40,40,40,40	0
57	MG	2A	3127	1/1	0.94	0.15	61,61,61,61	0
57	MG	2a	1635	1/1	0.94	0.35	69,69,69,69	0
57	MG	1a	1786	1/1	0.94	0.13	44,44,44,44	0
57	MG	2a	1700	1/1	0.94	0.11	53,53,53,53	0
57	MG	1A	3447	1/1	0.94	0.17	34,34,34,34	0
57	MG	2a	1690	1/1	0.94	0.14	59,59,59,59	0
57	MG	1A	3653	1/1	0.94	0.15	33,33,33,33	0
57	MG	2A	3412	1/1	0.94	0.21	47,47,47,47	0
57	MG	1E	312	1/1	0.94	0.17	45,45,45,45	0
57	MG	2a	1654	1/1	0.94	0.11	51,51,51,51	0
57	MG	1A	3400	1/1	0.94	0.31	40,40,40,40	0
57	MG	1x	109	1/1	0.94	0.10	60,60,60,60	0
57	MG	1A	4073	1/1	0.94	0.11	35,35,35,35	0
57	MG	2A	3181	1/1	0.94	0.10	63,63,63,63	0
57	MG	1A	3727	1/1	0.94	0.17	43,43,43,43	0
57	MG	2A	3266	1/1	0.94	0.12	43,43,43,43	0
57	MG	2A	3494	1/1	0.94	0.11	57,57,57,57	0
57	MG	2A	3877	1/1	0.94	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3629	1/1	0.94	0.21	29,29,29,29	0
57	MG	2A	3332	1/1	0.94	0.17	44,44,44,44	0
57	MG	2A	3727	1/1	0.94	0.17	49,49,49,49	0
57	MG	1A	3409	1/1	0.94	0.10	53,53,53,53	0
57	MG	2A	3547	1/1	0.94	0.11	54,54,54,54	0
57	MG	1a	1790	1/1	0.94	0.11	44,44,44,44	0
57	MG	1A	3608	1/1	0.94	0.21	43,43,43,43	0
57	MG	1a	1704	1/1	0.94	0.31	57,57,57,57	0
57	MG	1Q	207	1/1	0.94	0.14	41,41,41,41	0
57	MG	2A	3304	1/1	0.94	0.15	48,48,48,48	0
57	MG	1A	3942	1/1	0.94	0.16	48,48,48,48	0
57	MG	1A	4106	1/1	0.94	0.12	50,50,50,50	0
57	MG	1A	3392	1/1	0.94	0.22	61,61,61,61	0
57	MG	2A	3635	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3262	1/1	0.94	0.16	55,55,55,55	0
57	MG	2A	3427	1/1	0.94	0.26	43,43,43,43	0
57	MG	2A	3058	1/1	0.94	0.13	61,61,61,61	0
57	MG	2A	3261	1/1	0.94	0.09	60,60,60,60	0
57	MG	15	104	1/1	0.94	0.14	25,25,25,25	0
57	MG	1T	204	1/1	0.94	0.12	50,50,50,50	0
57	MG	1A	3187	1/1	0.94	0.13	31,31,31,31	0
57	MG	1A	3782	1/1	0.94	0.18	30,30,30,30	0
57	MG	1a	1743	1/1	0.94	0.18	53,53,53,53	0
57	MG	2A	3420	1/1	0.94	0.14	68,68,68,68	0
57	MG	1x	114	1/1	0.94	0.10	53,53,53,53	0
57	MG	2A	3431	1/1	0.94	0.23	52,52,52,52	0
57	MG	1B	218	1/1	0.94	0.26	52,52,52,52	0
57	MG	2A	3845	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3271	1/1	0.94	0.20	58,58,58,58	0
57	MG	1A	3827	1/1	0.94	0.13	37,37,37,37	0
57	MG	2A	3152	1/1	0.94	0.20	57,57,57,57	0
57	MG	1A	3339	1/1	0.94	0.30	69,69,69,69	0
57	MG	1A	3575	1/1	0.94	0.18	32,32,32,32	0
57	MG	1a	1753	1/1	0.94	0.15	48,48,48,48	0
57	MG	2a	1781	1/1	0.94	0.22	56,56,56,56	0
57	MG	1A	3219	1/1	0.94	0.10	39,39,39,39	0
57	MG	1A	3113	1/1	0.94	0.14	25,25,25,25	0
57	MG	1w	104	1/1	0.94	0.13	66,66,66,66	0
57	MG	2A	3646	1/1	0.94	0.14	56,56,56,56	0
57	MG	1B	224	1/1	0.94	0.20	34,34,34,34	0
57	MG	1A	3378	1/1	0.94	0.25	46,46,46,46	0
57	MG	1A	3130	1/1	0.94	0.23	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3694	1/1	0.94	0.15	38,38,38,38	0
57	MG	2A	3237	1/1	0.94	0.20	39,39,39,39	0
57	MG	2A	3200	1/1	0.94	0.16	56,56,56,56	0
57	MG	2a	1608	1/1	0.94	0.19	60,60,60,60	0
57	MG	2A	3740	1/1	0.94	0.14	51,51,51,51	0
57	MG	1A	3025	1/1	0.94	0.13	38,38,38,38	0
57	MG	2A	3026	1/1	0.94	0.16	43,43,43,43	0
57	MG	19	101	1/1	0.94	0.14	53,53,53,53	0
57	MG	2A	3478	1/1	0.94	0.10	61,61,61,61	0
57	MG	1A	4091	1/1	0.94	0.11	31,31,31,31	0
57	MG	2A	3207	1/1	0.94	0.19	49,49,49,49	0
57	MG	1A	3281	1/1	0.94	0.13	36,36,36,36	0
57	MG	1A	3637	1/1	0.94	0.07	33,33,33,33	0
57	MG	1a	1637	1/1	0.94	0.28	51,51,51,51	0
57	MG	2A	3806	1/1	0.94	0.12	65,65,65,65	0
57	MG	2a	1766	1/1	0.94	0.09	43,43,43,43	0
57	MG	2A	3175	1/1	0.94	0.18	47,47,47,47	0
57	MG	1A	3100	1/1	0.94	0.14	36,36,36,36	0
57	MG	1A	3471	1/1	0.94	0.33	48,48,48,48	0
57	MG	1A	3995	1/1	0.94	0.10	35,35,35,35	0
57	MG	2A	3063	1/1	0.94	0.14	62,62,62,62	0
57	MG	17	103	1/1	0.94	0.16	51,51,51,51	0
57	MG	2y	102	1/1	0.94	0.23	74,74,74,74	0
57	MG	1A	3254	1/1	0.94	0.16	27,27,27,27	0
57	MG	1a	1632	1/1	0.94	0.26	22,22,22,22	0
57	MG	1A	3538	1/1	0.94	0.22	40,40,40,40	0
57	MG	1A	3527	1/1	0.94	0.14	54,54,54,54	0
57	MG	2A	3839	1/1	0.94	0.12	51,51,51,51	0
57	MG	2A	3588	1/1	0.94	0.10	43,43,43,43	0
57	MG	1S	202	1/1	0.94	0.11	53,53,53,53	0
57	MG	1A	3962	1/1	0.94	0.12	41,41,41,41	0
57	MG	1A	4092	1/1	0.94	0.16	19,19,19,19	0
57	MG	2w	105	1/1	0.94	0.07	79,79,79,79	0
57	MG	2a	1736	1/1	0.94	0.09	64,64,64,64	0
57	MG	2A	3204	1/1	0.94	0.16	52,52,52,52	0
57	MG	1A	3716	1/1	0.94	0.21	37,37,37,37	0
57	MG	2A	3048	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3055	1/1	0.94	0.11	46,46,46,46	0
57	MG	1A	3454	1/1	0.94	0.15	45,45,45,45	0
57	MG	1a	1798	1/1	0.94	0.07	43,43,43,43	0
57	MG	1a	1715	1/1	0.94	0.22	51,51,51,51	0
57	MG	2v	102	1/1	0.94	0.14	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	3145	1/1	0.94	0.20	44,44,44,44	0
57	MG	2A	3522	1/1	0.94	0.12	35,35,35,35	0
57	MG	2A	3157	1/1	0.94	0.17	34,34,34,34	0
57	MG	2B	213	1/1	0.94	0.29	49,49,49,49	0
57	MG	2a	1645	1/1	0.94	0.07	67,67,67,67	0
57	MG	1A	3093	1/1	0.94	0.16	22,22,22,22	0
57	MG	1A	4062	1/1	0.94	0.06	43,43,43,43	0
57	MG	1A	4020	1/1	0.94	0.12	33,33,33,33	0
57	MG	1A	3870	1/1	0.94	0.12	45,45,45,45	0
57	MG	2A	3095	1/1	0.94	0.13	39,39,39,39	0
57	MG	1A	3379	1/1	0.94	0.27	25,25,25,25	0
57	MG	1a	1754	1/1	0.94	0.14	63,63,63,63	0
57	MG	2A	3607	1/1	0.94	0.11	43,43,43,43	0
57	MG	1A	3635	1/1	0.94	0.21	18,18,18,18	0
57	MG	1A	3284	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3506	1/1	0.94	0.11	51,51,51,51	0
57	MG	2a	1792	1/1	0.94	0.15	42,42,42,42	0
57	MG	2A	3129	1/1	0.94	0.11	51,51,51,51	0
57	MG	1F	311	1/1	0.94	0.17	54,54,54,54	0
57	MG	1F	304	1/1	0.94	0.17	38,38,38,38	0
57	MG	1A	3786	1/1	0.94	0.12	31,31,31,31	0
57	MG	1A	3099	1/1	0.94	0.16	36,36,36,36	0
57	MG	1A	3293	1/1	0.94	0.15	55,55,55,55	0
57	MG	1A	3277	1/1	0.94	0.25	42,42,42,42	0
57	MG	2A	3002	1/1	0.94	0.30	53,53,53,53	0
57	MG	1A	3554	1/1	0.94	0.16	27,27,27,27	0
57	MG	2A	3626	1/1	0.94	0.14	48,48,48,48	0
57	MG	1A	3903	1/1	0.94	0.25	22,22,22,22	0
57	MG	1A	3980	1/1	0.94	0.17	27,27,27,27	0
57	MG	1A	3272	1/1	0.94	0.11	33,33,33,33	0
57	MG	2f	202	1/1	0.94	0.15	57,57,57,57	0
57	MG	1A	3845	1/1	0.94	0.18	60,60,60,60	0
57	MG	2A	3190	1/1	0.94	0.09	57,57,57,57	0
57	MG	1A	3726	1/1	0.94	0.11	36,36,36,36	0
57	MG	2A	3701	1/1	0.94	0.09	73,73,73,73	0
57	MG	1l	106	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3833	1/1	0.94	0.14	34,34,34,34	0
57	MG	2a	1634	1/1	0.94	0.26	57,57,57,57	0
57	MG	2A	3010	1/1	0.94	0.18	54,54,54,54	0
57	MG	1A	3398	1/1	0.94	0.14	27,27,27,27	0
57	MG	2a	1805	1/1	0.94	0.28	57,57,57,57	0
57	MG	2A	3597	1/1	0.94	0.22	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	3050	1/1	0.94	0.17	61,61,61,61	0
57	MG	1A	3071	1/1	0.94	0.14	13,13,13,13	0
57	MG	2A	3076	1/1	0.94	0.18	39,39,39,39	0
57	MG	2A	3614	1/1	0.94	0.10	40,40,40,40	0
57	MG	1a	1718	1/1	0.94	0.23	45,45,45,45	0
57	MG	1A	3697	1/1	0.94	0.23	35,35,35,35	0
57	MG	1A	3502	1/1	0.94	0.16	56,56,56,56	0
57	MG	23	101	1/1	0.94	0.19	55,55,55,55	0
57	MG	1A	4100	1/1	0.94	0.27	40,40,40,40	0
57	MG	1N	201	1/1	0.94	0.24	43,43,43,43	0
57	MG	2A	3247	1/1	0.94	0.27	48,48,48,48	0
57	MG	1A	3263	1/1	0.94	0.18	44,44,44,44	0
57	MG	1A	3180	1/1	0.94	0.21	49,49,49,49	0
57	MG	1A	3212	1/1	0.94	0.19	44,44,44,44	0
57	MG	2a	1779	1/1	0.94	0.08	50,50,50,50	0
57	MG	2a	1688	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3638	1/1	0.94	0.16	44,44,44,44	0
57	MG	1a	1620	1/1	0.94	0.29	62,62,62,62	0
57	MG	2A	3283	1/1	0.94	0.15	52,52,52,52	0
57	MG	2a	1714	1/1	0.94	0.38	67,67,67,67	0
57	MG	1A	3168	1/1	0.94	0.49	42,42,42,42	0
57	MG	1A	3450	1/1	0.94	0.21	43,43,43,43	0
57	MG	1A	3372	1/1	0.94	0.24	43,43,43,43	0
57	MG	1A	3944	1/1	0.94	0.12	40,40,40,40	0
57	MG	2A	3351	1/1	0.94	0.19	42,42,42,42	0
57	MG	1a	1665	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3510	1/1	0.94	0.11	63,63,63,63	0
57	MG	1A	3404	1/1	0.94	0.15	34,34,34,34	0
57	MG	1A	3509	1/1	0.94	0.12	43,43,43,43	0
57	MG	2a	1703	1/1	0.94	0.18	55,55,55,55	0
57	MG	1a	1717	1/1	0.94	0.16	49,49,49,49	0
57	MG	1D	306	1/1	0.94	0.17	39,39,39,39	0
57	MG	1A	3153	1/1	0.94	0.15	29,29,29,29	0
57	MG	1E	303	1/1	0.94	0.20	33,33,33,33	0
57	MG	2A	3114	1/1	0.94	0.18	57,57,57,57	0
57	MG	1A	4063	1/1	0.94	0.11	37,37,37,37	0
57	MG	2A	3079	1/1	0.94	0.13	55,55,55,55	0
57	MG	18	104	1/1	0.94	0.15	52,52,52,52	0
57	MG	1A	3831	1/1	0.94	0.20	28,28,28,28	0
57	MG	1D	301	1/1	0.94	0.59	42,42,42,42	0
57	MG	1A	3439	1/1	0.94	0.16	43,43,43,43	0
57	MG	1A	3797	1/1	0.94	0.18	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4117	1/1	0.94	0.17	43,43,43,43	0
57	MG	2A	3268	1/1	0.94	0.14	50,50,50,50	0
57	MG	2A	3458	1/1	0.94	0.18	49,49,49,49	0
57	MG	1A	3152	1/1	0.94	0.17	41,41,41,41	0
57	MG	1a	1684	1/1	0.94	0.11	59,59,59,59	0
57	MG	2A	3524	1/1	0.95	0.12	31,31,31,31	0
57	MG	2A	3361	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	4025	1/1	0.95	0.11	34,34,34,34	0
57	MG	1A	3863	1/1	0.95	0.21	20,20,20,20	0
57	MG	1A	3540	1/1	0.95	0.35	56,56,56,56	0
57	MG	2a	1675	1/1	0.95	0.14	56,56,56,56	0
57	MG	2A	3139	1/1	0.95	0.17	39,39,39,39	0
57	MG	1A	3488	1/1	0.95	0.16	34,34,34,34	0
57	MG	2A	3842	1/1	0.95	0.10	37,37,37,37	0
57	MG	2A	3292	1/1	0.95	0.11	41,41,41,41	0
57	MG	2A	3205	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3806	1/1	0.95	0.17	30,30,30,30	0
57	MG	1A	3747	1/1	0.95	0.10	52,52,52,52	0
57	MG	1A	3236	1/1	0.95	0.23	35,35,35,35	0
57	MG	1A	3891	1/1	0.95	0.18	42,42,42,42	0
57	MG	1A	3465	1/1	0.95	0.17	33,33,33,33	0
57	MG	2A	3652	1/1	0.95	0.12	55,55,55,55	0
57	MG	1A	3084	1/1	0.95	0.15	30,30,30,30	0
57	MG	1A	3493	1/1	0.95	0.12	61,61,61,61	0
57	MG	1A	3656	1/1	0.95	0.17	28,28,28,28	0
57	MG	1A	3431	1/1	0.95	0.11	53,53,53,53	0
57	MG	2a	1816	1/1	0.95	0.12	62,62,62,62	0
57	MG	1A	3871	1/1	0.95	0.15	44,44,44,44	0
57	MG	1A	3664	1/1	0.95	0.19	39,39,39,39	0
57	MG	1X	102	1/1	0.95	0.14	34,34,34,34	0
57	MG	1a	1669	1/1	0.95	0.13	56,56,56,56	0
57	MG	2A	3039	1/1	0.95	0.12	47,47,47,47	0
57	MG	1a	1616	1/1	0.95	0.14	37,37,37,37	0
57	MG	1A	3864	1/1	0.95	0.20	31,31,31,31	0
57	MG	1A	3543	1/1	0.95	0.26	37,37,37,37	0
57	MG	1a	1688	1/1	0.95	0.14	63,63,63,63	0
57	MG	1A	3739	1/1	0.95	0.13	28,28,28,28	0
57	MG	2A	3570	1/1	0.95	0.10	58,58,58,58	0
57	MG	1A	4019	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3132	1/1	0.95	0.16	44,44,44,44	0
57	MG	1A	3249	1/1	0.95	0.20	47,47,47,47	0
57	MG	1A	3490	1/1	0.95	0.18	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3123	1/1	0.95	0.13	37,37,37,37	0
57	MG	2A	3329	1/1	0.95	0.31	54,54,54,54	0
57	MG	1x	111	1/1	0.95	0.11	63,63,63,63	0
57	MG	1A	3334	1/1	0.95	0.20	44,44,44,44	0
57	MG	1a	1610	1/1	0.95	0.20	51,51,51,51	0
57	MG	2a	1777	1/1	0.95	0.07	49,49,49,49	0
57	MG	2A	3059	1/1	0.95	0.11	53,53,53,53	0
57	MG	2A	3759	1/1	0.95	0.12	39,39,39,39	0
57	MG	17	101	1/1	0.95	0.15	35,35,35,35	0
57	MG	2A	3492	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3581	1/1	0.95	0.19	53,53,53,53	0
57	MG	1T	201	1/1	0.95	0.23	49,49,49,49	0
57	MG	1A	3771	1/1	0.95	0.23	43,43,43,43	0
57	MG	2A	3456	1/1	0.95	0.14	56,56,56,56	0
57	MG	1A	3424	1/1	0.95	0.19	33,33,33,33	0
57	MG	2A	3156	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	4071	1/1	0.95	0.23	28,28,28,28	0
57	MG	1A	3541	1/1	0.95	0.21	51,51,51,51	0
57	MG	2A	3682	1/1	0.95	0.18	51,51,51,51	0
57	MG	1B	231	1/1	0.95	0.14	67,67,67,67	0
57	MG	2D	306	1/1	0.95	0.46	40,40,40,40	0
57	MG	15	106	1/1	0.95	0.10	38,38,38,38	0
57	MG	1A	3691	1/1	0.95	0.18	21,21,21,21	0
57	MG	2A	3293	1/1	0.95	0.14	49,49,49,49	0
57	MG	2B	205	1/1	0.95	0.22	53,53,53,53	0
57	MG	1a	1775	1/1	0.95	0.18	44,44,44,44	0
57	MG	1A	3574	1/1	0.95	0.31	43,43,43,43	0
57	MG	2A	3117	1/1	0.95	0.18	47,47,47,47	0
57	MG	1a	1762	1/1	0.95	0.10	46,46,46,46	0
57	MG	1A	3306	1/1	0.95	0.21	40,40,40,40	0
57	MG	2A	3110	1/1	0.95	0.08	53,53,53,53	0
57	MG	2A	3126	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3427	1/1	0.95	0.12	48,48,48,48	0
57	MG	2R	201	1/1	0.95	0.27	46,46,46,46	0
57	MG	1A	3195	1/1	0.95	0.20	35,35,35,35	0
57	MG	1a	1707	1/1	0.95	0.17	53,53,53,53	0
57	MG	2A	3389	1/1	0.95	0.11	51,51,51,51	0
57	MG	2A	3216	1/1	0.95	0.13	70,70,70,70	0
57	MG	1B	229	1/1	0.95	0.12	39,39,39,39	0
57	MG	2a	1742	1/1	0.95	0.17	68,68,68,68	0
57	MG	1A	3571	1/1	0.95	0.20	31,31,31,31	0
57	MG	1A	3895	1/1	0.95	0.25	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3642	1/1	0.95	0.18	45,45,45,45	0
57	MG	1A	3303	1/1	0.95	0.14	26,26,26,26	0
57	MG	1a	1811	1/1	0.95	0.12	57,57,57,57	0
57	MG	1a	1721	1/1	0.95	0.26	49,49,49,49	0
57	MG	2A	3543	1/1	0.95	0.14	41,41,41,41	0
57	MG	1a	1770	1/1	0.95	0.13	43,43,43,43	0
57	MG	1A	3070	1/1	0.95	0.63	37,37,37,37	0
57	MG	2a	1733	1/1	0.95	0.14	42,42,42,42	0
57	MG	1A	3627	1/1	0.95	0.28	33,33,33,33	0
57	MG	1A	3807	1/1	0.95	0.11	37,37,37,37	0
57	MG	2A	3744	1/1	0.95	0.13	61,61,61,61	0
57	MG	1A	3020	1/1	0.95	0.18	37,37,37,37	0
57	MG	1A	3496	1/1	0.95	0.22	26,26,26,26	0
57	MG	1A	3259	1/1	0.95	0.10	63,63,63,63	0
57	MG	1V	206	1/1	0.95	0.26	37,37,37,37	0
57	MG	1A	3165	1/1	0.95	0.17	29,29,29,29	0
57	MG	1a	1617	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3132	1/1	0.95	0.12	67,67,67,67	0
57	MG	2X	102	1/1	0.95	0.37	66,66,66,66	0
57	MG	1x	102	1/1	0.95	0.29	42,42,42,42	0
57	MG	1A	3945	1/1	0.95	0.06	59,59,59,59	0
57	MG	1A	3507	1/1	0.95	0.13	24,24,24,24	0
57	MG	1A	3835	1/1	0.95	0.17	47,47,47,47	0
57	MG	1A	3065	1/1	0.95	0.22	33,33,33,33	0
57	MG	1A	3897	1/1	0.95	0.18	40,40,40,40	0
57	MG	2A	3852	1/1	0.95	0.13	55,55,55,55	0
57	MG	2a	1768	1/1	0.95	0.14	71,71,71,71	0
57	MG	1A	3217	1/1	0.95	0.15	34,34,34,34	0
57	MG	1A	3668	1/1	0.95	0.19	27,27,27,27	0
57	MG	2A	3604	1/1	0.95	0.14	59,59,59,59	0
57	MG	1A	3535	1/1	0.95	0.23	43,43,43,43	0
57	MG	2A	3462	1/1	0.95	0.22	51,51,51,51	0
57	MG	1A	3676	1/1	0.95	0.12	23,23,23,23	0
57	MG	1A	3889	1/1	0.95	0.18	29,29,29,29	0
57	MG	2A	3212	1/1	0.95	0.29	45,45,45,45	0
57	MG	1A	3743	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3055	1/1	0.95	0.13	33,33,33,33	0
57	MG	1a	1608	1/1	0.95	0.15	62,62,62,62	0
57	MG	1A	3159	1/1	0.95	0.31	31,31,31,31	0
57	MG	2a	1786	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3780	1/1	0.95	0.14	42,42,42,42	0
57	MG	1A	3449	1/1	0.95	0.09	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	2A	3077	1/1	0.95	0.16	44,44,44,44	0
57	MG	20	101	1/1	0.95	0.14	48,48,48,48	0
57	MG	2B	220	1/1	0.95	0.08	70,70,70,70	0
57	MG	2A	3009	1/1	0.95	0.15	44,44,44,44	0
57	MG	1E	302	1/1	0.95	0.14	38,38,38,38	0
57	MG	1A	3569	1/1	0.95	0.21	23,23,23,23	0
57	MG	1X	105	1/1	0.95	0.23	35,35,35,35	0
57	MG	1a	1666	1/1	0.95	0.11	50,50,50,50	0
57	MG	1A	3642	1/1	0.95	0.23	39,39,39,39	0
57	MG	2B	215	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3274	1/1	0.95	0.14	42,42,42,42	0
57	MG	1A	3838	1/1	0.95	0.15	52,52,52,52	0
57	MG	2A	3535	1/1	0.95	0.13	63,63,63,63	0
57	MG	1A	3907	1/1	0.95	0.11	42,42,42,42	0
57	MG	15	105	1/1	0.95	0.14	24,24,24,24	0
57	MG	1A	3412	1/1	0.95	0.26	33,33,33,33	0
57	MG	2A	3346	1/1	0.95	0.30	47,47,47,47	0
57	MG	1e	201	1/1	0.95	0.10	67,67,67,67	0
57	MG	25	102	1/1	0.95	0.18	42,42,42,42	0
57	MG	2A	3542	1/1	0.95	0.11	46,46,46,46	0
57	MG	2A	3382	1/1	0.95	0.29	43,43,43,43	0
57	MG	2A	3659	1/1	0.95	0.12	50,50,50,50	0
57	MG	2a	1696	1/1	0.95	0.10	67,67,67,67	0
57	MG	1X	101	1/1	0.95	0.21	51,51,51,51	0
57	MG	2D	301	1/1	0.95	0.12	47,47,47,47	0
57	MG	2A	3489	1/1	0.95	0.14	57,57,57,57	0
57	MG	2A	3103	1/1	0.95	0.15	26,26,26,26	0
57	MG	1Q	205	1/1	0.95	0.22	37,37,37,37	0
57	MG	1A	3555	1/1	0.95	0.15	24,24,24,24	0
57	MG	1A	4053	1/1	0.95	0.09	66,66,66,66	0
57	MG	1A	3198	1/1	0.95	0.14	39,39,39,39	0
57	MG	2A	3594	1/1	0.95	0.38	53,53,53,53	0
57	MG	2A	3231	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3445	1/1	0.95	0.13	25,25,25,25	0
57	MG	1A	3455	1/1	0.95	0.14	49,49,49,49	0
57	MG	2A	3480	1/1	0.95	0.19	24,24,24,24	0
57	MG	1A	3482	1/1	0.95	0.20	54,54,54,54	0
57	MG	1A	3587	1/1	0.95	0.22	44,44,44,44	0
57	MG	2a	1762	1/1	0.95	0.08	51,51,51,51	0
57	MG	1x	113	1/1	0.95	0.10	64,64,64,64	0
57	MG	2A	3172	1/1	0.95	0.12	62,62,62,62	0
57	MG	1A	3757	1/1	0.95	0.14	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	3060	1/1	0.95	0.32	50,50,50,50	0
57	MG	1A	3001	1/1	0.95	0.15	39,39,39,39	0
57	MG	1A	3958	1/1	0.95	0.17	23,23,23,23	0
57	MG	2A	3452	1/1	0.95	0.14	47,47,47,47	0
57	MG	1a	1756	1/1	0.95	0.12	45,45,45,45	0
57	MG	2A	3223	1/1	0.95	0.11	50,50,50,50	0
59	ZN	14	102	1/1	0.95	0.07	94,94,94,94	0
57	MG	1A	3108	1/1	0.95	0.13	31,31,31,31	0
57	MG	15	103	1/1	0.95	0.12	24,24,24,24	0
57	MG	1a	1714	1/1	0.95	0.09	58,58,58,58	0
57	MG	1F	308	1/1	0.95	0.17	41,41,41,41	0
57	MG	2A	3662	1/1	0.95	0.07	54,54,54,54	0
57	MG	2A	3350	1/1	0.95	0.13	65,65,65,65	0
57	MG	2A	3303	1/1	0.95	0.13	45,45,45,45	0
57	MG	1A	3679	1/1	0.95	0.16	34,34,34,34	0
57	MG	1P	202	1/1	0.95	0.19	31,31,31,31	0
57	MG	1A	3766	1/1	0.95	0.16	42,42,42,42	0
57	MG	1A	3524	1/1	0.95	0.13	68,68,68,68	0
57	MG	2A	3093	1/1	0.95	0.34	51,51,51,51	0
57	MG	2A	3486	1/1	0.95	0.12	53,53,53,53	0
57	MG	2A	3446	1/1	0.95	0.19	56,56,56,56	0
57	MG	2a	1823	1/1	0.95	0.21	49,49,49,49	0
57	MG	2A	3750	1/1	0.95	0.08	54,54,54,54	0
57	MG	1W	206	1/1	0.95	0.20	29,29,29,29	0
57	MG	2a	1663	1/1	0.95	0.11	56,56,56,56	0
57	MG	1A	3434	1/1	0.95	0.14	39,39,39,39	0
57	MG	1A	3013	1/1	0.95	0.14	24,24,24,24	0
57	MG	1D	308	1/1	0.95	0.19	31,31,31,31	0
57	MG	2a	1821	1/1	0.95	0.28	58,58,58,58	0
57	MG	2A	3183	1/1	0.95	0.13	47,47,47,47	0
57	MG	1A	3817	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3041	1/1	0.95	0.16	35,35,35,35	0
57	MG	1A	3350	1/1	0.95	0.15	44,44,44,44	0
57	MG	1B	223	1/1	0.95	0.21	37,37,37,37	0
57	MG	2B	211	1/1	0.95	0.12	57,57,57,57	0
57	MG	1a	1642	1/1	0.95	0.14	58,58,58,58	0
57	MG	2A	3732	1/1	0.95	0.14	56,56,56,56	0
57	MG	2A	3035	1/1	0.95	0.14	32,32,32,32	0
57	MG	2a	1658	1/1	0.95	0.12	57,57,57,57	0
57	MG	1A	3312	1/1	0.95	0.20	35,35,35,35	0
57	MG	2A	3108	1/1	0.95	0.40	49,49,49,49	0
57	MG	1a	1724	1/1	0.95	0.19	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1Y	202	1/1	0.95	0.21	64,64,64,64	0
57	MG	1A	3210	1/1	0.95	0.10	38,38,38,38	0
57	MG	2A	3007	1/1	0.95	0.17	46,46,46,46	0
57	MG	1S	201	1/1	0.95	0.12	38,38,38,38	0
57	MG	2A	3889	1/1	0.95	0.12	55,55,55,55	0
57	MG	2a	1802	1/1	0.95	0.18	50,50,50,50	0
57	MG	1A	3662	1/1	0.95	0.06	49,49,49,49	0
57	MG	2A	3843	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3693	1/1	0.95	0.15	26,26,26,26	0
57	MG	1A	3049	1/1	0.95	0.17	19,19,19,19	0
57	MG	1A	3547	1/1	0.95	0.11	41,41,41,41	0
57	MG	1A	3053	1/1	0.95	0.10	32,32,32,32	0
57	MG	1A	3921	1/1	0.95	0.14	31,31,31,31	0
57	MG	2A	3488	1/1	0.95	0.14	37,37,37,37	0
57	MG	1A	3188	1/1	0.95	0.14	34,34,34,34	0
57	MG	2A	3429	1/1	0.95	0.17	43,43,43,43	0
57	MG	2A	3243	1/1	0.95	0.13	63,63,63,63	0
57	MG	1a	1700	1/1	0.95	0.20	48,48,48,48	0
57	MG	10	103	1/1	0.95	0.46	46,46,46,46	0
57	MG	2A	3226	1/1	0.95	0.25	49,49,49,49	0
57	MG	1a	1729	1/1	0.95	0.22	44,44,44,44	0
57	MG	2T	203	1/1	0.95	0.17	42,42,42,42	0
57	MG	2A	3368	1/1	0.95	0.07	50,50,50,50	0
57	MG	1A	3517	1/1	0.95	0.27	31,31,31,31	0
57	MG	2a	1643	1/1	0.95	0.26	56,56,56,56	0
57	MG	2A	3333	1/1	0.95	0.37	59,59,59,59	0
57	MG	2I	101	1/1	0.95	0.35	47,47,47,47	0
57	MG	2a	1789	1/1	0.95	0.21	51,51,51,51	0
57	MG	1x	105	1/1	0.95	0.19	51,51,51,51	0
57	MG	1Q	203	1/1	0.95	0.17	40,40,40,40	0
57	MG	1A	3173	1/1	0.95	0.17	35,35,35,35	0
57	MG	1B	209	1/1	0.95	0.20	44,44,44,44	0
57	MG	1e	202	1/1	0.95	0.21	53,53,53,53	0
57	MG	2A	3697	1/1	0.95	0.11	44,44,44,44	0
57	MG	2a	1790	1/1	0.95	0.08	49,49,49,49	0
57	MG	1A	3591	1/1	0.95	0.27	32,32,32,32	0
57	MG	1A	3940	1/1	0.95	0.17	33,33,33,33	0
57	MG	1A	3435	1/1	0.95	0.11	43,43,43,43	0
57	MG	1A	3388	1/1	0.95	0.17	23,23,23,23	0
57	MG	1A	3841	1/1	0.95	0.20	60,60,60,60	0
57	MG	1W	205	1/1	0.95	0.15	36,36,36,36	0
57	MG	1a	1618	1/1	0.96	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1V	205	1/1	0.96	0.15	26,26,26,26	0
57	MG	1a	1613	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3154	1/1	0.96	0.21	37,37,37,37	0
57	MG	1A	3207	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3803	1/1	0.96	0.22	17,17,17,17	0
57	MG	1A	3612	1/1	0.96	0.13	29,29,29,29	0
57	MG	1A	3143	1/1	0.96	0.19	34,34,34,34	0
57	MG	1A	3578	1/1	0.96	0.19	33,33,33,33	0
57	MG	1A	3056	1/1	0.96	0.22	39,39,39,39	0
57	MG	1B	216	1/1	0.96	0.23	47,47,47,47	0
57	MG	1A	3476	1/1	0.96	0.17	45,45,45,45	0
57	MG	2A	3591	1/1	0.96	0.14	33,33,33,33	0
57	MG	2A	3158	1/1	0.96	0.18	48,48,48,48	0
57	MG	1E	309	1/1	0.96	0.20	24,24,24,24	0
57	MG	2A	3234	1/1	0.96	0.17	43,43,43,43	0
57	MG	1m	3001	1/1	0.96	0.13	49,49,49,49	0
57	MG	2A	3586	1/1	0.96	0.22	50,50,50,50	0
57	MG	2A	3580	1/1	0.96	0.12	46,46,46,46	0
57	MG	1A	3529	1/1	0.96	0.16	35,35,35,35	0
57	MG	1A	3485	1/1	0.96	0.14	41,41,41,41	0
57	MG	1G	202	1/1	0.96	0.25	50,50,50,50	0
57	MG	1w	105	1/1	0.96	0.20	50,50,50,50	0
57	MG	1A	3244	1/1	0.96	0.09	44,44,44,44	0
57	MG	2a	1836	1/1	0.96	0.17	54,54,54,54	0
57	MG	2a	1794	1/1	0.96	0.10	57,57,57,57	0
57	MG	1V	208	1/1	0.96	0.11	33,33,33,33	0
57	MG	2A	3363	1/1	0.96	0.11	59,59,59,59	0
57	MG	1B	215	1/1	0.96	0.25	38,38,38,38	0
57	MG	2A	3362	1/1	0.96	0.46	51,51,51,51	0
57	MG	2A	3771	1/1	0.96	0.12	33,33,33,33	0
57	MG	1a	1728	1/1	0.96	0.19	65,65,65,65	0
57	MG	1A	3926	1/1	0.96	0.19	31,31,31,31	0
57	MG	1A	3718	1/1	0.96	0.13	42,42,42,42	0
57	MG	1A	3877	1/1	0.96	0.22	33,33,33,33	0
57	MG	1A	3346	1/1	0.96	0.29	35,35,35,35	0
57	MG	1A	3882	1/1	0.96	0.17	35,35,35,35	0
57	MG	1A	3769	1/1	0.96	0.18	39,39,39,39	0
57	MG	2A	3031	1/1	0.96	0.11	52,52,52,52	0
57	MG	1a	1757	1/1	0.96	0.14	44,44,44,44	0
57	MG	2A	3481	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3489	1/1	0.96	0.14	32,32,32,32	0
57	MG	2A	3374	1/1	0.96	0.14	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	3675	1/1	0.96	0.15	48,48,48,48	0
57	MG	23	104	1/1	0.96	0.13	45,45,45,45	0
57	MG	2A	3491	1/1	0.96	0.18	59,59,59,59	0
57	MG	2A	3406	1/1	0.96	0.09	52,52,52,52	0
57	MG	1A	3617	1/1	0.96	0.20	42,42,42,42	0
57	MG	1A	3208	1/1	0.96	0.10	39,39,39,39	0
57	MG	1A	3196	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3561	1/1	0.96	0.24	31,31,31,31	0
57	MG	2a	1782	1/1	0.96	0.14	49,49,49,49	0
57	MG	1a	1686	1/1	0.96	0.10	48,48,48,48	0
57	MG	1A	3279	1/1	0.96	0.21	30,30,30,30	0
57	MG	1A	3473	1/1	0.96	0.14	43,43,43,43	0
57	MG	2a	1769	1/1	0.96	0.11	66,66,66,66	0
57	MG	1a	1612	1/1	0.96	0.27	52,52,52,52	0
57	MG	2A	3246	1/1	0.96	0.23	57,57,57,57	0
57	MG	1A	3862	1/1	0.96	0.15	51,51,51,51	0
57	MG	1a	1733	1/1	0.96	0.16	58,58,58,58	0
57	MG	1a	1685	1/1	0.96	0.13	61,61,61,61	0
57	MG	1A	3319	1/1	0.96	0.21	27,27,27,27	0
57	MG	1A	3923	1/1	0.96	0.15	20,20,20,20	0
57	MG	2A	3469	1/1	0.96	0.33	44,44,44,44	0
57	MG	1V	207	1/1	0.96	0.13	36,36,36,36	0
57	MG	1A	3107	1/1	0.96	0.14	32,32,32,32	0
57	MG	1A	3695	1/1	0.96	0.16	30,30,30,30	0
57	MG	2A	3051	1/1	0.96	0.18	54,54,54,54	0
57	MG	2l	202	1/1	0.96	0.29	60,60,60,60	0
57	MG	1A	3283	1/1	0.96	0.20	36,36,36,36	0
57	MG	2A	3523	1/1	0.96	0.14	54,54,54,54	0
57	MG	1A	4022	1/1	0.96	0.17	14,14,14,14	0
57	MG	2A	3540	1/1	0.96	0.16	43,43,43,43	0
57	MG	2A	3780	1/1	0.96	0.20	46,46,46,46	0
57	MG	1A	3814	1/1	0.96	0.14	25,25,25,25	0
57	MG	1A	3156	1/1	0.96	0.19	28,28,28,28	0
57	MG	1A	3596	1/1	0.96	0.16	28,28,28,28	0
57	MG	1A	3214	1/1	0.96	0.29	34,34,34,34	0
57	MG	1A	3078	1/1	0.96	0.23	30,30,30,30	0
57	MG	1A	3784	1/1	0.96	0.20	60,60,60,60	0
57	MG	1A	3375	1/1	0.96	0.17	33,33,33,33	0
57	MG	2a	1813	1/1	0.96	0.08	58,58,58,58	0
57	MG	1A	3018	1/1	0.96	0.19	23,23,23,23	0
57	MG	1A	3133	1/1	0.96	0.14	25,25,25,25	0
57	MG	2A	3399	1/1	0.96	0.22	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3407	1/1	0.96	0.15	40,40,40,40	0
59	ZN	29	501	1/1	0.96	0.11	62,62,62,62	0
57	MG	2A	3034	1/1	0.96	0.19	40,40,40,40	0
57	MG	1a	1679	1/1	0.96	0.07	60,60,60,60	0
57	MG	1A	3696	1/1	0.96	0.15	30,30,30,30	0
57	MG	1A	3459	1/1	0.96	0.17	43,43,43,43	0
57	MG	1A	3256	1/1	0.96	0.17	49,49,49,49	0
57	MG	1a	1690	1/1	0.96	0.15	54,54,54,54	0
57	MG	1A	3304	1/1	0.96	0.33	44,44,44,44	0
57	MG	1O	202	1/1	0.96	0.10	47,47,47,47	0
57	MG	2D	302	1/1	0.96	0.17	35,35,35,35	0
57	MG	1A	3512	1/1	0.96	0.21	28,28,28,28	0
57	MG	2A	3396	1/1	0.96	0.18	60,60,60,60	0
57	MG	2A	3668	1/1	0.96	0.15	57,57,57,57	0
57	MG	1A	3801	1/1	0.96	0.15	40,40,40,40	0
57	MG	1F	309	1/1	0.96	0.23	27,27,27,27	0
57	MG	1A	3238	1/1	0.96	0.20	28,28,28,28	0
57	MG	1A	3876	1/1	0.96	0.08	36,36,36,36	0
57	MG	1l	103	1/1	0.96	0.16	44,44,44,44	0
57	MG	2A	3879	1/1	0.96	0.18	43,43,43,43	0
57	MG	1A	3572	1/1	0.96	0.17	49,49,49,49	0
57	MG	2A	3404	1/1	0.96	0.38	62,62,62,62	0
57	MG	2A	3208	1/1	0.96	0.17	50,50,50,50	0
57	MG	2a	1633	1/1	0.96	0.10	73,73,73,73	0
57	MG	1a	1792	1/1	0.96	0.22	53,53,53,53	0
57	MG	2A	3436	1/1	0.96	0.31	46,46,46,46	0
57	MG	1A	3576	1/1	0.96	0.24	30,30,30,30	0
57	MG	2a	1640	1/1	0.96	0.35	65,65,65,65	0
57	MG	1A	3032	1/1	0.96	0.12	22,22,22,22	0
57	MG	1A	3717	1/1	0.96	0.16	35,35,35,35	0
57	MG	1A	3725	1/1	0.96	0.07	23,23,23,23	0
57	MG	2B	206	1/1	0.96	0.19	58,58,58,58	0
57	MG	1A	4107	1/1	0.96	0.14	38,38,38,38	0
57	MG	1a	1639	1/1	0.96	0.26	52,52,52,52	0
57	MG	1A	3089	1/1	0.96	0.10	53,53,53,53	0
58	K	1A	3565	1/1	0.96	0.12	31,31,31,31	0
57	MG	1A	3941	1/1	0.96	0.14	43,43,43,43	0
57	MG	2A	3498	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3656	1/1	0.96	0.17	48,48,48,48	0
57	MG	1A	3506	1/1	0.96	0.15	46,46,46,46	0
57	MG	1A	3760	1/1	0.96	0.13	35,35,35,35	0
57	MG	23	102	1/1	0.96	0.13	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	1A	3297	1/1	0.96	0.29	40,40,40,40	0
57	MG	1A	3270	1/1	0.96	0.11	28,28,28,28	0
57	MG	1A	3184	1/1	0.96	0.27	28,28,28,28	0
57	MG	1a	1653	1/1	0.96	0.17	45,45,45,45	0
57	MG	2A	3848	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3525	1/1	0.96	0.11	48,48,48,48	0
57	MG	2O	201	1/1	0.96	0.09	69,69,69,69	0
57	MG	1A	3508	1/1	0.96	0.13	45,45,45,45	0
57	MG	2w	101	1/1	0.96	0.10	64,64,64,64	0
57	MG	2F	301	1/1	0.96	0.11	41,41,41,41	0
57	MG	1A	3753	1/1	0.96	0.17	17,17,17,17	0
57	MG	1A	3732	1/1	0.96	0.14	47,47,47,47	0
57	MG	1A	3104	1/1	0.96	0.14	42,42,42,42	0
57	MG	2A	3722	1/1	0.96	0.10	56,56,56,56	0
57	MG	1A	3271	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3354	1/1	0.96	0.22	53,53,53,53	0
57	MG	1A	3344	1/1	0.96	0.36	51,51,51,51	0
57	MG	2F	304	1/1	0.96	0.19	48,48,48,48	0
57	MG	1A	3366	1/1	0.96	0.15	26,26,26,26	0
57	MG	1Q	201	1/1	0.96	0.17	28,28,28,28	0
57	MG	1A	3147	1/1	0.96	0.20	34,34,34,34	0
57	MG	1A	3973	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3501	1/1	0.96	0.17	52,52,52,52	0
57	MG	1A	3235	1/1	0.96	0.14	39,39,39,39	0
57	MG	10	104	1/1	0.96	0.14	49,49,49,49	0
57	MG	2a	1832	1/1	0.96	0.14	68,68,68,68	0
57	MG	2A	3871	1/1	0.96	0.12	57,57,57,57	0
57	MG	1A	3442	1/1	0.96	0.16	32,32,32,32	0
57	MG	2A	3068	1/1	0.96	0.15	49,49,49,49	0
57	MG	1A	3611	1/1	0.96	0.13	19,19,19,19	0
57	MG	2A	3785	1/1	0.96	0.07	40,40,40,40	0
57	MG	2a	1683	1/1	0.96	0.08	53,53,53,53	0
57	MG	2a	1656	1/1	0.96	0.29	66,66,66,66	0
57	MG	1A	3298	1/1	0.96	0.34	56,56,56,56	0
57	MG	2a	1697	1/1	0.96	0.13	47,47,47,47	0
57	MG	1A	3621	1/1	0.96	0.21	49,49,49,49	0
57	MG	2a	1628	1/1	0.96	0.11	58,58,58,58	0
57	MG	2a	1689	1/1	0.96	0.10	65,65,65,65	0
57	MG	2A	3178	1/1	0.96	0.18	37,37,37,37	0
57	MG	1A	3318	1/1	0.96	0.20	46,46,46,46	0
57	MG	1A	3666	1/1	0.96	0.19	35,35,35,35	0
57	MG	2a	1650	1/1	0.96	0.20	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	3783	1/1	0.96	0.15	35,35,35,35	0
57	MG	1N	204	1/1	0.96	0.15	39,39,39,39	0
57	MG	18	101	1/1	0.96	0.28	41,41,41,41	0
57	MG	1A	3811	1/1	0.96	0.10	25,25,25,25	0
57	MG	1A	3530	1/1	0.96	0.24	37,37,37,37	0
57	MG	1A	3751	1/1	0.96	0.13	24,24,24,24	0
57	MG	2d	301	1/1	0.96	0.31	58,58,58,58	0
57	MG	2a	1657	1/1	0.96	0.09	41,41,41,41	0
57	MG	2A	3441	1/1	0.96	0.14	38,38,38,38	0
57	MG	2A	3663	1/1	0.96	0.14	44,44,44,44	0
57	MG	1A	3432	1/1	0.96	0.18	26,26,26,26	0
57	MG	2A	3135	1/1	0.96	0.18	43,43,43,43	0
57	MG	2A	3083	1/1	0.96	0.12	44,44,44,44	0
57	MG	2A	3267	1/1	0.96	0.08	48,48,48,48	0
57	MG	2A	3262	1/1	0.96	0.14	39,39,39,39	0
57	MG	2a	1814	1/1	0.96	0.12	60,60,60,60	0
57	MG	2A	3159	1/1	0.96	0.14	55,55,55,55	0
57	MG	2A	3250	1/1	0.96	0.17	43,43,43,43	0
57	MG	2A	3787	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	4076	1/1	0.96	0.16	32,32,32,32	0
57	MG	1A	3096	1/1	0.96	0.11	39,39,39,39	0
57	MG	2A	3504	1/1	0.96	0.11	51,51,51,51	0
57	MG	1A	3221	1/1	0.96	0.25	40,40,40,40	0
57	MG	1A	4114	1/1	0.96	0.13	13,13,13,13	0
57	MG	1A	3673	1/1	0.96	0.19	34,34,34,34	0
57	MG	2A	3189	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3080	1/1	0.96	0.17	32,32,32,32	0
57	MG	1A	3322	1/1	0.96	0.17	41,41,41,41	0
57	MG	2a	1758	1/1	0.96	0.11	73,73,73,73	0
57	MG	2A	3405	1/1	0.96	0.22	53,53,53,53	0
57	MG	2A	3769	1/1	0.96	0.09	58,58,58,58	0
57	MG	1A	4023	1/1	0.96	0.19	19,19,19,19	0
57	MG	1A	3583	1/1	0.96	0.11	51,51,51,51	0
57	MG	1A	3738	1/1	0.96	0.13	51,51,51,51	0
57	MG	1A	3118	1/1	0.96	0.23	43,43,43,43	0
57	MG	2A	3460	1/1	0.96	0.16	41,41,41,41	0
57	MG	2A	3870	1/1	0.96	0.14	34,34,34,34	0
57	MG	1A	3886	1/1	0.96	0.23	34,34,34,34	0
57	MG	1A	3713	1/1	0.96	0.23	31,31,31,31	0
57	MG	1A	3438	1/1	0.96	0.12	39,39,39,39	0
57	MG	1D	312	1/1	0.96	0.18	34,34,34,34	0
57	MG	1A	3413	1/1	0.96	0.12	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	1A	4120	1/1	0.96	0.19	37,37,37,37	0
57	MG	2A	3708	1/1	0.96	0.13	43,43,43,43	0
57	MG	1A	3730	1/1	0.96	0.21	22,22,22,22	0
57	MG	1A	3122	1/1	0.96	0.13	34,34,34,34	0
57	MG	2A	3317	1/1	0.96	0.07	62,62,62,62	0
57	MG	1A	3276	1/1	0.96	0.12	29,29,29,29	0
57	MG	2A	3838	1/1	0.96	0.19	38,38,38,38	0
57	MG	1A	3652	1/1	0.96	0.23	29,29,29,29	0
57	MG	2A	3289	1/1	0.96	0.21	46,46,46,46	0
57	MG	2a	1820	1/1	0.96	0.17	53,53,53,53	0
57	MG	1A	3610	1/1	0.96	0.21	42,42,42,42	0
57	MG	2A	3120	1/1	0.96	0.18	34,34,34,34	0
57	MG	1A	4099	1/1	0.96	0.19	28,28,28,28	0
57	MG	1A	3062	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3182	1/1	0.96	0.14	38,38,38,38	0
57	MG	1a	1656	1/1	0.96	0.18	46,46,46,46	0
57	MG	1A	3076	1/1	0.96	0.17	34,34,34,34	0
57	MG	2A	3627	1/1	0.96	0.17	38,38,38,38	0
57	MG	2a	1774	1/1	0.96	0.12	62,62,62,62	0
57	MG	1A	3185	1/1	0.96	0.21	54,54,54,54	0
57	MG	1A	3002	1/1	0.96	0.22	42,42,42,42	0
57	MG	2E	301	1/1	0.96	0.14	63,63,63,63	0
57	MG	2A	3163	1/1	0.96	0.22	42,42,42,42	0
57	MG	1A	3403	1/1	0.96	0.14	35,35,35,35	0
57	MG	2A	3881	1/1	0.96	0.06	50,50,50,50	0
57	MG	1A	3261	1/1	0.96	0.25	46,46,46,46	0
57	MG	1a	1759	1/1	0.96	0.14	55,55,55,55	0
57	MG	1D	310	1/1	0.96	0.19	44,44,44,44	0
57	MG	2a	1647	1/1	0.96	0.05	62,62,62,62	0
57	MG	2A	3192	1/1	0.96	0.24	51,51,51,51	0
57	MG	2A	3112	1/1	0.96	0.15	36,36,36,36	0
57	MG	1A	3650	1/1	0.96	0.24	55,55,55,55	0
57	MG	1A	3823	1/1	0.96	0.15	19,19,19,19	0
57	MG	2T	202	1/1	0.96	0.20	52,52,52,52	0
57	MG	1a	1747	1/1	0.96	0.09	37,37,37,37	0
57	MG	2U	202	1/1	0.96	0.36	46,46,46,46	0
57	MG	1a	1635	1/1	0.96	0.39	56,56,56,56	0
57	MG	1A	3072	1/1	0.96	0.18	21,21,21,21	0
57	MG	1A	3669	1/1	0.96	0.17	19,19,19,19	0
57	MG	2a	1828	1/1	0.96	0.08	60,60,60,60	0
57	MG	2A	3359	1/1	0.96	0.08	52,52,52,52	0
57	MG	1A	3865	1/1	0.96	0.17	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3356	1/1	0.96	0.16	66,66,66,66	0
57	MG	1D	305	1/1	0.96	0.13	32,32,32,32	0
57	MG	1A	3083	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3794	1/1	0.96	0.16	33,33,33,33	0
57	MG	1w	107	1/1	0.96	0.15	59,59,59,59	0
57	MG	2A	3130	1/1	0.96	0.13	41,41,41,41	0
57	MG	2A	3648	1/1	0.96	0.23	38,38,38,38	0
57	MG	2A	3514	1/1	0.96	0.15	58,58,58,58	0
57	MG	2A	3337	1/1	0.96	0.38	48,48,48,48	0
57	MG	1A	3197	1/1	0.96	0.20	27,27,27,27	0
57	MG	2A	3698	1/1	0.96	0.12	45,45,45,45	0
57	MG	2A	3621	1/1	0.96	0.10	34,34,34,34	0
57	MG	1A	3117	1/1	0.96	0.13	36,36,36,36	0
57	MG	2A	3502	1/1	0.96	0.10	62,62,62,62	0
57	MG	2y	101	1/1	0.96	0.15	60,60,60,60	0
57	MG	1A	3342	1/1	0.96	0.26	45,45,45,45	0
57	MG	1A	4080	1/1	0.96	0.17	29,29,29,29	0
57	MG	1B	211	1/1	0.96	0.14	45,45,45,45	0
57	MG	1A	3341	1/1	0.96	0.14	34,34,34,34	0
57	MG	2A	3657	1/1	0.96	0.20	57,57,57,57	0
57	MG	2q	203	1/1	0.96	0.12	70,70,70,70	0
57	MG	2a	1722	1/1	0.96	0.13	69,69,69,69	0
57	MG	1A	3423	1/1	0.96	0.22	42,42,42,42	0
57	MG	1A	3887	1/1	0.96	0.16	37,37,37,37	0
57	MG	2A	3038	1/1	0.97	0.20	31,31,31,31	0
57	MG	1A	3278	1/1	0.97	0.21	32,32,32,32	0
57	MG	1A	3021	1/1	0.97	0.11	21,21,21,21	0
57	MG	1A	3915	1/1	0.97	0.11	39,39,39,39	0
57	MG	2A	3658	1/1	0.97	0.07	59,59,59,59	0
57	MG	1A	3389	1/1	0.97	0.10	52,52,52,52	0
57	MG	1A	3503	1/1	0.97	0.12	43,43,43,43	0
57	MG	2A	3471	1/1	0.97	0.17	49,49,49,49	0
57	MG	2A	3148	1/1	0.97	0.19	43,43,43,43	0
57	MG	1G	205	1/1	0.97	0.15	45,45,45,45	0
57	MG	1A	3364	1/1	0.97	0.24	44,44,44,44	0
57	MG	1F	310	1/1	0.97	0.16	44,44,44,44	0
57	MG	2A	3473	1/1	0.97	0.11	58,58,58,58	0
57	MG	2a	1784	1/1	0.97	0.17	45,45,45,45	0
57	MG	1a	1627	1/1	0.97	0.15	41,41,41,41	0
57	MG	2a	1810	1/1	0.97	0.15	56,56,56,56	0
57	MG	13	103	1/1	0.97	0.17	33,33,33,33	0
57	MG	1B	217	1/1	0.97	0.21	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	1795	1/1	0.97	0.14	47,47,47,47	0
57	MG	1A	3684	1/1	0.97	0.14	20,20,20,20	0
57	MG	1a	1694	1/1	0.97	0.22	33,33,33,33	0
57	MG	2A	3162	1/1	0.97	0.11	35,35,35,35	0
57	MG	1A	3289	1/1	0.97	0.15	52,52,52,52	0
57	MG	2A	3119	1/1	0.97	0.16	49,49,49,49	0
57	MG	1A	3229	1/1	0.97	0.11	58,58,58,58	0
57	MG	1A	3532	1/1	0.97	0.19	36,36,36,36	0
57	MG	1A	4070	1/1	0.97	0.11	37,37,37,37	0
57	MG	2A	3561	1/1	0.97	0.15	54,54,54,54	0
57	MG	1A	3046	1/1	0.97	0.18	22,22,22,22	0
57	MG	1A	3898	1/1	0.97	0.08	36,36,36,36	0
57	MG	1T	203	1/1	0.97	0.17	39,39,39,39	0
57	MG	2A	3484	1/1	0.97	0.09	47,47,47,47	0
57	MG	1a	1647	1/1	0.97	0.14	48,48,48,48	0
57	MG	2A	3171	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	3950	1/1	0.97	0.12	30,30,30,30	0
57	MG	1A	3064	1/1	0.97	0.16	35,35,35,35	0
57	MG	1A	3157	1/1	0.97	0.20	22,22,22,22	0
57	MG	2A	3099	1/1	0.97	0.11	39,39,39,39	0
57	MG	1A	3175	1/1	0.97	0.15	28,28,28,28	0
57	MG	1U	205	1/1	0.97	0.14	30,30,30,30	0
57	MG	2w	107	1/1	0.97	0.28	55,55,55,55	0
57	MG	2A	3218	1/1	0.97	0.17	55,55,55,55	0
57	MG	2A	3516	1/1	0.97	0.17	49,49,49,49	0
57	MG	1A	4006	1/1	0.97	0.15	22,22,22,22	0
57	MG	10	109	1/1	0.97	0.17	38,38,38,38	0
57	MG	1A	3781	1/1	0.97	0.17	19,19,19,19	0
57	MG	1A	3301	1/1	0.97	0.23	39,39,39,39	0
57	MG	2A	3025	1/1	0.97	0.28	53,53,53,53	0
57	MG	1A	3166	1/1	0.97	0.17	41,41,41,41	0
57	MG	2A	3490	1/1	0.97	0.34	62,62,62,62	0
57	MG	2A	3885	1/1	0.97	0.07	49,49,49,49	0
57	MG	1A	3644	1/1	0.97	0.17	22,22,22,22	0
57	MG	2A	3672	1/1	0.97	0.11	53,53,53,53	0
57	MG	1A	3349	1/1	0.97	0.17	57,57,57,57	0
57	MG	1A	3051	1/1	0.97	0.16	19,19,19,19	0
57	MG	1t	201	1/1	0.97	0.13	51,51,51,51	0
57	MG	1a	1664	1/1	0.97	0.10	41,41,41,41	0
57	MG	1B	221	1/1	0.97	0.20	49,49,49,49	0
57	MG	2a	1691	1/1	0.97	0.12	55,55,55,55	0
57	MG	1a	1609	1/1	0.97	0.21	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4088	1/1	0.97	0.14	44,44,44,44	0
57	MG	1A	3251	1/1	0.97	0.19	28,28,28,28	0
57	MG	1A	3868	1/1	0.97	0.10	42,42,42,42	0
57	MG	10	105	1/1	0.97	0.12	43,43,43,43	0
57	MG	1A	3872	1/1	0.97	0.19	35,35,35,35	0
57	MG	1A	4068	1/1	0.97	0.18	35,35,35,35	0
57	MG	1A	3039	1/1	0.97	0.38	33,33,33,33	0
57	MG	2A	3315	1/1	0.97	0.13	58,58,58,58	0
57	MG	2A	3733	1/1	0.97	0.15	51,51,51,51	0
57	MG	1a	1692	1/1	0.97	0.27	50,50,50,50	0
57	MG	1A	3416	1/1	0.97	0.22	39,39,39,39	0
57	MG	2A	3519	1/1	0.97	0.13	67,67,67,67	0
57	MG	1A	3213	1/1	0.97	0.16	38,38,38,38	0
57	MG	1A	3163	1/1	0.97	0.20	28,28,28,28	0
57	MG	1X	104	1/1	0.97	0.22	44,44,44,44	0
57	MG	1B	202	1/1	0.97	0.24	42,42,42,42	0
57	MG	13	105	1/1	0.97	0.14	41,41,41,41	0
57	MG	2A	3665	1/1	0.97	0.15	29,29,29,29	0
57	MG	1X	106	1/1	0.97	0.14	44,44,44,44	0
57	MG	2A	3660	1/1	0.97	0.14	48,48,48,48	0
57	MG	2A	3070	1/1	0.97	0.21	51,51,51,51	0
57	MG	2A	3609	1/1	0.97	0.28	47,47,47,47	0
57	MG	1A	3736	1/1	0.97	0.17	55,55,55,55	0
57	MG	1U	208	1/1	0.97	0.16	34,34,34,34	0
57	MG	2A	3121	1/1	0.97	0.11	41,41,41,41	0
59	ZN	2n	501	1/1	0.97	0.09	73,73,73,73	0
57	MG	1a	1671	1/1	0.97	0.05	51,51,51,51	0
57	MG	1A	3987	1/1	0.97	0.14	50,50,50,50	0
57	MG	1E	305	1/1	0.97	0.21	31,31,31,31	0
57	MG	2A	3021	1/1	0.97	0.24	40,40,40,40	0
57	MG	1a	1607	1/1	0.97	0.24	45,45,45,45	0
57	MG	1a	1675	1/1	0.97	0.09	55,55,55,55	0
57	MG	1A	3614	1/1	0.97	0.19	21,21,21,21	0
57	MG	2A	3092	1/1	0.97	0.21	31,31,31,31	0
57	MG	2A	3734	1/1	0.97	0.06	54,54,54,54	0
57	MG	2A	3624	1/1	0.97	0.14	57,57,57,57	0
57	MG	1A	3670	1/1	0.97	0.16	24,24,24,24	0
57	MG	1Y	203	1/1	0.97	0.23	37,37,37,37	0
57	MG	1A	3014	1/1	0.97	0.15	30,30,30,30	0
57	MG	2A	3176	1/1	0.97	0.32	58,58,58,58	0
57	MG	1A	3160	1/1	0.97	0.14	50,50,50,50	0
57	MG	1A	3355	1/1	0.97	0.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3818	1/1	0.97	0.11	32,32,32,32	0
59	ZN	1n	102	1/1	0.97	0.15	56,56,56,56	0
57	MG	1a	1806	1/1	0.97	0.12	53,53,53,53	0
57	MG	1A	3243	1/1	0.97	0.19	47,47,47,47	0
57	MG	1a	1651	1/1	0.97	0.20	42,42,42,42	0
57	MG	1A	3645	1/1	0.97	0.18	41,41,41,41	0
57	MG	1A	3422	1/1	0.97	0.14	29,29,29,29	0
57	MG	1A	3658	1/1	0.97	0.15	50,50,50,50	0
57	MG	1f	202	1/1	0.97	0.30	49,49,49,49	0
57	MG	1A	4104	1/1	0.97	0.15	33,33,33,33	0
57	MG	1A	3142	1/1	0.97	0.28	19,19,19,19	0
57	MG	1A	3004	1/1	0.97	0.15	20,20,20,20	0
57	MG	1A	3237	1/1	0.97	0.21	37,37,37,37	0
57	MG	1W	204	1/1	0.97	0.26	39,39,39,39	0
57	MG	1A	3282	1/1	0.97	0.21	53,53,53,53	0
57	MG	1D	304	1/1	0.97	0.18	43,43,43,43	0
57	MG	1U	204	1/1	0.97	0.13	27,27,27,27	0
57	MG	2A	3094	1/1	0.97	0.19	40,40,40,40	0
57	MG	1a	1745	1/1	0.97	0.19	45,45,45,45	0
57	MG	1A	3799	1/1	0.97	0.15	49,49,49,49	0
57	MG	2D	305	1/1	0.97	0.14	30,30,30,30	0
57	MG	1A	3654	1/1	0.97	0.17	29,29,29,29	0
57	MG	1A	3232	1/1	0.97	0.29	57,57,57,57	0
57	MG	1a	1615	1/1	0.97	0.17	35,35,35,35	0
57	MG	2a	1826	1/1	0.97	0.12	61,61,61,61	0
57	MG	1a	1739	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3883	1/1	0.97	0.17	33,33,33,33	0
57	MG	2A	3726	1/1	0.97	0.13	31,31,31,31	0
57	MG	1A	3588	1/1	0.97	0.11	42,42,42,42	0
57	MG	2A	3812	1/1	0.97	0.19	41,41,41,41	0
57	MG	15	101	1/1	0.97	0.13	18,18,18,18	0
57	MG	11	102	1/1	0.97	0.13	56,56,56,56	0
57	MG	2A	3763	1/1	0.97	0.11	54,54,54,54	0
57	MG	1a	1732	1/1	0.97	0.12	58,58,58,58	0
57	MG	1A	3528	1/1	0.97	0.17	40,40,40,40	0
57	MG	2A	3415	1/1	0.97	0.12	51,51,51,51	0
57	MG	2A	3013	1/1	0.97	0.14	42,42,42,42	0
57	MG	1A	3176	1/1	0.97	0.20	13,13,13,13	0
57	MG	2A	3883	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3047	1/1	0.97	0.16	24,24,24,24	0
57	MG	2A	3168	1/1	0.97	0.16	38,38,38,38	0
57	MG	2A	3536	1/1	0.97	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3762	1/1	0.97	0.12	19,19,19,19	0
57	MG	1A	3146	1/1	0.97	0.19	24,24,24,24	0
57	MG	1A	3223	1/1	0.97	0.21	42,42,42,42	0
57	MG	2A	3222	1/1	0.97	0.23	46,46,46,46	0
57	MG	2A	3644	1/1	0.97	0.19	47,47,47,47	0
57	MG	1A	3560	1/1	0.97	0.15	39,39,39,39	0
57	MG	2a	1818	1/1	0.97	0.06	55,55,55,55	0
57	MG	2A	3583	1/1	0.97	0.12	50,50,50,50	0
57	MG	1a	1606	1/1	0.97	0.19	43,43,43,43	0
57	MG	1G	201	1/1	0.97	0.20	35,35,35,35	0
57	MG	2a	1622	1/1	0.97	0.06	59,59,59,59	0
57	MG	2A	3440	1/1	0.97	0.24	54,54,54,54	0
57	MG	1A	3331	1/1	0.97	0.12	46,46,46,46	0
57	MG	1A	3362	1/1	0.97	0.09	55,55,55,55	0
57	MG	1A	3314	1/1	0.97	0.33	46,46,46,46	0
57	MG	1a	1734	1/1	0.97	0.15	46,46,46,46	0
57	MG	1A	3086	1/1	0.97	0.25	33,33,33,33	0
57	MG	1W	201	1/1	0.97	0.21	34,34,34,34	0
57	MG	1A	3976	1/1	0.97	0.12	32,32,32,32	0
57	MG	1A	3912	1/1	0.97	0.15	29,29,29,29	0
57	MG	2A	3012	1/1	0.97	0.13	32,32,32,32	0
57	MG	1A	3893	1/1	0.97	0.14	27,27,27,27	0
57	MG	2A	3713	1/1	0.97	0.15	27,27,27,27	0
57	MG	2A	3596	1/1	0.97	0.12	47,47,47,47	0
57	MG	1A	3129	1/1	0.97	0.21	30,30,30,30	0
57	MG	12	101	1/1	0.97	0.26	45,45,45,45	0
57	MG	1A	3061	1/1	0.97	0.23	30,30,30,30	0
57	MG	1A	3681	1/1	0.97	0.18	28,28,28,28	0
57	MG	1A	3057	1/1	0.97	0.24	40,40,40,40	0
57	MG	2A	3840	1/1	0.97	0.09	54,54,54,54	0
57	MG	1a	1619	1/1	0.97	0.17	47,47,47,47	0
57	MG	1A	3131	1/1	0.97	0.19	34,34,34,34	0
57	MG	2Q	203	1/1	0.97	0.20	48,48,48,48	0
57	MG	1A	3031	1/1	0.97	0.17	24,24,24,24	0
57	MG	2A	3692	1/1	0.97	0.19	36,36,36,36	0
57	MG	1B	212	1/1	0.97	0.23	50,50,50,50	0
57	MG	1A	3605	1/1	0.97	0.16	48,48,48,48	0
57	MG	2a	1791	1/1	0.97	0.11	66,66,66,66	0
57	MG	1A	3373	1/1	0.97	0.24	43,43,43,43	0
57	MG	1A	3137	1/1	0.97	0.14	25,25,25,25	0
57	MG	2A	3388	1/1	0.97	0.24	52,52,52,52	0
57	MG	28	102	1/1	0.97	0.15	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	3648	1/1	0.97	0.15	19,19,19,19	0
57	MG	1A	3830	1/1	0.97	0.15	22,22,22,22	0
57	MG	2a	1701	1/1	0.97	0.24	31,31,31,31	0
57	MG	2a	1708	1/1	0.97	0.28	63,63,63,63	0
57	MG	1A	3374	1/1	0.97	0.14	39,39,39,39	0
57	MG	17	105	1/1	0.97	0.14	46,46,46,46	0
57	MG	1A	3092	1/1	0.97	0.29	38,38,38,38	0
57	MG	1A	3804	1/1	0.97	0.16	32,32,32,32	0
57	MG	2O	202	1/1	0.97	0.12	57,57,57,57	0
57	MG	1A	3639	1/1	0.97	0.13	20,20,20,20	0
57	MG	1A	3347	1/1	0.97	0.23	30,30,30,30	0
57	MG	1A	3724	1/1	0.97	0.35	54,54,54,54	0
57	MG	2A	3512	1/1	0.97	0.15	37,37,37,37	0
57	MG	2A	3042	1/1	0.97	0.17	47,47,47,47	0
57	MG	2A	3206	1/1	0.97	0.13	49,49,49,49	0
57	MG	2A	3619	1/1	0.97	0.14	47,47,47,47	0
57	MG	1A	3557	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3659	1/1	0.97	0.13	28,28,28,28	0
57	MG	1A	3019	1/1	0.97	0.27	35,35,35,35	0
57	MG	1a	1698	1/1	0.97	0.33	39,39,39,39	0
57	MG	1U	209	1/1	0.97	0.14	33,33,33,33	0
57	MG	1A	3484	1/1	0.97	0.15	40,40,40,40	0
57	MG	2A	3794	1/1	0.97	0.08	62,62,62,62	0
57	MG	2A	3636	1/1	0.97	0.16	41,41,41,41	0
57	MG	1B	222	1/1	0.97	0.18	56,56,56,56	0
57	MG	1A	4038	1/1	0.97	0.21	34,34,34,34	0
57	MG	1A	3623	1/1	0.97	0.14	22,22,22,22	0
57	MG	15	102	1/1	0.97	0.12	30,30,30,30	0
57	MG	2A	3520	1/1	0.97	0.12	42,42,42,42	0
57	MG	1a	1682	1/1	0.97	0.12	43,43,43,43	0
57	MG	1A	3011	1/1	0.97	0.18	33,33,33,33	0
57	MG	2A	3044	1/1	0.97	0.23	57,57,57,57	0
57	MG	2A	3395	1/1	0.97	0.17	58,58,58,58	0
57	MG	1A	3007	1/1	0.97	0.17	35,35,35,35	0
57	MG	1A	3330	1/1	0.97	0.23	51,51,51,51	0
57	MG	2A	3510	1/1	0.97	0.12	20,20,20,20	0
57	MG	1Q	202	1/1	0.97	0.23	31,31,31,31	0
57	MG	2a	1757	1/1	0.97	0.09	50,50,50,50	0
57	MG	2A	3757	1/1	0.97	0.23	44,44,44,44	0
57	MG	2V	202	1/1	0.97	0.20	41,41,41,41	0
57	MG	2A	3214	1/1	0.97	0.09	54,54,54,54	0
57	MG	1A	3953	1/1	0.97	0.14	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	3840	1/1	0.97	0.12	44,44,44,44	0
57	MG	1B	206	1/1	0.97	0.16	47,47,47,47	0
57	MG	1U	206	1/1	0.97	0.13	32,32,32,32	0
57	MG	2A	3776	1/1	0.97	0.09	55,55,55,55	0
57	MG	1A	3177	1/1	0.97	0.22	34,34,34,34	0
57	MG	2A	3016	1/1	0.97	0.14	56,56,56,56	0
57	MG	2A	3027	1/1	0.97	0.36	54,54,54,54	0
57	MG	1A	3045	1/1	0.97	0.14	29,29,29,29	0
57	MG	1A	3371	1/1	0.97	0.10	40,40,40,40	0
57	MG	2a	1629	1/1	0.97	0.17	51,51,51,51	0
57	MG	2A	3277	1/1	0.97	0.16	50,50,50,50	0
57	MG	1A	3227	1/1	0.97	0.18	26,26,26,26	0
57	MG	2A	3390	1/1	0.97	0.18	39,39,39,39	0
57	MG	1A	3199	1/1	0.97	0.15	28,28,28,28	0
57	MG	1A	3911	1/1	0.98	0.12	46,46,46,46	0
57	MG	2D	303	1/1	0.98	0.20	46,46,46,46	0
57	MG	1A	3164	1/1	0.98	0.18	27,27,27,27	0
57	MG	2A	3075	1/1	0.98	0.29	39,39,39,39	0
57	MG	1A	3307	1/1	0.98	0.16	26,26,26,26	0
57	MG	1A	3151	1/1	0.98	0.37	34,34,34,34	0
57	MG	1A	3616	1/1	0.98	0.21	20,20,20,20	0
57	MG	1A	3622	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3537	1/1	0.98	0.28	35,35,35,35	0
57	MG	2A	3705	1/1	0.98	0.15	50,50,50,50	0
57	MG	1A	3042	1/1	0.98	0.23	26,26,26,26	0
57	MG	1A	3134	1/1	0.98	0.12	38,38,38,38	0
57	MG	1A	3599	1/1	0.98	0.20	57,57,57,57	0
57	MG	1A	3037	1/1	0.98	0.21	20,20,20,20	0
57	MG	1a	1740	1/1	0.98	0.17	48,48,48,48	0
57	MG	2A	3874	1/1	0.98	0.20	47,47,47,47	0
57	MG	1A	3545	1/1	0.98	0.21	51,51,51,51	0
57	MG	1E	313	1/1	0.98	0.08	30,30,30,30	0
57	MG	2A	3526	1/1	0.98	0.09	37,37,37,37	0
57	MG	1A	3778	1/1	0.98	0.17	23,23,23,23	0
57	MG	2A	3141	1/1	0.98	0.15	30,30,30,30	0
57	MG	1A	3568	1/1	0.98	0.25	26,26,26,26	0
57	MG	2A	3249	1/1	0.98	0.22	49,49,49,49	0
57	MG	1A	3225	1/1	0.98	0.16	22,22,22,22	0
57	MG	1A	3703	1/1	0.98	0.18	42,42,42,42	0
57	MG	1A	3114	1/1	0.98	0.18	26,26,26,26	0
57	MG	1a	1644	1/1	0.98	0.35	55,55,55,55	0
57	MG	1A	3192	1/1	0.98	0.11	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3275	1/1	0.98	0.23	20,20,20,20	0
57	MG	2A	3457	1/1	0.98	0.12	56,56,56,56	0
57	MG	1R	202	1/1	0.98	0.18	31,31,31,31	0
57	MG	1A	3003	1/1	0.98	0.19	25,25,25,25	0
57	MG	2A	3746	1/1	0.98	0.18	38,38,38,38	0
57	MG	1D	303	1/1	0.98	0.23	18,18,18,18	0
57	MG	2A	3786	1/1	0.98	0.09	42,42,42,42	0
57	MG	2a	1679	1/1	0.98	0.14	44,44,44,44	0
57	MG	1A	3300	1/1	0.98	0.39	38,38,38,38	0
57	MG	1A	3531	1/1	0.98	0.22	31,31,31,31	0
57	MG	1A	3081	1/1	0.98	0.22	31,31,31,31	0
57	MG	1A	3708	1/1	0.98	0.20	46,46,46,46	0
57	MG	17	102	1/1	0.98	0.17	28,28,28,28	0
57	MG	1A	3009	1/1	0.98	0.16	22,22,22,22	0
59	ZN	25	106	1/1	0.98	0.19	65,65,65,65	0
57	MG	1A	3348	1/1	0.98	0.13	23,23,23,23	0
57	MG	1A	3267	1/1	0.98	0.12	49,49,49,49	0
57	MG	1A	3966	1/1	0.98	0.19	38,38,38,38	0
57	MG	1A	3859	1/1	0.98	0.20	17,17,17,17	0
57	MG	2a	1648	1/1	0.98	0.33	59,59,59,59	0
57	MG	1A	3874	1/1	0.98	0.14	24,24,24,24	0
57	MG	1A	3286	1/1	0.98	0.18	31,31,31,31	0
57	MG	2A	3595	1/1	0.98	0.14	54,54,54,54	0
57	MG	1A	3969	1/1	0.98	0.22	46,46,46,46	0
57	MG	2A	3082	1/1	0.98	0.09	52,52,52,52	0
57	MG	2A	3173	1/1	0.98	0.23	55,55,55,55	0
57	MG	1A	3191	1/1	0.98	0.18	24,24,24,24	0
57	MG	1A	3226	1/1	0.98	0.17	30,30,30,30	0
57	MG	2A	3772	1/1	0.98	0.16	41,41,41,41	0
57	MG	1A	3209	1/1	0.98	0.14	27,27,27,27	0
57	MG	1w	109	1/1	0.98	0.22	46,46,46,46	0
57	MG	2A	3549	1/1	0.98	0.21	37,37,37,37	0
57	MG	2A	3867	1/1	0.98	0.14	24,24,24,24	0
57	MG	1A	3174	1/1	0.98	0.20	28,28,28,28	0
57	MG	1n	101	1/1	0.98	0.12	50,50,50,50	0
57	MG	2A	3196	1/1	0.98	0.31	53,53,53,53	0
57	MG	1A	3791	1/1	0.98	0.19	19,19,19,19	0
57	MG	1A	3812	1/1	0.98	0.20	19,19,19,19	0
57	MG	2A	3628	1/1	0.98	0.12	51,51,51,51	0
57	MG	1A	3595	1/1	0.98	0.28	26,26,26,26	0
57	MG	1A	3632	1/1	0.98	0.14	32,32,32,32	0
57	MG	1A	3106	1/1	0.98	0.14	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3643	1/1	0.98	0.11	31,31,31,31	0
57	MG	13	102	1/1	0.98	0.17	31,31,31,31	0
57	MG	1A	3052	1/1	0.98	0.23	21,21,21,21	0
57	MG	2A	3425	1/1	0.98	0.17	38,38,38,38	0
57	MG	1A	3201	1/1	0.98	0.21	20,20,20,20	0
57	MG	2a	1644	1/1	0.98	0.32	61,61,61,61	0
57	MG	2A	3625	1/1	0.98	0.10	38,38,38,38	0
57	MG	1A	3158	1/1	0.98	0.12	23,23,23,23	0
57	MG	1A	3581	1/1	0.98	0.20	32,32,32,32	0
57	MG	1E	301	1/1	0.98	0.22	29,29,29,29	0
57	MG	1E	311	1/1	0.98	0.10	34,34,34,34	0
57	MG	2A	3264	1/1	0.98	0.09	54,54,54,54	0
57	MG	2A	3154	1/1	0.98	0.15	39,39,39,39	0
57	MG	1A	3706	1/1	0.98	0.24	30,30,30,30	0
59	ZN	15	108	1/1	0.98	0.17	40,40,40,40	0
57	MG	1E	306	1/1	0.98	0.17	24,24,24,24	0
57	MG	2F	305	1/1	0.98	0.17	41,41,41,41	0
57	MG	1A	3028	1/1	0.98	0.11	27,27,27,27	0
57	MG	1V	201	1/1	0.98	0.13	19,19,19,19	0
57	MG	2A	3880	1/1	0.98	0.17	44,44,44,44	0
57	MG	1A	3023	1/1	0.98	0.20	12,12,12,12	0
57	MG	1A	3660	1/1	0.98	0.09	34,34,34,34	0
57	MG	1a	1755	1/1	0.98	0.18	32,32,32,32	0
57	MG	1D	309	1/1	0.98	0.26	34,34,34,34	0
57	MG	1A	3365	1/1	0.98	0.16	45,45,45,45	0
57	MG	1A	3837	1/1	0.98	0.17	32,32,32,32	0
57	MG	1A	3586	1/1	0.98	0.14	42,42,42,42	0
57	MG	2A	3019	1/1	0.98	0.14	46,46,46,46	0
57	MG	1A	3230	1/1	0.98	0.18	45,45,45,45	0
57	MG	1A	3264	1/1	0.98	0.11	29,29,29,29	0
57	MG	1w	110	1/1	0.98	0.13	65,65,65,65	0
57	MG	1A	3719	1/1	0.98	0.20	52,52,52,52	0
57	MG	2A	3576	1/1	0.98	0.15	37,37,37,37	0
57	MG	1a	1673	1/1	0.98	0.17	45,45,45,45	0
57	MG	2A	3585	1/1	0.98	0.10	35,35,35,35	0
57	MG	1V	203	1/1	0.98	0.17	26,26,26,26	0
57	MG	1A	4037	1/1	0.98	0.08	40,40,40,40	0
57	MG	1A	3800	1/1	0.98	0.17	41,41,41,41	0
57	MG	2A	3538	1/1	0.98	0.17	40,40,40,40	0
57	MG	2A	3020	1/1	0.98	0.10	28,28,28,28	0
57	MG	1A	3867	1/1	0.98	0.27	36,36,36,36	0
57	MG	2A	3789	1/1	0.98	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	3850	1/1	0.98	0.13	41,41,41,41	0
57	MG	2a	1751	1/1	0.98	0.12	58,58,58,58	0
57	MG	2A	3029	1/1	0.98	0.11	40,40,40,40	0
57	MG	2A	3632	1/1	0.98	0.10	43,43,43,43	0
57	MG	2A	3562	1/1	0.98	0.12	34,34,34,34	0
57	MG	1A	3075	1/1	0.98	0.16	37,37,37,37	0
57	MG	1A	3686	1/1	0.98	0.14	35,35,35,35	0
57	MG	1A	3030	1/1	0.98	0.20	26,26,26,26	0
57	MG	1A	3215	1/1	0.98	0.19	31,31,31,31	0
57	MG	1a	1670	1/1	0.98	0.24	59,59,59,59	0
57	MG	1B	214	1/1	0.98	0.27	36,36,36,36	0
57	MG	2a	1720	1/1	0.98	0.11	66,66,66,66	0
57	MG	1A	3546	1/1	0.98	0.21	43,43,43,43	0
60	SF4	2d	303	8/8	0.98	0.11	64,67,77,77	0
57	MG	2A	3078	1/1	0.98	0.21	24,24,24,24	0
57	MG	2A	3263	1/1	0.98	0.17	49,49,49,49	0
57	MG	2v	104	1/1	0.98	0.16	47,47,47,47	0
57	MG	2X	103	1/1	0.98	0.16	40,40,40,40	0
57	MG	1U	201	1/1	0.98	0.18	28,28,28,28	0
57	MG	1U	202	1/1	0.98	0.19	41,41,41,41	0
57	MG	1a	1725	1/1	0.98	0.18	37,37,37,37	0
57	MG	2A	3875	1/1	0.98	0.18	26,26,26,26	0
57	MG	1A	3380	1/1	0.98	0.15	31,31,31,31	0
57	MG	1A	4108	1/1	0.98	0.20	33,33,33,33	0
57	MG	1A	3397	1/1	0.98	0.18	31,31,31,31	0
57	MG	2A	3755	1/1	0.98	0.10	38,38,38,38	0
57	MG	1A	3302	1/1	0.98	0.31	27,27,27,27	0
57	MG	1V	202	1/1	0.98	0.15	32,32,32,32	0
57	MG	2Q	201	1/1	0.98	0.10	58,58,58,58	0
57	MG	1A	3010	1/1	0.98	0.20	30,30,30,30	0
57	MG	1A	3387	1/1	0.98	0.13	29,29,29,29	0
57	MG	1A	3477	1/1	0.98	0.18	30,30,30,30	0
57	MG	1A	3641	1/1	0.98	0.15	18,18,18,18	0
57	MG	1F	306	1/1	0.98	0.15	26,26,26,26	0
57	MG	1A	3079	1/1	0.98	0.23	31,31,31,31	0
57	MG	1a	1689	1/1	0.98	0.13	55,55,55,55	0
57	MG	1A	3363	1/1	0.98	0.34	32,32,32,32	0
57	MG	2A	3061	1/1	0.98	0.10	40,40,40,40	0
57	MG	1N	203	1/1	0.98	0.26	33,33,33,33	0
57	MG	2A	3724	1/1	0.98	0.17	44,44,44,44	0
57	MG	1A	3464	1/1	0.98	0.20	33,33,33,33	0
57	MG	1A	3008	1/1	0.98	0.18	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3529	1/1	0.98	0.11	27,27,27,27	0
57	MG	1A	3828	1/1	0.98	0.10	30,30,30,30	0
57	MG	1E	304	1/1	0.98	0.13	26,26,26,26	0
57	MG	1A	3048	1/1	0.98	0.20	27,27,27,27	0
57	MG	2A	3122	1/1	0.98	0.08	57,57,57,57	0
57	MG	1A	3997	1/1	0.98	0.17	53,53,53,53	0
57	MG	1A	3036	1/1	0.98	0.12	37,37,37,37	0
57	MG	1A	3033	1/1	0.98	0.12	26,26,26,26	0
57	MG	1A	3468	1/1	0.98	0.13	53,53,53,53	0
57	MG	2A	3537	1/1	0.98	0.18	30,30,30,30	0
57	MG	18	102	1/1	0.98	0.19	41,41,41,41	0
57	MG	1a	1660	1/1	0.98	0.07	48,48,48,48	0
57	MG	1A	3234	1/1	0.98	0.17	28,28,28,28	0
57	MG	2a	1638	1/1	0.98	0.21	49,49,49,49	0
57	MG	1A	3858	1/1	0.98	0.17	32,32,32,32	0
57	MG	1A	4034	1/1	0.99	0.16	19,19,19,19	0
57	MG	1a	1819	1/1	0.99	0.25	47,47,47,47	0
57	MG	25	104	1/1	0.99	0.10	35,35,35,35	0
57	MG	1A	3552	1/1	0.99	0.17	47,47,47,47	0
57	MG	1A	3167	1/1	0.99	0.14	14,14,14,14	0
57	MG	1A	3012	1/1	0.99	0.17	20,20,20,20	0
57	MG	1A	3094	1/1	0.99	0.22	20,20,20,20	0
57	MG	1A	3128	1/1	0.99	0.24	27,27,27,27	0
57	MG	1A	3120	1/1	0.99	0.17	27,27,27,27	0
57	MG	1A	3558	1/1	0.99	0.17	20,20,20,20	0
57	MG	1A	3097	1/1	0.99	0.11	33,33,33,33	0
59	ZN	26	102	1/1	0.99	0.18	47,47,47,47	0
57	MG	2A	3600	1/1	0.99	0.15	51,51,51,51	0
57	MG	1A	3787	1/1	0.99	0.13	23,23,23,23	0
57	MG	1A	3058	1/1	0.99	0.18	23,23,23,23	0
57	MG	1A	3737	1/1	0.99	0.16	43,43,43,43	0
57	MG	1A	3951	1/1	0.99	0.17	30,30,30,30	0
57	MG	1A	4109	1/1	0.99	0.11	49,49,49,49	0
57	MG	1A	3138	1/1	0.99	0.24	13,13,13,13	0
57	MG	1A	3885	1/1	0.99	0.16	31,31,31,31	0
57	MG	1A	3515	1/1	0.99	0.18	31,31,31,31	0
58	K	2A	3479	1/1	0.99	0.12	52,52,52,52	0
57	MG	1U	207	1/1	0.99	0.16	27,27,27,27	0
57	MG	1A	3419	1/1	0.99	0.19	40,40,40,40	0
57	MG	1A	3829	1/1	0.99	0.21	21,21,21,21	0
57	MG	1A	3038	1/1	0.99	0.13	21,21,21,21	0
57	MG	1A	3315	1/1	0.99	0.23	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3700	1/1	0.99	0.14	56,56,56,56	0
57	MG	2e	201	1/1	0.99	0.12	58,58,58,58	0
57	MG	2A	3674	1/1	0.99	0.23	40,40,40,40	0
57	MG	1a	1667	1/1	0.99	0.11	65,65,65,65	0
57	MG	1A	3630	1/1	0.99	0.20	24,24,24,24	0
57	MG	1A	3922	1/1	0.99	0.15	29,29,29,29	0
57	MG	2A	3532	1/1	0.99	0.20	39,39,39,39	0
57	MG	1A	3034	1/1	0.99	0.21	28,28,28,28	0
57	MG	2A	3670	1/1	0.99	0.13	33,33,33,33	0
57	MG	1A	4101	1/1	0.99	0.23	20,20,20,20	0
57	MG	1A	3172	1/1	0.99	0.14	19,19,19,19	0
57	MG	1A	4113	1/1	0.99	0.22	25,25,25,25	0
57	MG	1F	302	1/1	0.99	0.18	25,25,25,25	0
57	MG	1D	302	1/1	0.99	0.14	37,37,37,37	0
57	MG	1A	3280	1/1	0.99	0.20	28,28,28,28	0
57	MG	1A	3649	1/1	0.99	0.15	14,14,14,14	0
57	MG	1A	3386	1/1	0.99	0.32	24,24,24,24	0
57	MG	1A	3426	1/1	0.99	0.26	39,39,39,39	0
60	SF4	1d	302	8/8	0.99	0.14	46,56,61,69	0
57	MG	1A	3711	1/1	0.99	0.12	17,17,17,17	0
57	MG	1A	3839	1/1	0.99	0.22	46,46,46,46	0
57	MG	1A	4098	1/1	0.99	0.23	14,14,14,14	0
57	MG	1a	1631	1/1	0.99	0.26	40,40,40,40	0
57	MG	1a	1731	1/1	0.99	0.13	63,63,63,63	0
57	MG	1A	3928	1/1	0.99	0.22	29,29,29,29	0
59	ZN	19	102	1/1	0.99	0.21	41,41,41,41	0
57	MG	1F	305	1/1	0.99	0.22	25,25,25,25	0
57	MG	2A	3603	1/1	0.99	0.17	55,55,55,55	0
57	MG	1A	3723	1/1	0.99	0.14	13,13,13,13	0
57	MG	1a	1723	1/1	0.99	0.17	45,45,45,45	0
57	MG	2A	3647	1/1	0.99	0.12	57,57,57,57	0
57	MG	1A	3202	1/1	0.99	0.22	26,26,26,26	0
57	MG	1A	3946	1/1	0.99	0.17	12,12,12,12	0
57	MG	2a	1680	1/1	0.99	0.14	44,44,44,44	0
57	MG	2A	3149	1/1	0.99	0.18	26,26,26,26	0
57	MG	2A	3381	1/1	0.99	0.11	45,45,45,45	0
57	MG	2A	3049	1/1	0.99	0.20	21,21,21,21	0
59	ZN	16	102	1/1	0.99	0.20	40,40,40,40	0
57	MG	1A	3085	1/1	0.99	0.25	37,37,37,37	0
57	MG	2A	3634	1/1	0.99	0.12	38,38,38,38	0
57	MG	1A	3825	1/1	1.00	0.11	26,26,26,26	0
57	MG	1A	3707	1/1	1.00	0.24	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3625	1/1	1.00	0.16	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.