



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2022 – 03:43 PM EDT

PDB ID : 8CVK
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Phe-NH-tRNA^{phe}, peptidyl P-site fMRC-NH-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.50Å resolution
Authors : Syroegin, E.A.; Aleksandrova, E.V.; Polikanov, Y.S.
Deposited on : 2022-05-18
Resolution : 2.50 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 types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

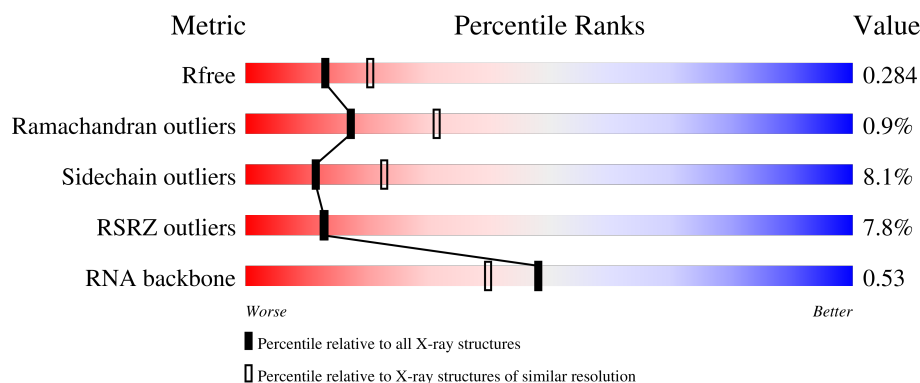
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



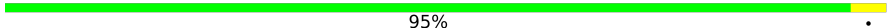

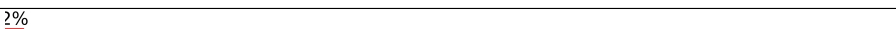
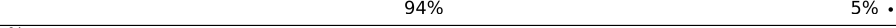


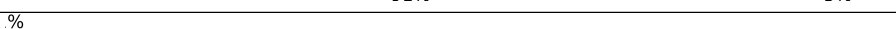
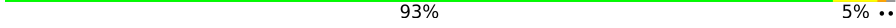


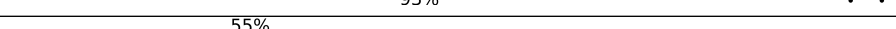


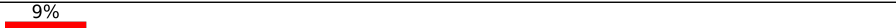
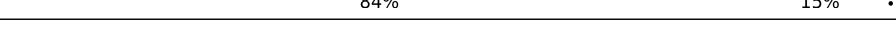
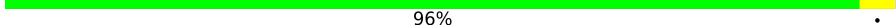

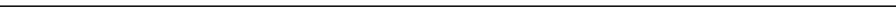
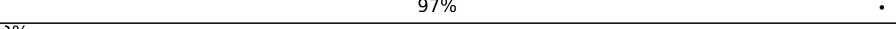
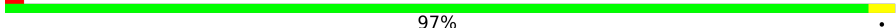



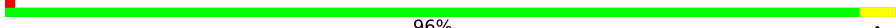

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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>5%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
1	2A	2915	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>.</div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
2	2B	121	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>19%</div> <div>.</div> </div> </div>
3	1D	276	<div> <div></div> <div> <div></div> <div>97%</div> <div>.</div> </div> </div>

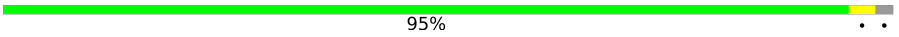
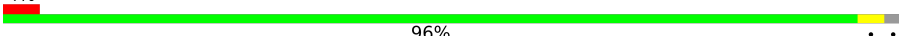
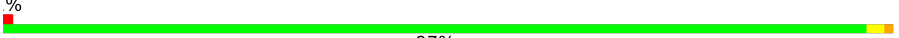
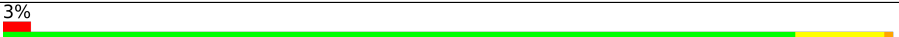
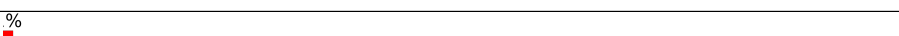
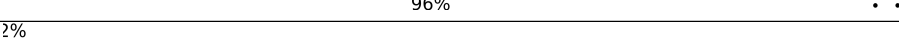
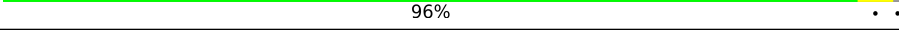
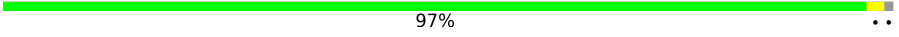
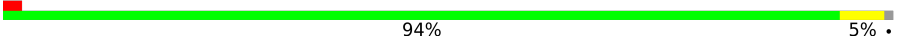


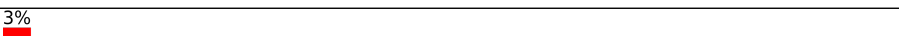

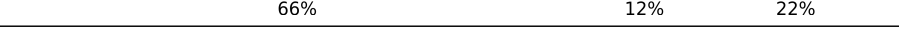
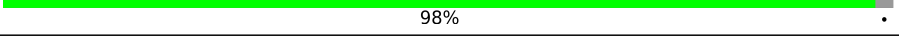
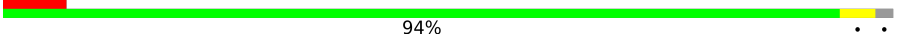
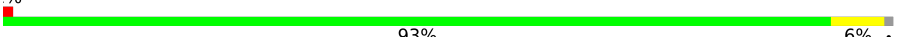


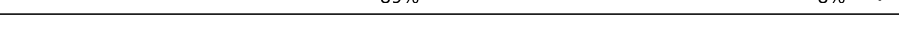

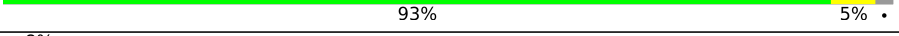
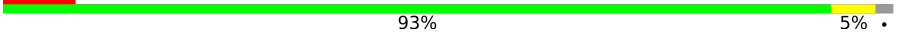


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Mol	Chain	Length	Quality of chain
3	2D	276	 95% .
4	1E	206	 93% 6% .
4	2E	206	 94% 5% .
5	1F	210	 88% 8% .
5	2F	210	 91% 5% .
6	1G	182	 93% 5% ..
6	2G	182	 86% 13% ..
7	1H	180	 93% . .
7	2H	180	 55% 87% 10% .
8	1I	148	 86% 12% ..
8	2I	148	 9% 84% 15% .
9	1N	140	 96% .
9	2N	140	 5% 96% .
10	1O	122	 97% .
10	2O	122	 2% 97% .
11	1P	150	 92% 7% .
11	2P	150	 18% 90% 9% .
12	1Q	141	 96% .
12	2Q	141	 9% 96% .
13	1R	118	 97% .
13	2R	118	 97% .
14	1S	112	 93% 5% .
14	2S	112	 6% 92% 6% .
15	1T	146	 87% . 10%
15	2T	146	 2% 84% 6% 10%

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Mol	Chain	Length	Quality of chain
16	1U	118	 95% ..
16	2U	118	 96% ..
17	1V	101	 97% ..
17	2V	101	 89% 10% ..
18	1W	113	 96% ..
18	2W	113	 96% ..
19	1X	96	 97% ..
19	2X	96	 94% 5% ..
20	1Y	110	 93% 5% ..
20	2Y	110	 87% 10% ..
21	1Z	206	 66% 9% 25%
21	2Z	206	 66% 12% 22%
22	10	85	 98% ..
22	20	85	 94% ..
23	11	98	 93% 6% ..
23	21	98	 93% 6% ..
24	12	72	 89% 8% ..
24	22	72	 90% 7% ..
25	13	60	 93% 5% ..
25	23	60	 93% 5% ..
26	14	71	 83% 10% ..
26	24	71	 77% 18% ..
27	15	60	 95% ..
27	25	60	 95% ..
28	16	54	 87% 11% ..

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Mol	Chain	Length	Quality of chain
28	26	54	<div> <div>9%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
29	17	49	<div> <div>92%</div> <div>6%</div> <div>.</div> </div>
29	27	49	<div> <div>4%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
30	18	65	<div> <div>89%</div> <div>9%</div> <div>.</div> </div>
30	28	65	<div> <div>12%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
31	19	37	<div> <div>97%</div> <div>.</div> </div>
31	29	37	<div> <div>16%</div> <div>100%</div> </div>
32	1a	1521	<div> <div>5%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
32	2a	1521	<div> <div>8%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
33	1b	256	<div> <div>15%</div> <div>77%</div> <div>13%</div> <div>10%</div> </div>
33	2b	256	<div> <div>25%</div> <div>74%</div> <div>16%</div> <div>10%</div> </div>
34	1c	239	<div> <div>8%</div> <div>81%</div> <div>5%</div> <div>14%</div> </div>
34	2c	239	<div> <div>27%</div> <div>81%</div> <div>5%</div> <div>14%</div> </div>
35	1d	209	<div> <div>2%</div> <div>93%</div> <div>7%</div> </div>
35	2d	209	<div> <div>%</div> <div>93%</div> <div>7%</div> </div>
36	1e	162	<div> <div>4%</div> <div>86%</div> <div>6%</div> <div>9%</div> </div>
36	2e	162	<div> <div>9%</div> <div>84%</div> <div>7%</div> <div>9%</div> </div>
37	1f	101	<div> <div>95%</div> <div>.</div> <div>.</div> </div>
37	2f	101	<div> <div>95%</div> <div>.</div> <div>.</div> </div>
38	1g	156	<div> <div>9%</div> <div>88%</div> <div>12%</div> <div>.</div> </div>
38	2g	156	<div> <div>19%</div> <div>87%</div> <div>13%</div> <div>.</div> </div>
39	1h	138	<div> <div>3%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
39	2h	138	<div> <div>9%</div> <div>91%</div> <div>9%</div> <div>.</div> </div>
40	1i	128	<div> <div>27%</div> <div>91%</div> <div>9%</div> <div>.</div> </div>
40	2i	128	<div> <div>57%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>

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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	1z	3	
56	2z	3	
57	1y	76	
57	2y	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MIA	1y	37	-	-	-	X
57	PSU	1y	39	-	-	-	X
57	5MU	1y	54	-	-	-	X
57	PSU	1y	55	-	-	-	X
57	PSU	2y	32	-	-	-	X
57	MIA	2y	37	-	-	-	X
57	PSU	2y	39	-	-	-	X
57	5MU	2y	54	-	-	-	X
57	PSU	2y	55	-	-	-	X
58	MG	1A	3074	-	-	-	X
58	MG	1A	3951	-	-	-	X
58	MG	1U	209	-	-	-	X
58	MG	2A	3128	-	-	-	X
58	MG	2A	3351	-	-	-	X
58	MG	2A	3443	-	-	-	X
58	MG	2A	3463	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 300017 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	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 MF-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 Aminoacyl-tRNA Phe-NH-tRNA_{phe}.

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

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMRC-NH-tRNA_{met} RNA-part.

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

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMRC-NH-tRNA_{met} Peptide-part.

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

- Molecule 57 is a RNA chain called E-site Deacylated tRNA_{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
57	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1098	Total	Mg	0	0
			1098	1098		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	37	Total 37	Mg 37	0	0
58	1D	12	Total 12	Mg 12	0	0
58	1E	13	Total 13	Mg 13	0	0
58	1F	14	Total 14	Mg 14	0	0
58	1G	5	Total 5	Mg 5	0	0
58	1I	1	Total 1	Mg 1	0	0
58	1N	6	Total 6	Mg 6	0	0
58	1O	5	Total 5	Mg 5	0	0
58	1P	4	Total 4	Mg 4	0	0
58	1Q	8	Total 8	Mg 8	0	0
58	1R	4	Total 4	Mg 4	0	0
58	1S	3	Total 3	Mg 3	0	0
58	1T	4	Total 4	Mg 4	0	0
58	1U	9	Total 9	Mg 9	0	0
58	1V	7	Total 7	Mg 7	0	0
58	1W	7	Total 7	Mg 7	0	0
58	1X	6	Total 6	Mg 6	0	0
58	1Y	5	Total 5	Mg 5	0	0
58	1Z	2	Total 2	Mg 2	0	0
58	10	9	Total 9	Mg 9	0	0
58	11	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	12	3	Total 3	Mg 3	0	0
58	13	3	Total 3	Mg 3	0	0
58	14	1	Total 1	Mg 1	0	0
58	15	7	Total 7	Mg 7	0	0
58	16	1	Total 1	Mg 1	0	0
58	17	4	Total 4	Mg 4	0	0
58	18	9	Total 9	Mg 9	0	0
58	19	1	Total 1	Mg 1	0	0
58	1a	214	Total 214	Mg 214	0	0
58	1b	1	Total 1	Mg 1	0	0
58	1d	1	Total 1	Mg 1	0	0
58	1e	2	Total 2	Mg 2	0	0
58	1f	2	Total 2	Mg 2	0	0
58	1k	1	Total 1	Mg 1	0	0
58	1l	2	Total 2	Mg 2	0	0
58	1m	1	Total 1	Mg 1	0	0
58	1n	2	Total 2	Mg 2	0	0
58	1t	1	Total 1	Mg 1	0	0
58	1v	1	Total 1	Mg 1	0	0
58	1w	8	Total 8	Mg 8	0	0
58	1x	12	Total 12	Mg 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	2A	870	Total Mg 870 870	0	0
58	2B	20	Total Mg 20 20	0	0
58	2D	8	Total Mg 8 8	0	0
58	2E	10	Total Mg 10 10	0	0
58	2F	8	Total Mg 8 8	0	0
58	2G	1	Total Mg 1 1	0	0
58	2O	1	Total Mg 1 1	0	0
58	2P	2	Total Mg 2 2	0	0
58	2Q	2	Total Mg 2 2	0	0
58	2R	1	Total Mg 1 1	0	0
58	2T	1	Total Mg 1 1	0	0
58	2U	2	Total Mg 2 2	0	0
58	2V	2	Total Mg 2 2	0	0
58	2W	4	Total Mg 4 4	0	0
58	2X	3	Total Mg 3 3	0	0
58	2Y	1	Total Mg 1 1	0	0
58	2Z	1	Total Mg 1 1	0	0
58	20	2	Total Mg 2 2	0	0
58	23	3	Total Mg 3 3	0	0
58	25	5	Total Mg 5 5	0	0
58	26	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	27	3	Total 3 Mg 3	0	0
58	28	3	Total 3 Mg 3	0	0
58	29	1	Total 1 Mg 1	0	0
58	2a	235	Total 235 Mg 235	0	0
58	2d	2	Total 2 Mg 2	0	0
58	2e	1	Total 1 Mg 1	0	0
58	2f	2	Total 2 Mg 2	0	0
58	2g	1	Total 1 Mg 1	0	0
58	2i	1	Total 1 Mg 1	0	0
58	2j	1	Total 1 Mg 1	0	0
58	2k	1	Total 1 Mg 1	0	0
58	2l	4	Total 4 Mg 4	0	0
58	2n	2	Total 2 Mg 2	0	0
58	2q	3	Total 3 Mg 3	0	0
58	2r	1	Total 1 Mg 1	0	0
58	2t	1	Total 1 Mg 1	0	0
58	2v	3	Total 3 Mg 3	0	0
58	2w	5	Total 5 Mg 5	0	0
58	2x	7	Total 7 Mg 7	0	0
58	2y	1	Total 1 Mg 1	0	0

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1968	Total	O	0	0
			1968	1968		
62	1B	61	Total	O	0	0
			61	61		
62	1D	31	Total	O	0	0
			31	31		
62	1E	29	Total	O	0	0
			29	29		
62	1F	22	Total	O	0	0
			22	22		
62	1G	2	Total	O	0	0
			2	2		
62	1H	2	Total	O	0	0
			2	2		
62	1I	1	Total	O	0	0
			1	1		
62	1N	5	Total	O	0	0
			5	5		
62	1O	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1P	20	Total 20	O 20	0	0
62	1Q	6	Total 6	O 6	0	0
62	1R	15	Total 15	O 15	0	0
62	1S	5	Total 5	O 5	0	0
62	1T	8	Total 8	O 8	0	0
62	1U	11	Total 11	O 11	0	0
62	1V	7	Total 7	O 7	0	0
62	1W	5	Total 5	O 5	0	0
62	1X	5	Total 5	O 5	0	0
62	1Y	3	Total 3	O 3	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	14	Total 14	O 14	0	0
62	11	10	Total 10	O 10	0	0
62	12	3	Total 3	O 3	0	0
62	13	5	Total 5	O 5	0	0
62	14	1	Total 1	O 1	0	0
62	15	7	Total 7	O 7	0	0
62	16	3	Total 3	O 3	0	0
62	17	10	Total 10	O 10	0	0
62	18	10	Total 10	O 10	0	0
62	1a	340	Total 340	O 340	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1b	1	Total 1	O 1	0	0
62	1e	2	Total 2	O 2	0	0
62	1f	1	Total 1	O 1	0	0
62	1i	1	Total 1	O 1	0	0
62	1l	8	Total 8	O 8	0	0
62	1m	1	Total 1	O 1	0	0
62	1p	1	Total 1	O 1	0	0
62	1q	2	Total 2	O 2	0	0
62	1u	1	Total 1	O 1	0	0
62	1v	4	Total 4	O 4	0	0
62	1w	9	Total 9	O 9	0	0
62	1x	9	Total 9	O 9	0	0
62	1z	1	Total 1	O 1	0	0
62	1y	1	Total 1	O 1	0	0
62	2A	1091	Total 1091	O 1091	0	0
62	2B	23	Total 23	O 23	0	0
62	2D	21	Total 21	O 21	0	0
62	2E	11	Total 11	O 11	0	0
62	2F	13	Total 13	O 13	0	0
62	2O	2	Total 2	O 2	0	0
62	2P	13	Total 13	O 13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2Q	1	Total	O	0	0
			1	1		
62	2R	4	Total	O	0	0
			4	4		
62	2T	6	Total	O	0	0
			6	6		
62	2U	3	Total	O	0	0
			3	3		
62	2W	1	Total	O	0	0
			1	1		
62	2X	3	Total	O	0	0
			3	3		
62	2Y	1	Total	O	0	0
			1	1		
62	2Z	1	Total	O	0	0
			1	1		
62	20	4	Total	O	0	0
			4	4		
62	21	9	Total	O	0	0
			9	9		
62	23	2	Total	O	0	0
			2	2		
62	25	1	Total	O	0	0
			1	1		
62	27	4	Total	O	0	0
			4	4		
62	28	3	Total	O	0	0
			3	3		
62	29	1	Total	O	0	0
			1	1		
62	2a	216	Total	O	0	0
			216	216		
62	2d	2	Total	O	0	0
			2	2		
62	2e	1	Total	O	0	0
			1	1		
62	2i	1	Total	O	0	0
			1	1		
62	2j	2	Total	O	0	0
			2	2		
62	2l	6	Total	O	0	0
			6	6		

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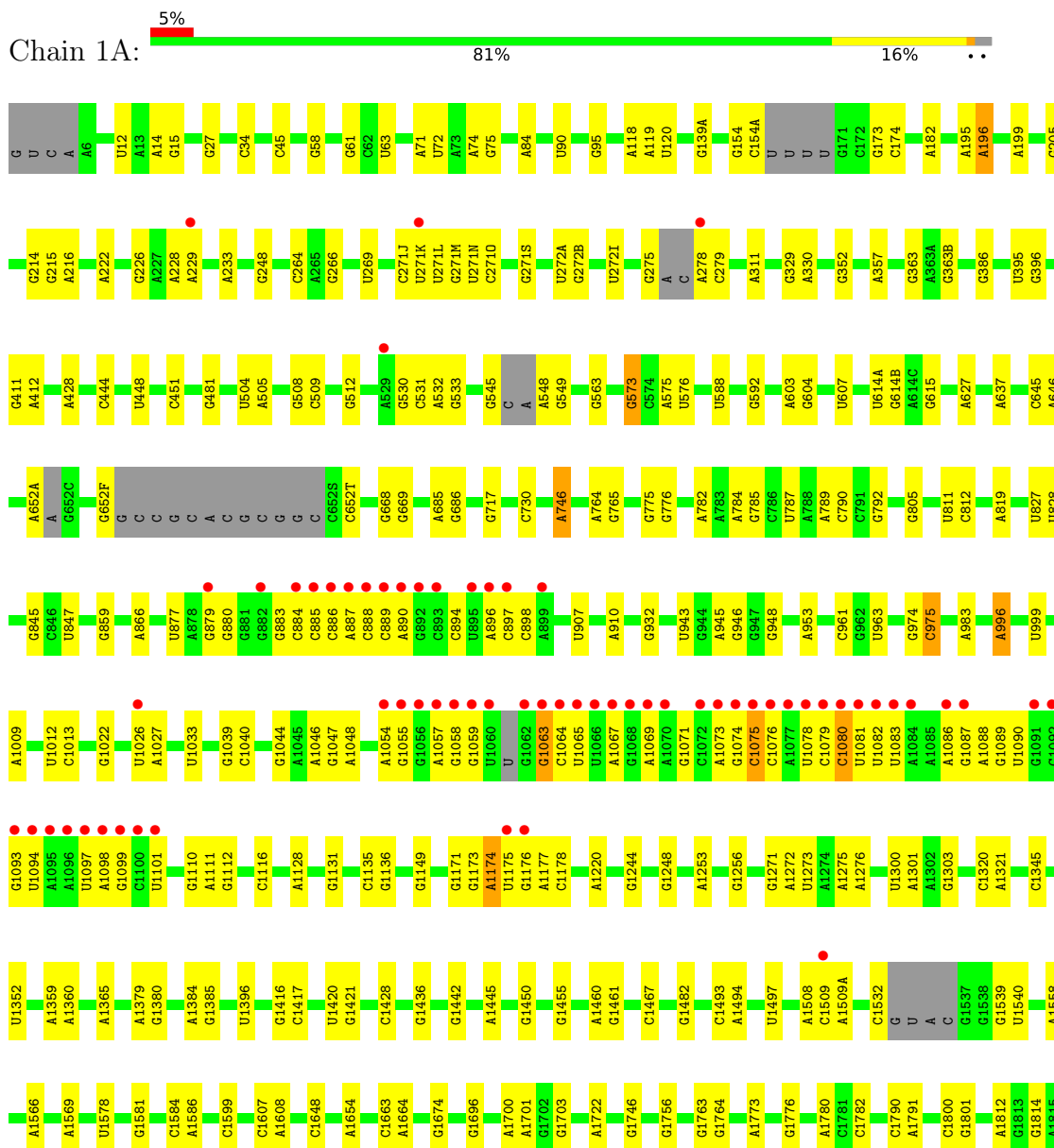
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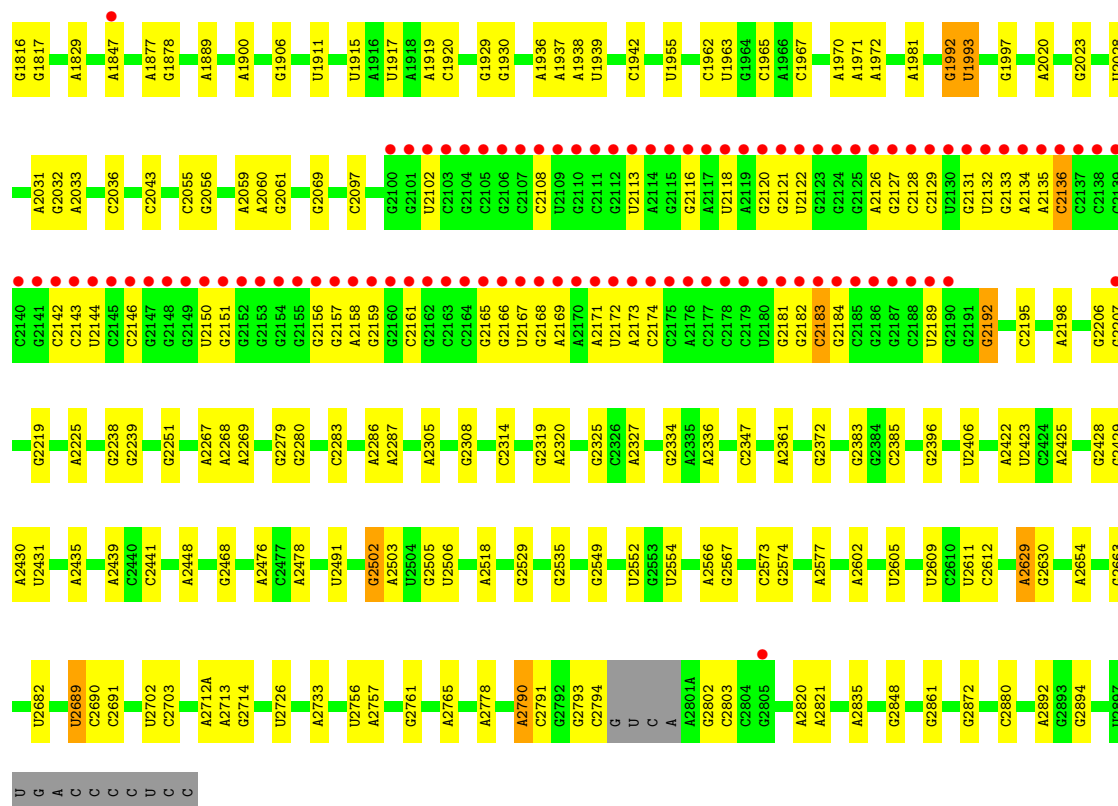
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2p	1	Total 1	O 1	0	0
62	2q	1	Total 1	O 1	0	0
62	2r	1	Total 1	O 1	0	0
62	2t	1	Total 1	O 1	0	0
62	2v	1	Total 1	O 1	0	0
62	2w	3	Total 3	O 3	0	0
62	2x	4	Total 4	O 4	0	0
62	2z	1	Total 1	O 1	0	0
62	2y	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

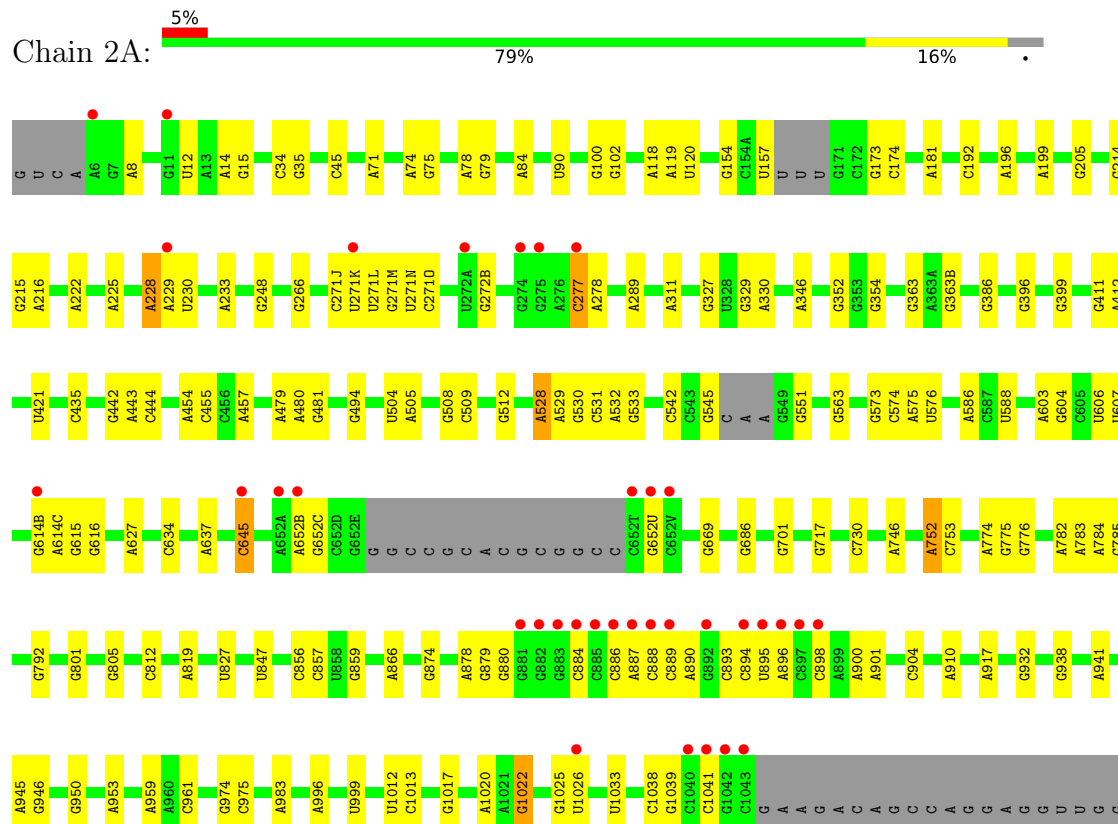
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

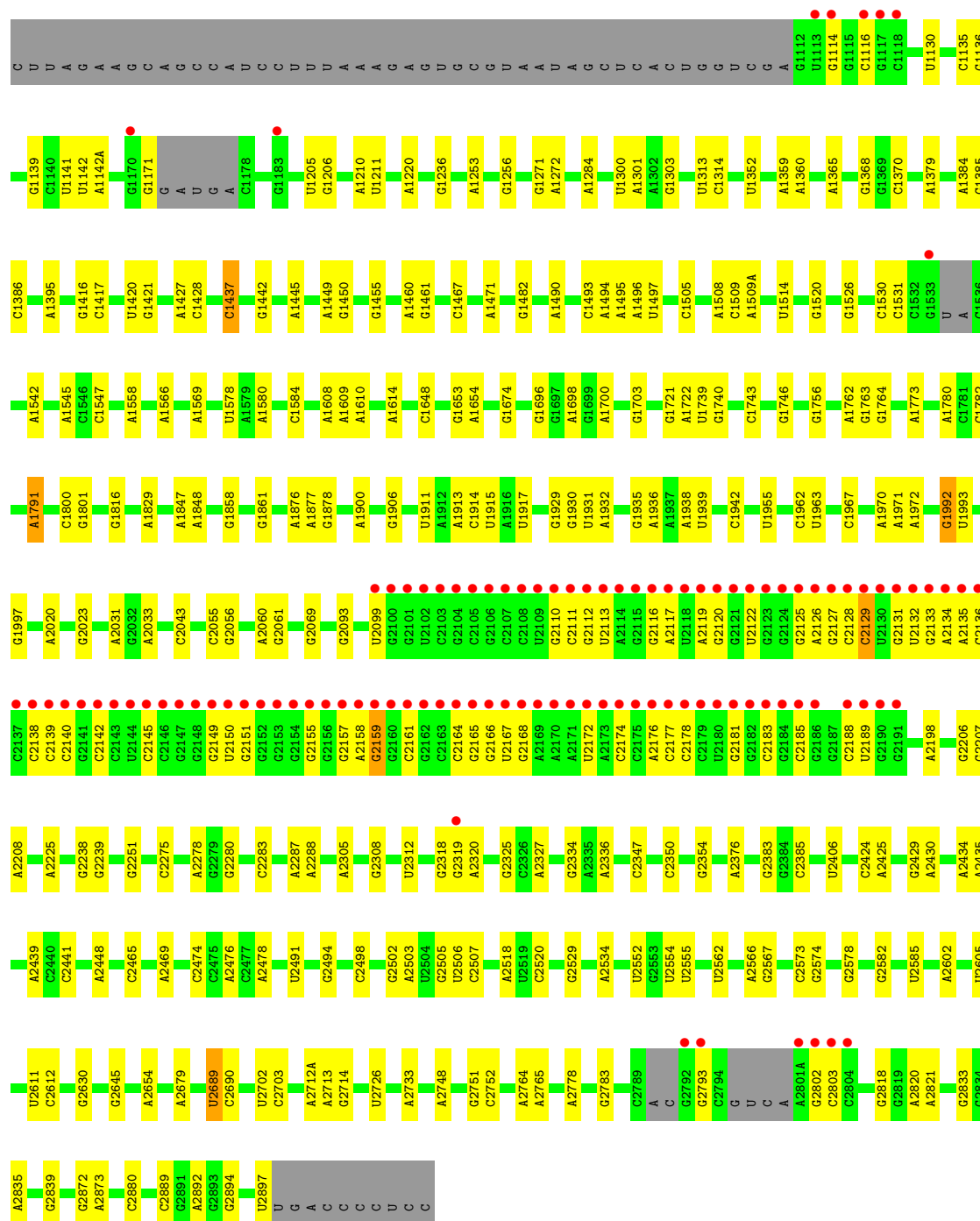
• Molecule 1: 23S Ribosomal RNA





• Molecule 1: 23S Ribosomal RNA






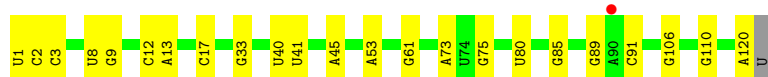
- Molecule 2: 5S Ribosomal RNA

Chain 1B:  90% 9%



- Molecule 2: 5S Ribosomal RNA

Chain 2B:  %



- Molecule 3: 50S ribosomal protein L2

Chain 1D: 97%



- Molecule 3: 50S ribosomal protein L2

Chain 2D: 95%



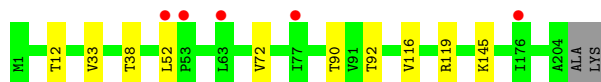
- Molecule 4: 50S ribosomal protein L3

Chain 1E: 93% 6%



- Molecule 4: 50S ribosomal protein L3

Chain 2E: 94% 5%



- Molecule 5: 50S ribosomal protein L4

Chain 1F: 88% 8%



- Molecule 5: 50S ribosomal protein L4

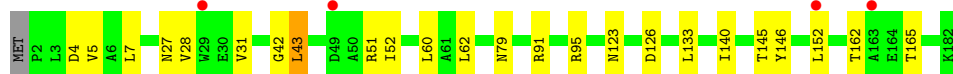
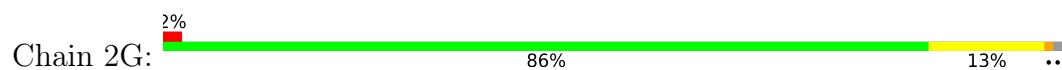
Chain 2F: 91% 5%



- Molecule 6: 50S ribosomal protein L5



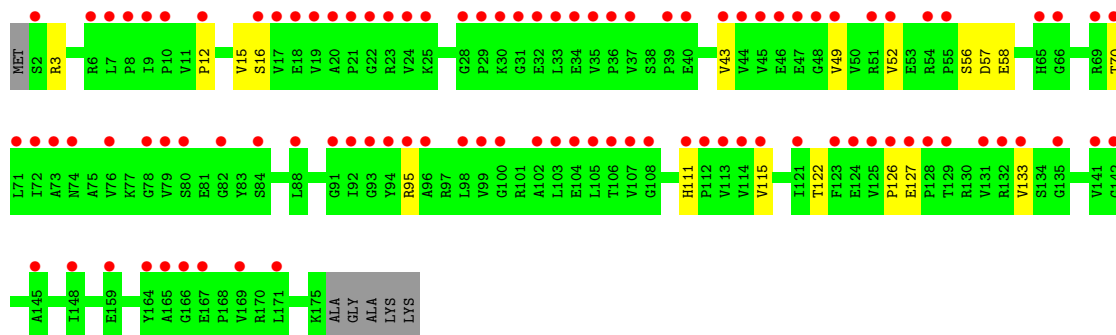
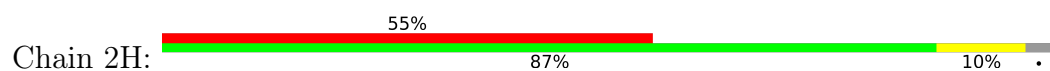
- Molecule 6: 50S ribosomal protein L5



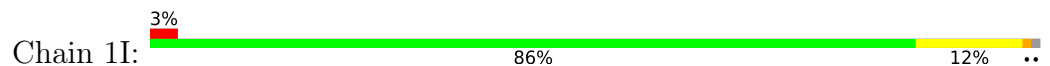
- Molecule 7: 50S ribosomal protein L6



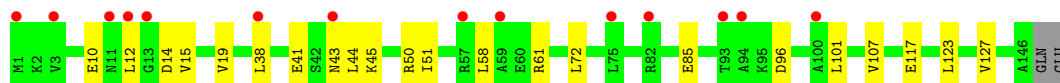
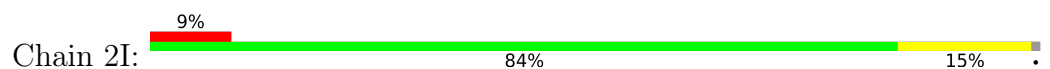
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13

Chain 1N:  96% .



- Molecule 9: 50S ribosomal protein L13

Chain 2N:  5% 96% .



- Molecule 10: 50S ribosomal protein L14

Chain 1O:  97% .



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  2% 97% .




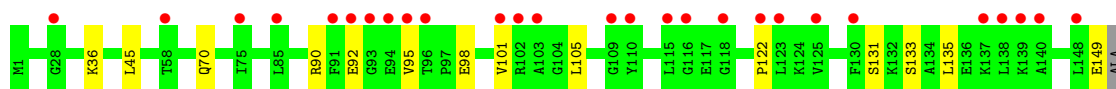
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  % 92% 7% .



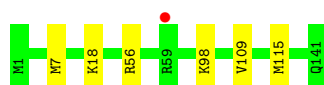
- Molecule 11: 50S ribosomal protein L15

Chain 2P:  18% 90% 9% .

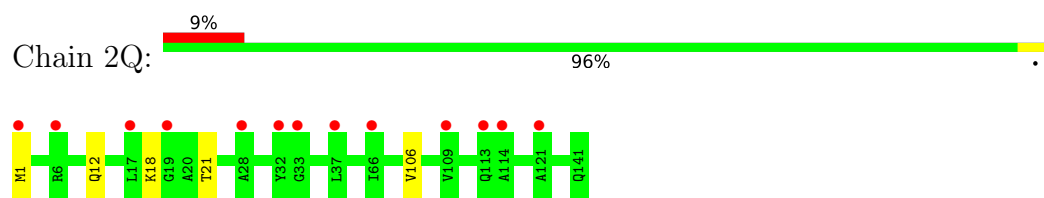


- Molecule 12: 50S ribosomal protein L16

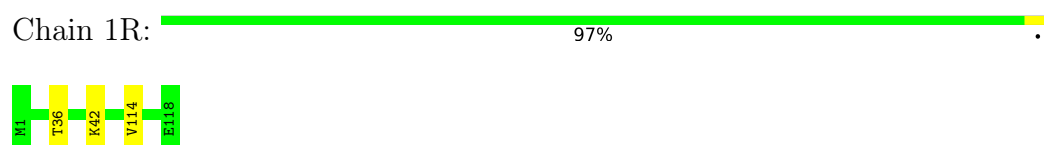
Chain 1Q:  % 96% .



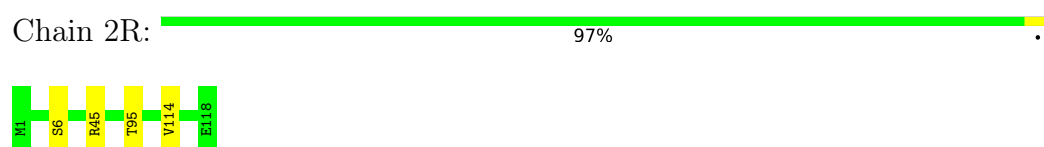
- Molecule 12: 50S ribosomal protein L16



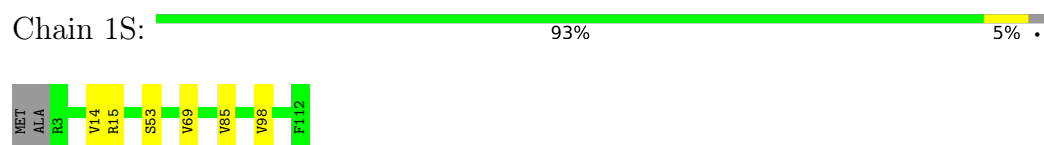
- Molecule 13: 50S ribosomal protein L17



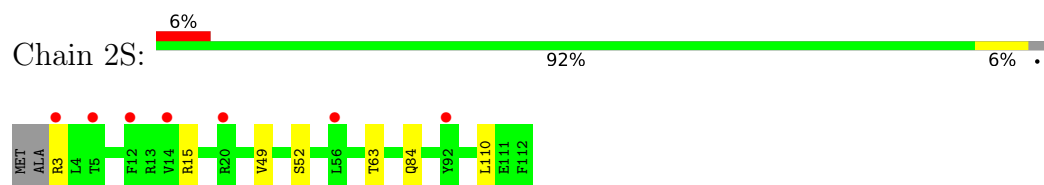
- Molecule 13: 50S ribosomal protein L17



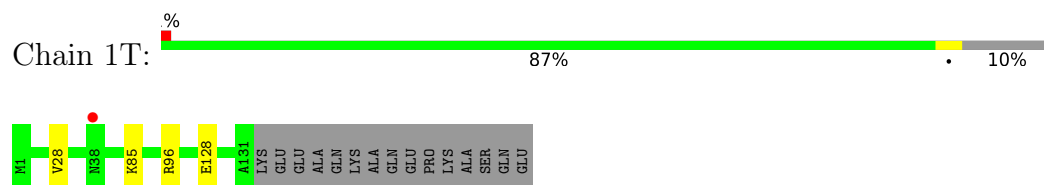
- Molecule 14: 50S ribosomal protein L18



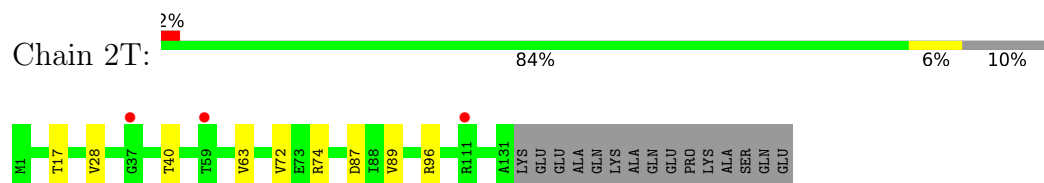
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



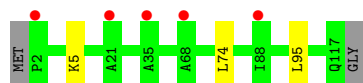
- Molecule 16: 50S ribosomal protein L20

Chain 1U:  95% ..



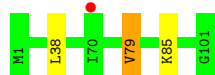
- Molecule 16: 50S ribosomal protein L20

Chain 2U:  96% ..




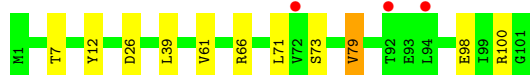
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  97% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  89% 10% ..



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  96% ..



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  96% ..

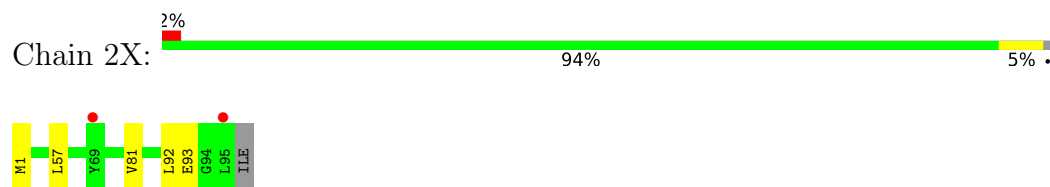


- Molecule 19: 50S ribosomal protein L23

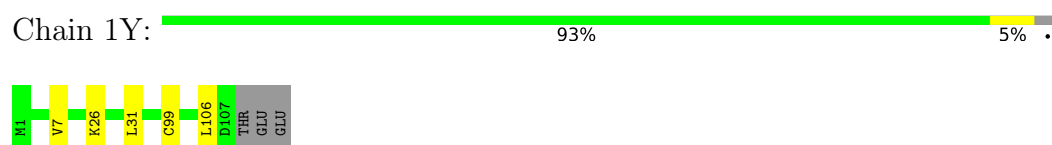
Chain 1X:  97% ..



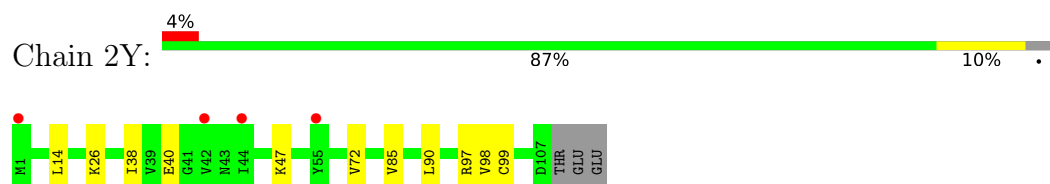
- Molecule 19: 50S ribosomal protein L23



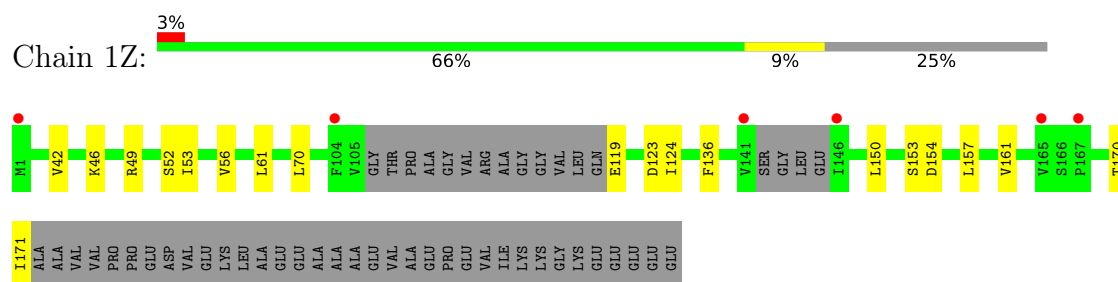
- Molecule 20: 50S ribosomal protein L24



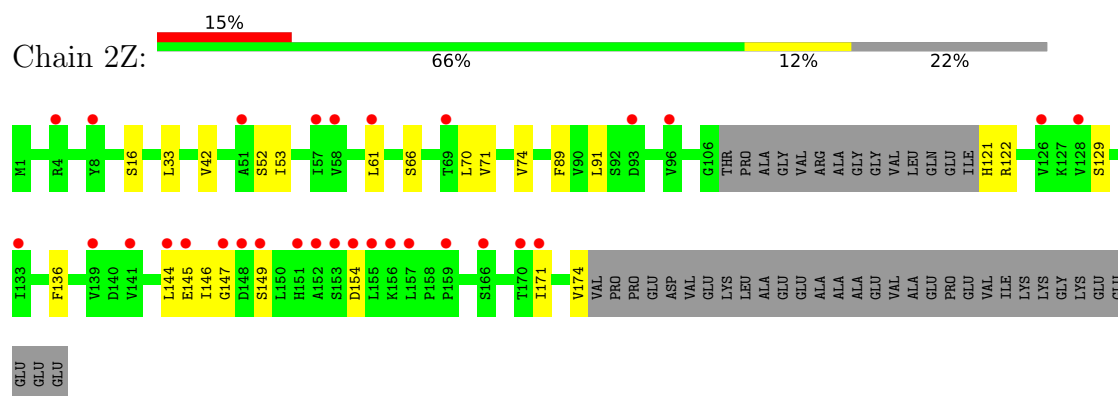
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25

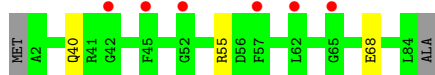


- Molecule 22: 50S ribosomal protein L27





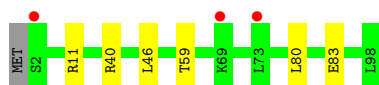
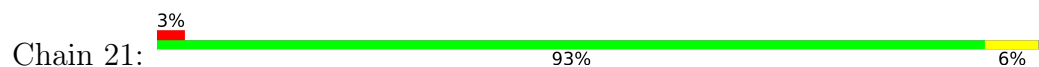
- Molecule 22: 50S ribosomal protein L27



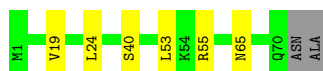
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



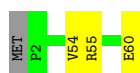
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29

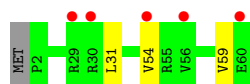


- Molecule 25: 50S ribosomal protein L30

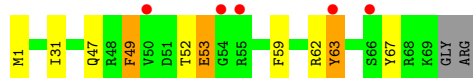
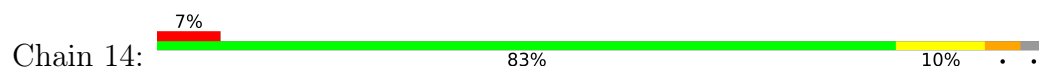


- Molecule 25: 50S ribosomal protein L30

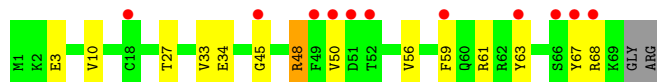
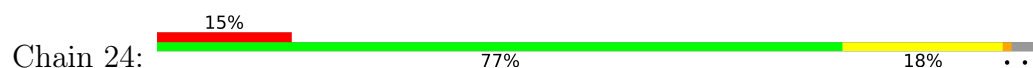




- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



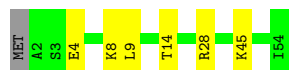
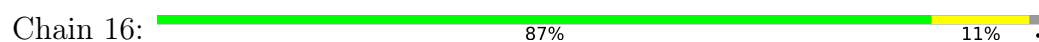
- Molecule 27: 50S ribosomal protein L32



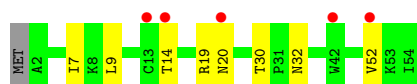
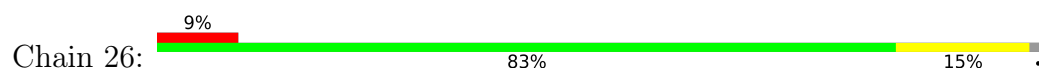
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

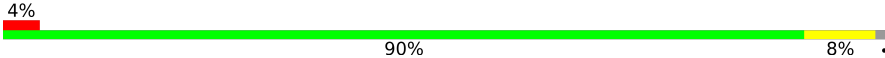


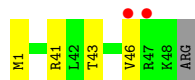
- Molecule 29: 50S ribosomal protein L34

Chain 17:  92% 6% .




- Molecule 29: 50S ribosomal protein L34

Chain 27:  4% 90% 8% .



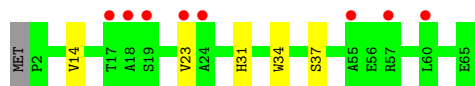
- Molecule 30: 50S ribosomal protein L35

Chain 18:  89% 9% .



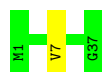
- Molecule 30: 50S ribosomal protein L35

Chain 28:  12% 91% 8% .



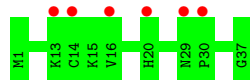
- Molecule 31: 50S ribosomal protein L36

Chain 19:  97% .




- Molecule 31: 50S ribosomal protein L36

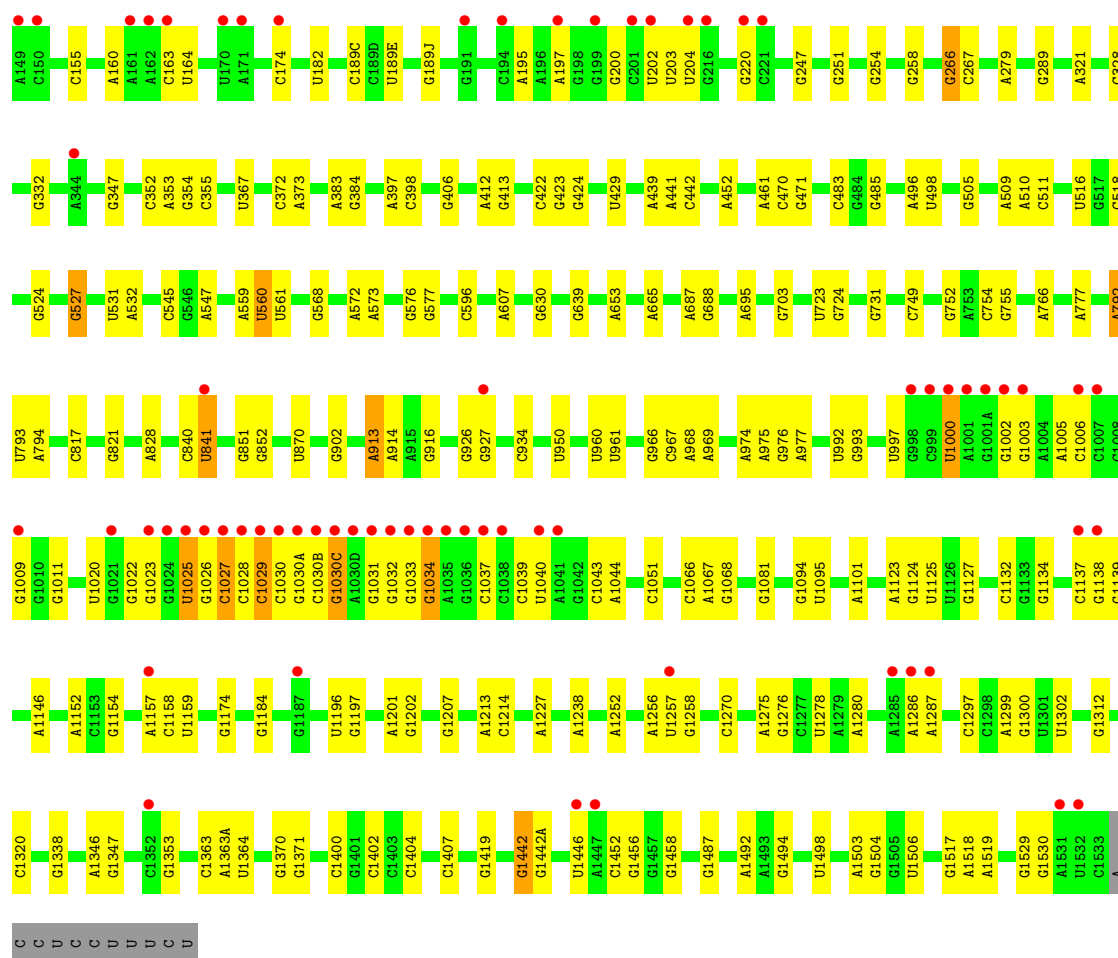
Chain 29:  16% 100%



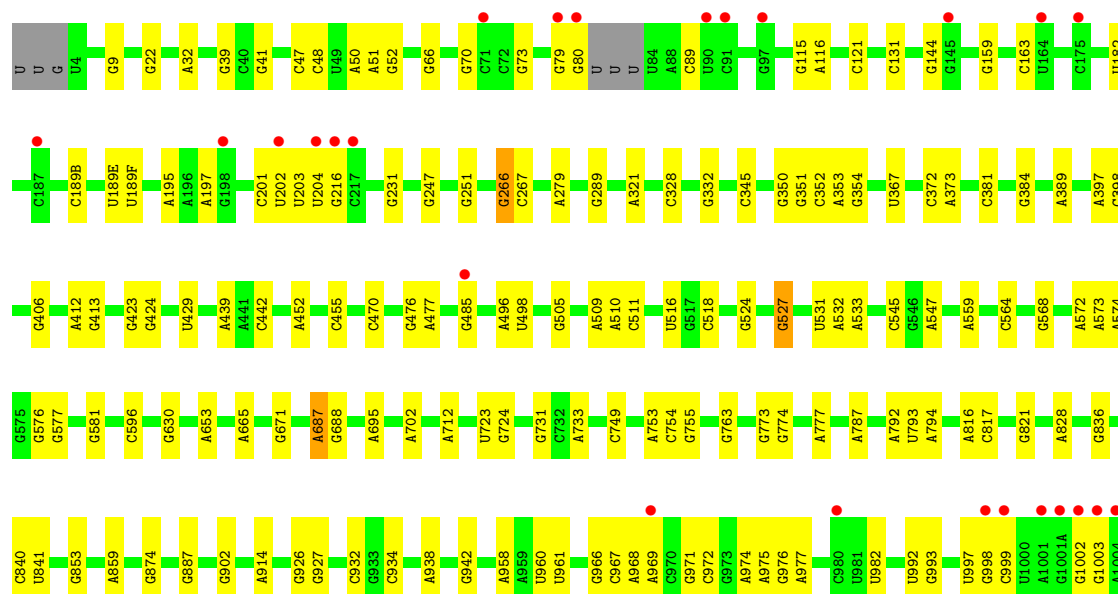
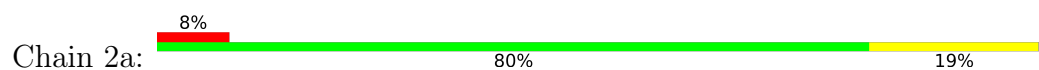
- Molecule 32: 16S Ribosomal RNA

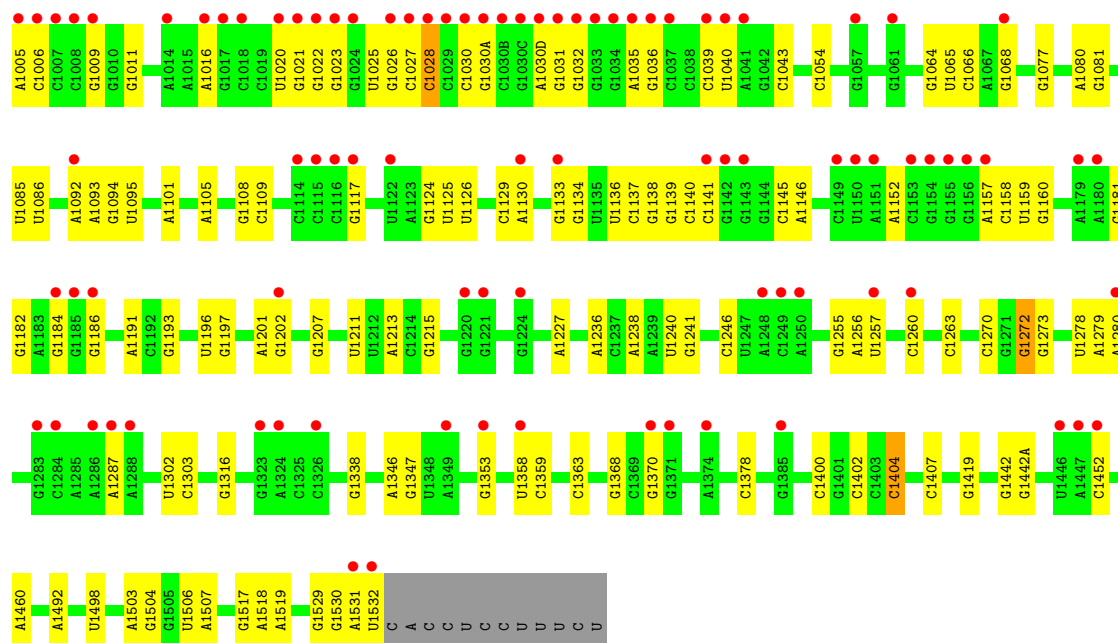
Chain 1a:  5% 81% 16% ..



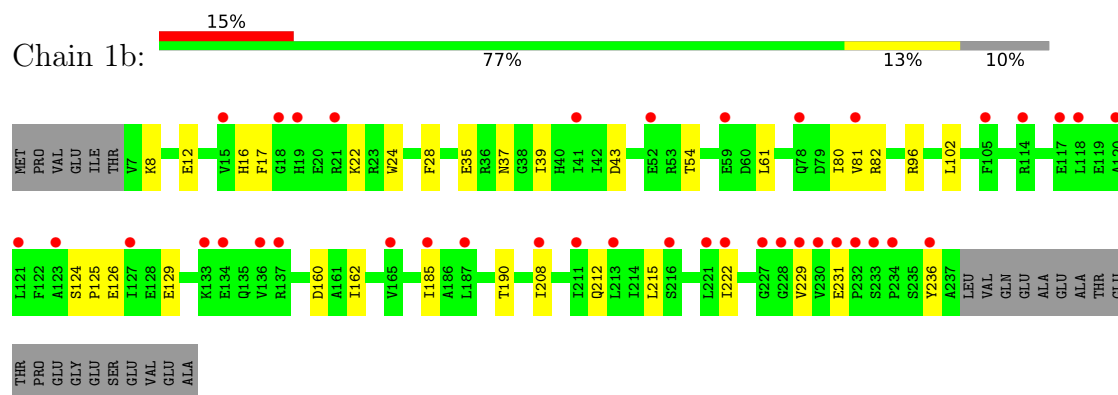


• Molecule 32: 16S Ribosomal RNA

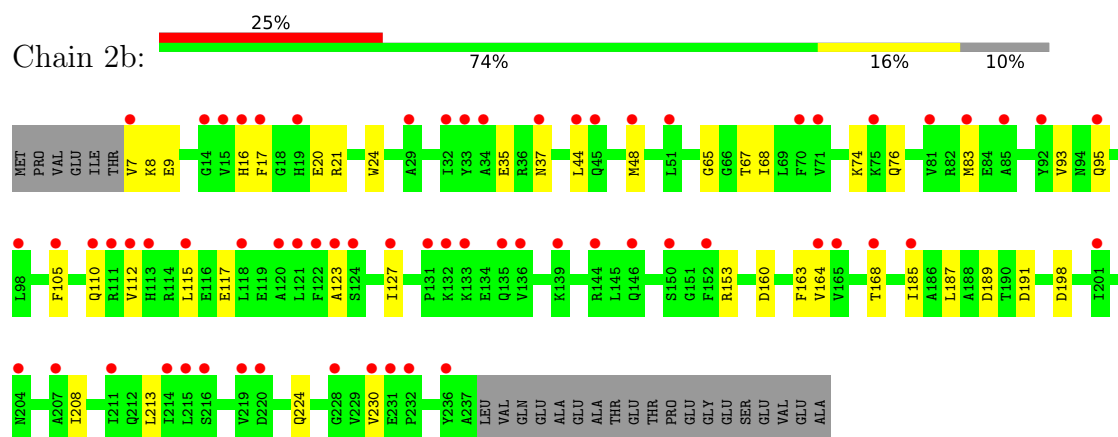




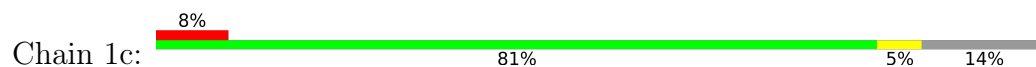
• Molecule 33: 30S ribosomal protein S2

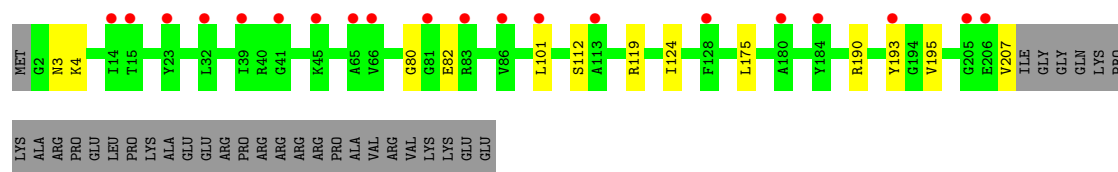


• Molecule 33: 30S ribosomal protein S2

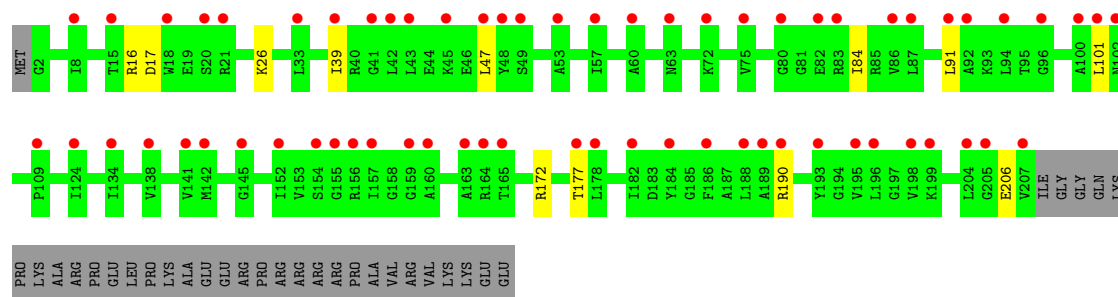
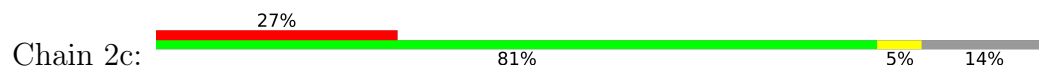


• Molecule 34: 30S ribosomal protein S3





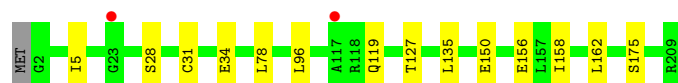
- Molecule 34: 30S ribosomal protein S3



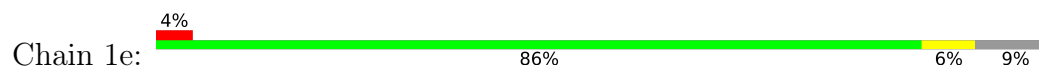
- Molecule 35: 30S ribosomal protein S4



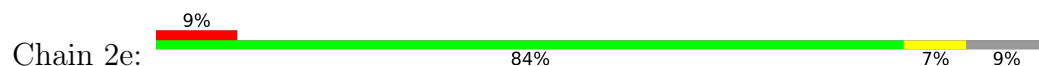
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5

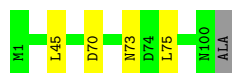


- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6

Chain 1f:  95% . .




- Molecule 37: 30S ribosomal protein S6

Chain 2f:  95% . .




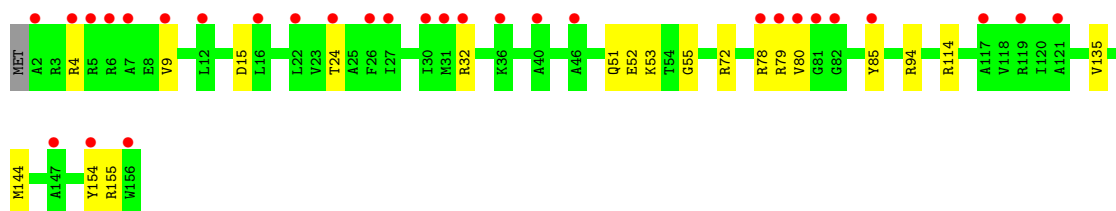
- Molecule 38: 30S ribosomal protein S7

Chain 1g:  9% 88% 12% .

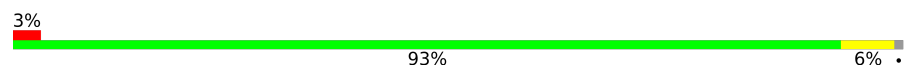


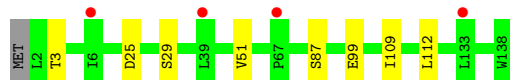
- Molecule 38: 30S ribosomal protein S7

Chain 2g:  19% 87% 13% .

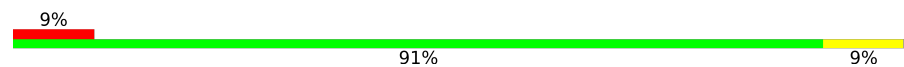


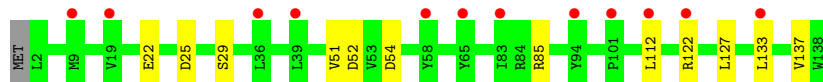
- Molecule 39: 30S ribosomal protein S8

Chain 1h:  3% 93% 6% .

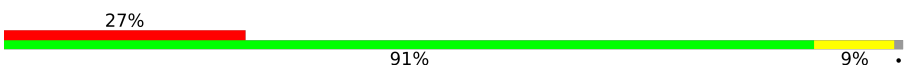


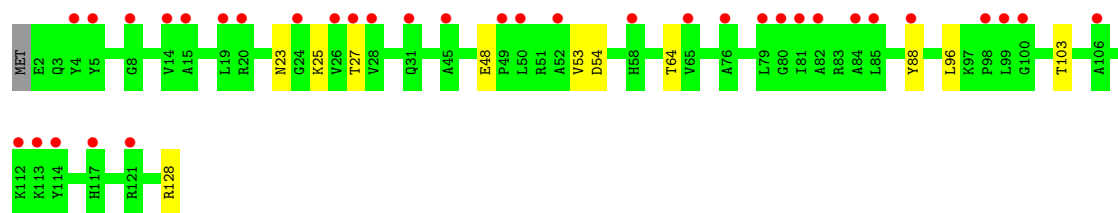
- Molecule 39: 30S ribosomal protein S8

Chain 2h:  9% 91% 9% .

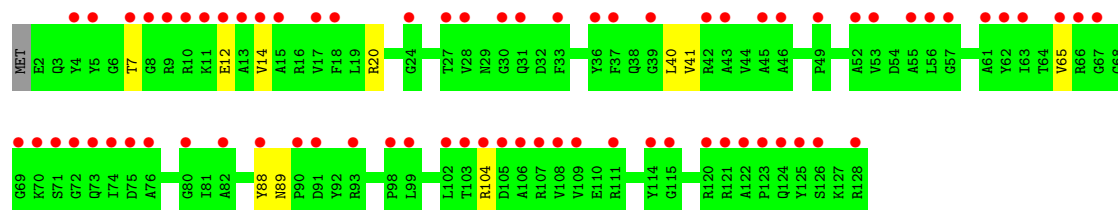
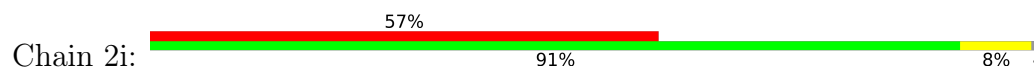


- Molecule 40: 30S ribosomal protein S9

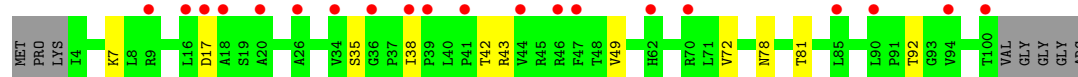
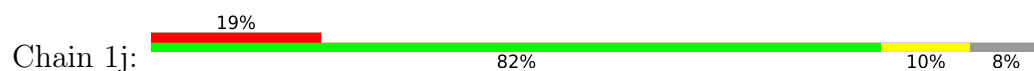
Chain 1i:  27% 91% 9% .



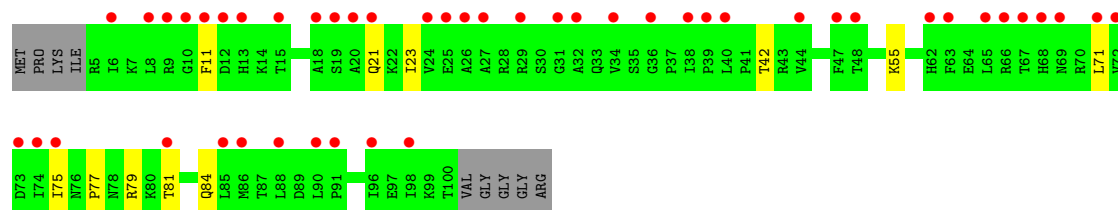
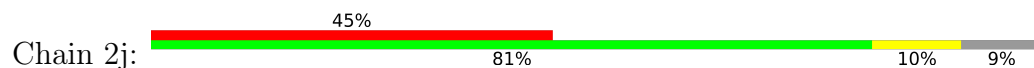
- Molecule 40: 30S ribosomal protein S9



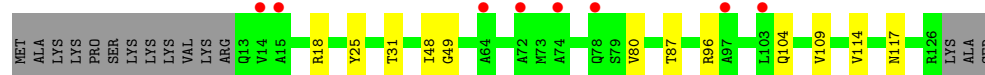
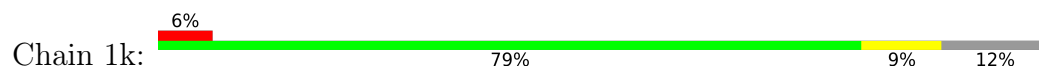
- Molecule 41: 30S ribosomal protein S10



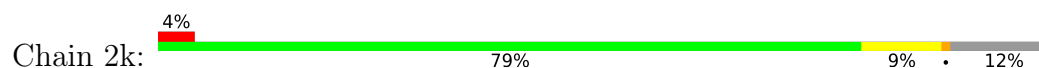
- Molecule 41: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S11

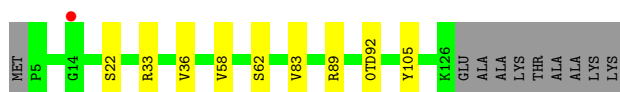
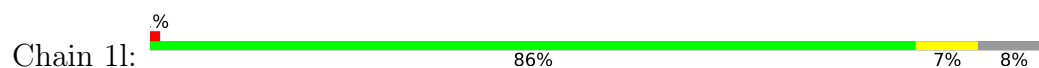


- Molecule 42: 30S ribosomal protein S11

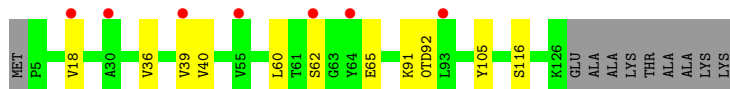
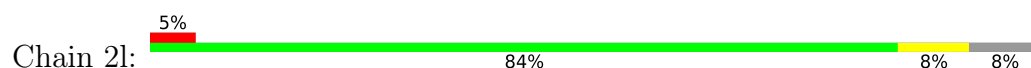




- Molecule 43: 30S ribosomal protein S12



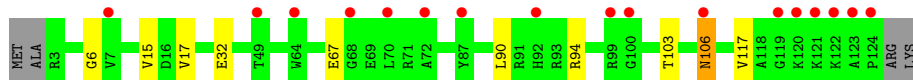
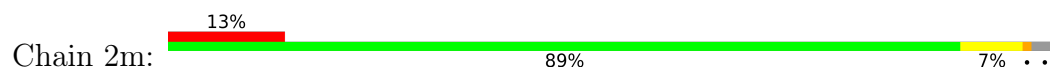
- Molecule 43: 30S ribosomal protein S12



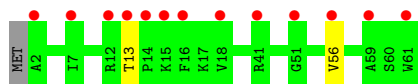
- Molecule 44: 30S ribosomal protein S13



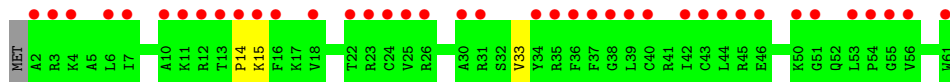
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



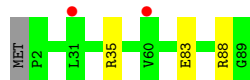
- Molecule 45: 30S ribosomal protein S14 type Z



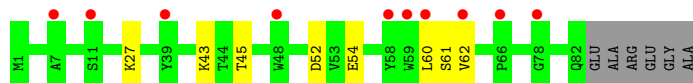
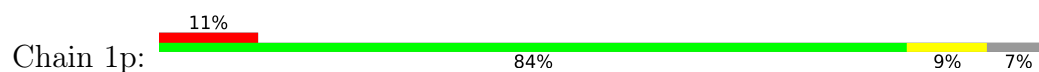
- Molecule 46: 30S ribosomal protein S15



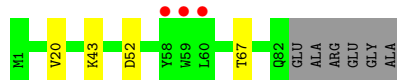
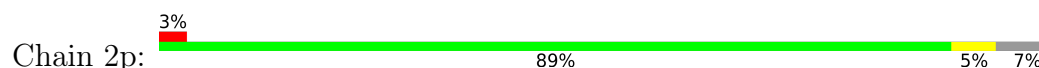
- Molecule 46: 30S ribosomal protein S15



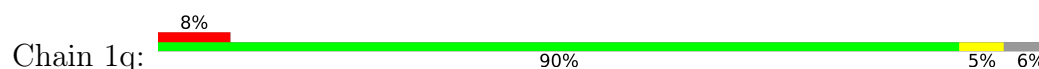
- Molecule 47: 30S ribosomal protein S16



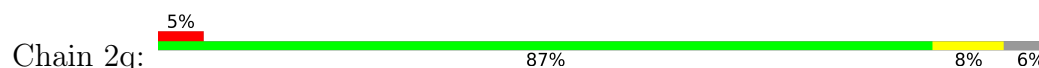
- Molecule 47: 30S ribosomal protein S16



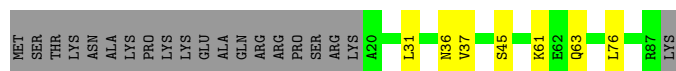
- Molecule 48: 30S ribosomal protein S17



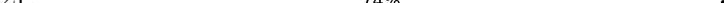
- Molecule 48: 30S ribosomal protein S17

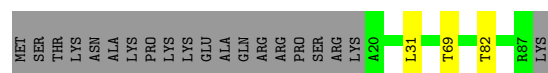


- Molecule 49: 30S ribosomal protein S18




- Molecule 49: 30S ribosomal protein S18

Chain 2r:  74% . 23%




- Molecule 50: 30S ribosomal protein S19

Chain 1s: 




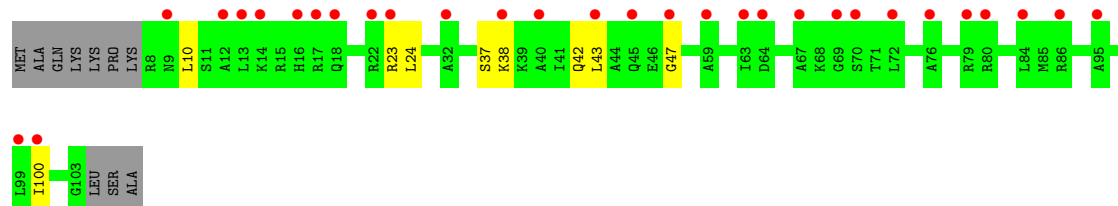
- Molecule 50: 30S ribosomal protein S19

Chain 2s: 

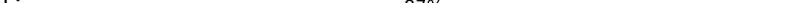


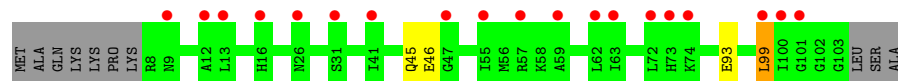
- Molecule 51: 30S ribosomal protein S20

Chain 1t: 

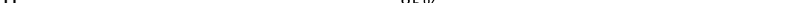


- Molecule 51: 30S ribosomal protein S20

Chain 2t:  18% 87% 9%

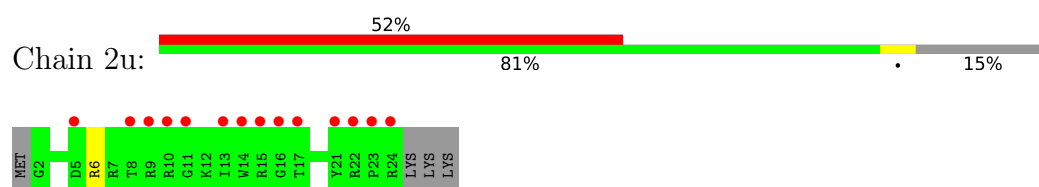


- Molecule 52: 30S ribosomal protein Thx

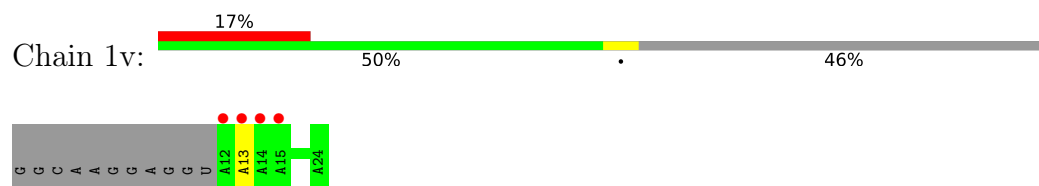
Chain 1u: 



- Molecule 52: 30S ribosomal protein Thx



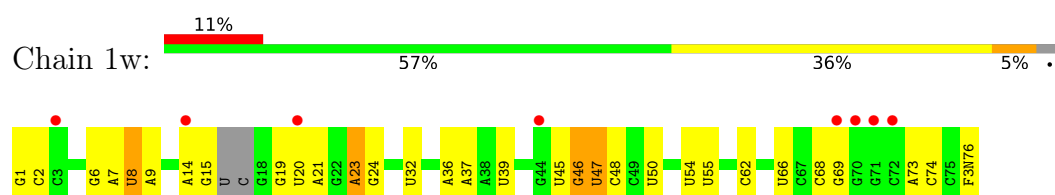
- Molecule 53: MF-mRNA



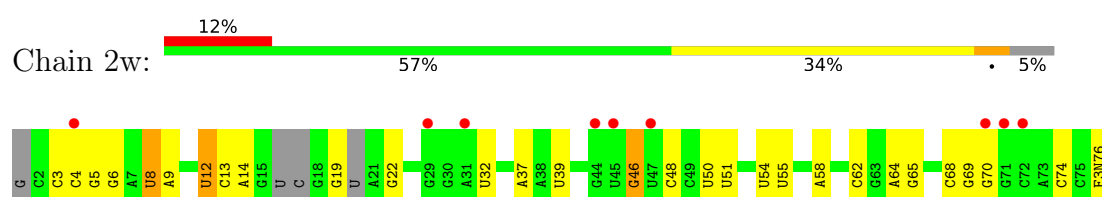
- Molecule 53: MF-mRNA



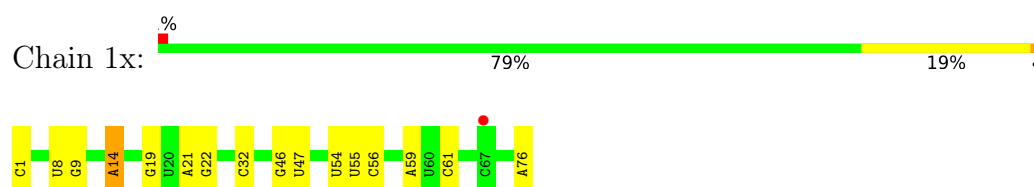
- Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNA_{phe}



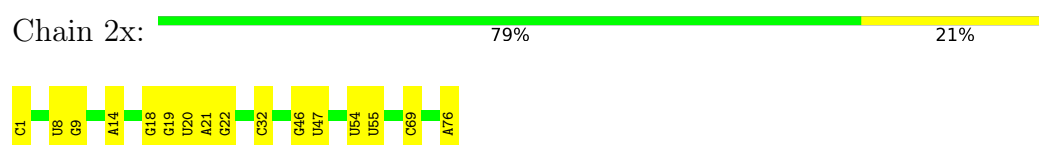
- Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNA_{phe}



- Molecule 55: P-site Peptidyl-tRNA fMRC-NH-tRNA_{met} RNA-part



- Molecule 55: P-site Peptidyl-tRNA fMRC-NH-tRNA_{met} RNA-part



- Molecule 56: P-site Peptidyl-tRNA fMRC-NH-tRNA^{met} Peptide-part

Chain 1z:  67% 33%




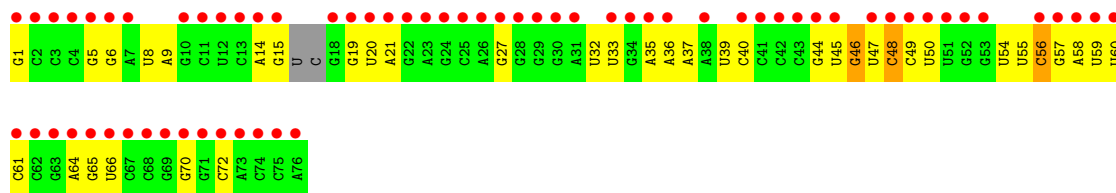
- Molecule 56: P-site Peptidyl-tRNA fMRC-NH-tRNA^{met} Peptide-part

Chain 2z:  67% 33%




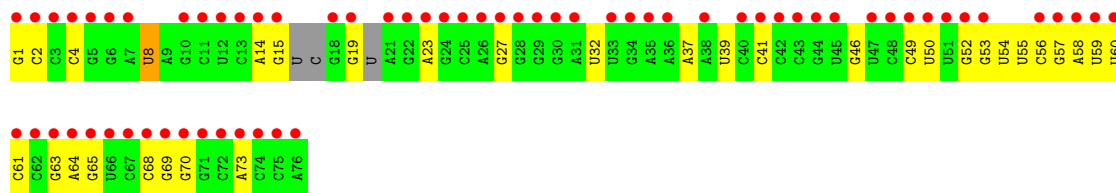
- Molecule 57: E-site Deacylated tRNA^{phe}

Chain 1y:  87% 47% 46%



- Molecule 57: E-site Deacylated tRNA^{phe}

Chain 2y:  86% 53% 42%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.16Å 452.74Å 623.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	128.40 – 2.50 182.30 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (128.40-2.50) 99.6 (182.30-2.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.235 , 0.284 0.235 , 0.284	Depositor DCC
R_{free} test set	101013 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	300017	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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: ZN, 5MC, 5MU, 0TD, 2MG, MA6, SF4, 4SU, UR3, K, 4OC, 8AN, OMU, F3N, MIA, M2G, OMG, 2MA, MG, OMC, PSU, FME, G7M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.48	0/69011	0.98	62/107720 (0.1%)
1	2A	0.38	0/67295	0.88	35/105042 (0.0%)
2	1B	0.43	1/2882 (0.0%)	0.85	0/4494
2	2B	0.38	1/2879 (0.0%)	0.85	3/4487 (0.1%)
3	1D	0.35	0/2186	0.56	0/2944
3	2D	0.31	0/2186	0.51	0/2944
4	1E	0.33	0/1592	0.54	0/2149
4	2E	0.30	0/1592	0.50	0/2149
5	1F	0.32	0/1618	0.52	0/2191
5	2F	0.29	0/1614	0.50	0/2186
6	1G	0.30	0/1448	0.49	0/1957
6	2G	0.28	0/1453	0.47	0/1963
7	1H	0.31	0/1356	0.49	0/1834
7	2H	0.28	0/1356	0.47	1/1834 (0.1%)
8	1I	0.28	0/1112	0.49	0/1514
8	2I	0.26	0/1079	0.49	0/1475
9	1N	0.31	0/1144	0.49	0/1543
9	2N	0.28	0/1144	0.44	0/1543
10	1O	0.32	0/943	0.52	0/1269
10	2O	0.30	0/943	0.51	0/1269
11	1P	0.32	0/1152	0.59	0/1533
11	2P	0.30	0/1152	0.54	0/1533
12	1Q	0.33	0/1143	0.54	0/1527
12	2Q	0.29	0/1143	0.49	0/1527
13	1R	0.31	0/982	0.53	0/1312
13	2R	0.26	0/982	0.49	0/1312
14	1S	0.31	0/883	0.52	0/1176
14	2S	0.30	0/880	0.49	0/1172
15	1T	0.31	0/1105	0.49	0/1477
15	2T	0.29	0/1097	0.48	0/1468
16	1U	0.33	0/977	0.52	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.29	0/977	0.43	0/1301
17	1V	0.31	0/782	0.54	0/1049
17	2V	0.29	0/782	0.50	0/1049
18	1W	0.32	0/897	0.51	0/1205
18	2W	0.30	0/897	0.47	0/1205
19	1X	0.35	0/764	0.56	0/1025
19	2X	0.31	0/764	0.53	0/1025
20	1Y	0.32	0/819	0.50	0/1095
20	2Y	0.30	0/819	0.50	0/1095
21	1Z	0.28	0/1267	0.51	0/1717
21	2Z	0.28	0/1299	0.50	0/1763
22	10	0.34	0/662	0.54	0/881
22	20	0.34	0/662	0.49	0/881
23	11	0.33	0/762	0.50	0/1014
23	21	0.29	0/762	0.49	0/1014
24	12	0.31	0/590	0.48	0/781
24	22	0.27	0/590	0.40	0/781
25	13	0.32	0/474	0.56	0/635
25	23	0.27	0/469	0.45	0/630
26	14	0.33	0/565	0.54	0/761
26	24	0.29	0/545	0.50	0/737
27	15	0.33	0/469	0.56	0/635
27	25	0.28	0/469	0.54	0/635
28	16	0.34	0/460	0.53	0/613
28	26	0.27	0/456	0.50	0/608
29	17	0.32	0/426	0.55	0/561
29	27	0.29	0/426	0.49	0/561
30	18	0.33	0/525	0.56	0/691
30	28	0.28	0/525	0.48	0/691
31	19	0.31	0/310	0.53	0/407
31	29	0.29	0/310	0.50	0/407
32	1a	0.36	0/35795	0.88	36/55864 (0.1%)
32	2a	0.35	2/35886 (0.0%)	0.90	36/56005 (0.1%)
33	1b	0.30	0/1881	0.49	0/2542
33	2b	0.29	0/1860	0.50	0/2518
34	1c	0.28	0/1572	0.47	0/2126
34	2c	0.28	0/1566	0.47	0/2119
35	1d	0.29	0/1685	0.47	0/2262
35	2d	0.28	0/1704	0.46	0/2284
36	1e	0.29	0/1145	0.51	0/1543
36	2e	0.29	0/1149	0.52	0/1548
37	1f	0.28	0/823	0.48	0/1115
37	2f	0.29	0/829	0.50	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	0.44	0/1683
39	1h	0.28	0/1108	0.47	0/1494
39	2h	0.27	0/1108	0.46	0/1494
40	1i	0.28	0/1002	0.50	0/1346
40	2i	0.29	0/997	0.50	0/1343
41	1j	0.28	0/722	0.49	0/982
41	2j	0.29	0/727	0.53	0/988
42	1k	0.29	0/844	0.48	0/1145
42	2k	0.28	0/848	0.47	0/1149
43	1l	0.30	0/937	0.51	0/1260
43	2l	0.30	0/937	0.50	0/1260
44	1m	0.28	0/969	0.51	0/1302
44	2m	0.26	0/961	0.46	0/1291
45	1n	0.29	0/501	0.46	0/664
45	2n	0.30	0/501	0.47	0/664
46	1o	0.28	0/739	0.41	0/985
46	2o	0.27	0/739	0.44	0/985
47	1p	0.27	0/697	0.51	0/939
47	2p	0.29	0/693	0.51	0/935
48	1q	0.28	0/836	0.48	0/1117
48	2q	0.28	0/836	0.47	0/1117
49	1r	0.28	0/560	0.47	0/746
49	2r	0.26	0/560	0.48	0/746
50	1s	0.27	0/667	0.52	0/900
50	2s	0.29	0/661	0.52	0/893
51	1t	0.27	0/730	0.50	0/965
51	2t	0.27	0/729	0.42	0/965
52	1u	0.25	0/203	0.47	0/266
52	2u	0.27	0/203	0.49	0/266
53	1v	0.42	0/310	0.84	0/480
53	2v	0.38	0/310	0.87	0/480
54	1w	0.53	1/1581 (0.1%)	1.12	4/2458 (0.2%)
54	2w	0.43	0/1531	1.11	1/2379 (0.0%)
55	1x	0.60	2/1723 (0.1%)	1.14	18/2684 (0.7%)
55	2x	0.54	2/1723 (0.1%)	1.06	14/2684 (0.5%)
56	1z	0.49	0/16	0.97	0/19
56	2z	0.31	0/16	0.69	0/19
57	1y	0.59	1/1606 (0.1%)	1.16	9/2497 (0.4%)
57	2y	0.56	1/1583 (0.1%)	1.09	5/2459 (0.2%)
All	All	0.38	11/316666 (0.0%)	0.83	224/474075 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	1	C	OP3-P	-10.66	1.48	1.61
54	1w	1	G	OP3-P	-10.64	1.48	1.61
2	1B	1	U	OP3-P	-10.38	1.48	1.61
57	2y	1	G	OP3-P	-10.21	1.48	1.61
57	1y	1	G	OP3-P	-10.18	1.49	1.61
2	2B	1	U	OP3-P	-10.17	1.49	1.61
55	2x	1	C	OP3-P	-10.14	1.49	1.61
32	2a	1272	G	N1-C2	-8.39	1.31	1.37
32	2a	1272	G	C6-N1	-7.88	1.34	1.39
55	1x	22	G	N7-C5	6.12	1.43	1.39
55	2x	22	G	N7-C5	5.14	1.42	1.39

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	22.79	132.57	118.90
32	2a	1272	G	N3-C2-N2	20.99	134.59	119.90
32	2a	1272	G	N1-C2-N2	-18.07	99.93	116.20
32	2a	1272	G	C5-C6-O6	17.68	139.21	128.60
32	2a	1263	C	C2-N3-C4	14.49	127.14	119.90
32	2a	1263	C	C5-C6-N1	12.41	127.20	121.00
32	2a	1272	G	C6-N1-C2	12.24	132.44	125.10
1	1A	999	U	O5'-P-OP2	-11.92	94.97	105.70
32	2a	1263	C	N3-C2-O2	-11.71	113.70	121.90
32	2a	1272	G	C5-C6-N1	-11.58	105.71	111.50
1	2A	2136	C	N1-C2-O2	10.58	125.25	118.90
55	2x	46	G	C6-N1-C2	-10.44	118.84	125.10
55	1x	46	G	C6-N1-C2	-10.17	119.00	125.10
1	2A	2155	G	C6-N1-C2	9.86	131.01	125.10
1	1A	1075	C	N1-C2-O2	9.58	124.65	118.90
1	1A	1063	G	C5-C6-O6	9.42	134.25	128.60
1	1A	1086	A	N1-C6-N6	-9.40	112.96	118.60
1	2A	2155	G	C5-C6-O6	9.13	134.07	128.60
32	2a	1263	C	C2-N1-C1'	9.06	128.77	118.80
55	1x	14	A	C4-C5-C6	9.04	121.52	117.00
2	2B	80	U	O4'-C1'-N1	8.99	115.39	108.20
1	1A	787	U	O5'-P-OP1	-8.93	97.66	105.70
32	2a	1263	C	C4-C5-C6	-8.81	113.00	117.40
1	1A	1075	C	C2-N3-C4	8.74	124.27	119.90
55	1x	14	A	C5-N7-C8	8.65	108.23	103.90
55	1x	22	G	C5-N7-C8	-8.59	100.00	104.30
32	2a	1272	G	C4-N9-C1'	8.55	137.62	126.50
32	2a	1272	G	C2-N3-C4	-8.50	107.65	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	576	U	O5'-P-OP1	-8.30	98.23	105.70
57	1y	48	C	N1-C2-O2	-8.22	113.97	118.90
32	2a	1272	G	C8-N9-C1'	-8.14	116.42	127.00
32	2a	1272	G	N1-C6-O6	-8.08	115.05	119.90
32	1a	1034	G	C5-C6-O6	7.94	133.36	128.60
32	2a	1263	C	C6-N1-C2	-7.92	117.13	120.30
32	2a	1263	C	N1-C2-N3	-7.87	113.69	119.20
32	2a	1054	C	C2-N1-C1'	7.81	127.39	118.80
55	2x	14	A	C5-N7-C8	7.81	107.81	103.90
1	1A	2577	A	O5'-P-OP1	-7.79	98.69	105.70
32	1a	1029	C	C2-N3-C4	7.69	123.75	119.90
55	1x	22	G	C4-C5-C6	-7.69	114.19	118.80
54	1w	47	U	N1-C2-O2	7.63	128.14	122.80
1	2A	2155	G	N3-C2-N2	7.49	125.14	119.90
55	2x	14	A	C4-C5-C6	7.39	120.70	117.00
32	1a	1034	G	C6-N1-C2	7.24	129.44	125.10
55	2x	22	G	C5-N7-C8	-7.24	100.68	104.30
54	1w	47	U	C2-N1-C1'	7.16	126.29	117.70
55	1x	14	A	C5-C6-N1	-7.11	114.15	117.70
1	2A	2129	C	N1-C2-O2	7.08	123.15	118.90
1	1A	2682	U	O5'-P-OP2	-7.06	99.35	105.70
1	1A	975	C	N1-C2-O2	-7.05	114.67	118.90
55	1x	46	G	C5-C6-O6	-7.01	124.39	128.60
32	1a	841	U	C5-C6-N1	7.01	126.20	122.70
54	1w	47	U	N3-C2-O2	-6.99	117.31	122.20
32	2a	754	C	N1-C2-O2	6.99	123.09	118.90
1	1A	1063	G	N3-C2-N2	6.95	124.76	119.90
32	1a	754	C	C2-N1-C1'	6.88	126.36	118.80
32	2a	754	C	C2-N1-C1'	6.83	126.31	118.80
2	2B	1	U	C2-N1-C1'	6.81	125.87	117.70
1	1A	1992	G	P-O3'-C3'	6.80	127.86	119.70
32	2a	1028	C	C2-N3-C4	6.74	123.27	119.90
57	1y	33	U	C2-N1-C1'	6.72	125.77	117.70
1	1A	512	G	O4'-C1'-N9	6.71	113.57	108.20
32	1a	841	U	C2-N1-C1'	6.69	125.73	117.70
1	1A	2167	U	C2-N1-C1'	6.69	125.72	117.70
32	1a	266	G	P-O3'-C3'	6.68	127.72	119.70
1	1A	1063	G	C6-N1-C2	6.67	129.10	125.10
1	1A	588	U	O5'-P-OP2	-6.67	99.70	105.70
1	2A	2136	C	C2-N3-C4	6.65	123.22	119.90
1	2A	847	U	C2-N1-C1'	6.64	125.67	117.70
32	1a	90	U	N3-C2-O2	-6.58	117.60	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1698	A	O4'-C1'-N9	6.54	113.44	108.20
1	1A	2167	U	N1-C2-O2	6.40	127.28	122.80
32	1a	1029	C	N1-C2-O2	6.39	122.73	118.90
32	1a	1027	C	C6-N1-C1'	6.38	128.46	120.80
55	2x	22	G	C4-C5-C6	-6.34	115.00	118.80
1	1A	576	U	O5'-P-OP1	-6.34	100.00	105.70
1	2A	1791	A	O5'-P-OP1	-6.33	100.00	105.70
1	1A	2629	A	P-O3'-C3'	6.31	127.27	119.70
1	2A	2689	U	P-O3'-C3'	6.30	127.26	119.70
32	1a	560	U	C2-N1-C1'	6.29	125.25	117.70
32	1a	1030(B)	C	C2-N1-C1'	6.27	125.70	118.80
57	1y	33	U	N1-C2-O2	6.26	127.19	122.80
32	1a	1158	C	C2-N1-C1'	6.25	125.68	118.80
32	1a	1067	A	P-O3'-C3'	6.24	127.19	119.70
55	1x	46	G	C5-C6-N1	6.24	114.62	111.50
55	2x	46	G	C5-C6-N1	6.24	114.62	111.50
1	1A	2502	G	O5'-P-OP2	-6.24	100.08	105.70
1	1A	1993	U	O5'-P-OP1	-6.23	100.10	105.70
1	2A	2159	G	N3-C2-N2	6.22	124.25	119.90
32	2a	1158	C	C2-N1-C1'	6.18	125.60	118.80
55	1x	22	G	N3-C4-N9	-6.18	122.29	126.00
1	2A	2136	C	N3-C2-O2	-6.17	117.58	121.90
1	1A	948	G	O5'-P-OP1	-6.16	100.15	105.70
32	1a	1030(B)	C	N1-C2-O2	6.16	122.60	118.90
32	2a	1054	C	C6-N1-C1'	-6.16	113.41	120.80
55	2x	14	A	C5-C6-N1	-6.15	114.62	117.70
1	1A	845	G	O4'-C1'-N9	6.15	113.12	108.20
1	1A	2136	C	N1-C2-O2	6.12	122.57	118.90
1	1A	196	A	OP2-P-O3'	6.08	118.58	105.20
32	1a	754	C	C6-N1-C2	-6.07	117.87	120.30
32	2a	1054	C	N1-C2-O2	6.06	122.54	118.90
1	1A	847	U	C2-N1-C1'	6.05	124.96	117.70
32	1a	1032	G	C5-C6-O6	6.05	132.23	128.60
55	2x	22	G	N1-C6-O6	-6.02	116.29	119.90
1	1A	1790	C	O5'-P-OP2	-6.01	100.29	105.70
55	1x	22	G	N1-C6-O6	-6.01	116.29	119.90
32	1a	254	G	O5'-P-OP1	-6.00	100.30	105.70
32	2a	1043	C	N1-C2-O2	6.00	122.50	118.90
1	1A	1080	C	N1-C2-O2	5.97	122.48	118.90
1	2A	1022	G	N3-C4-N9	-5.96	122.42	126.00
1	1A	1063	G	N1-C6-O6	-5.95	116.33	119.90
1	1A	2167	U	N3-C2-O2	-5.94	118.04	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2155	G	N1-C2-N3	-5.93	120.34	123.90
1	1A	1776	G	O5'-P-OP2	-5.90	100.39	105.70
1	1A	2028	U	N3-C4-O4	-5.90	115.27	119.40
1	1A	2036	C	O5'-P-OP1	-5.87	100.42	105.70
1	2A	1614	A	O5'-P-OP1	-5.87	100.42	105.70
57	1y	64	A	C5-C6-N6	5.86	128.38	123.70
1	1A	395	U	O4'-C1'-N1	5.85	112.88	108.20
32	1a	1158	C	N1-C2-O2	5.85	122.41	118.90
1	1A	1064	C	C2-N1-C1'	5.84	125.22	118.80
57	2y	14	A	P-O3'-C3'	5.83	126.69	119.70
32	1a	1027	C	C2-N1-C1'	-5.79	112.43	118.80
57	2y	4	C	C2-N3-C4	5.78	122.79	119.90
1	2A	1437	C	C2-N1-C1'	5.78	125.16	118.80
1	2A	1313	U	C2-N1-C1'	5.75	124.61	117.70
1	1A	2059	A	O4'-C1'-N9	5.72	112.78	108.20
55	1x	22	G	N7-C8-N9	5.71	115.95	113.10
1	2A	2155	G	N1-C6-O6	-5.70	116.48	119.90
32	2a	1263	C	C6-N1-C1'	-5.69	113.97	120.80
57	1y	56	C	N1-C2-O2	5.68	122.31	118.90
1	2A	1992	G	P-O3'-C3'	5.67	126.50	119.70
55	2x	46	G	N3-C4-C5	-5.65	125.78	128.60
32	1a	754	C	N1-C2-O2	5.64	122.28	118.90
32	1a	560	U	C5-C6-N1	5.63	125.52	122.70
32	1a	1025	U	N1-C2-O2	5.60	126.72	122.80
57	1y	15	G	N3-C2-N2	5.59	123.81	119.90
1	2A	752	A	P-O3'-C3'	5.58	126.40	119.70
1	2A	192	C	O5'-P-OP1	-5.57	100.69	105.70
32	1a	1032	G	C6-N1-C2	5.57	128.44	125.10
54	2w	12	U	C5-C4-O4	5.56	129.24	125.90
1	1A	2848	G	O4'-C1'-N9	5.56	112.65	108.20
1	2A	228	A	P-O3'-C3'	5.56	126.37	119.70
57	2y	4	C	N1-C2-O2	5.54	122.22	118.90
32	1a	1442	G	N3-C4-C5	-5.54	125.83	128.60
7	2H	115	VAL	C-N-CA	-5.53	107.89	121.70
32	1a	1030(B)	C	C6-N1-C2	-5.50	118.10	120.30
1	1A	2192	G	N3-C4-N9	5.50	129.30	126.00
55	2x	46	G	N1-C2-N3	5.49	127.19	123.90
55	1x	22	G	C5-C6-N1	5.49	114.24	111.50
1	2A	528	A	P-O3'-C3'	5.48	126.28	119.70
1	1A	226	G	O4'-C1'-N9	5.48	112.59	108.20
32	2a	1158	C	N1-C2-O2	5.47	122.18	118.90
57	1y	33	U	N3-C2-O2	-5.44	118.39	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	847	U	N1-C2-O2	5.44	126.61	122.80
1	1A	1936	A	O4'-C1'-N9	5.44	112.55	108.20
32	2a	754	C	C6-N1-C1'	-5.43	114.28	120.80
1	1A	2122	U	C5-C4-O4	5.43	129.16	125.90
1	1A	1599	C	N3-C2-O2	-5.42	118.10	121.90
55	1x	22	G	C8-N9-C1'	5.42	134.05	127.00
1	1A	996	A	O5'-P-OP1	-5.42	100.83	105.70
32	2a	266	G	P-O3'-C3'	5.41	126.20	119.70
1	1A	1131	G	O4'-C1'-N9	5.41	112.53	108.20
1	1A	1009	A	OP1-P-OP2	-5.40	111.49	119.60
1	2A	2689	U	N3-C2-O2	-5.40	118.42	122.20
32	2a	1263	C	C5-C4-N4	5.40	123.98	120.20
1	2A	847	U	N3-C2-O2	-5.38	118.43	122.20
1	1A	1082	U	N3-C4-O4	-5.38	115.64	119.40
55	1x	14	A	C8-N9-C1'	-5.38	118.03	127.70
1	2A	2318	G	C4-N9-C1'	5.35	133.45	126.50
1	2A	801	G	O5'-P-OP2	-5.35	100.89	105.70
55	2x	46	G	N3-C2-N2	-5.34	116.16	119.90
1	1A	746	A	O4'-C1'-N9	5.33	112.47	108.20
1	2A	2129	C	C2-N3-C4	5.33	122.57	119.90
1	2A	277	C	OP2-P-O3'	5.32	116.90	105.20
32	2a	687	A	P-O3'-C3'	5.32	126.08	119.70
57	1y	50	U	C2-N3-C4	5.32	130.19	127.00
1	1A	1174	A	OP1-P-O3'	5.30	116.87	105.20
1	1A	196	A	OP1-P-O3'	-5.30	93.55	105.20
2	2B	1	U	C6-N1-C1'	-5.28	113.81	121.20
32	1a	560	U	C3'-C2'-C1'	5.27	105.72	101.50
32	1a	754	C	N3-C2-O2	-5.27	118.21	121.90
1	1A	2183	C	C5-C6-N1	5.24	123.62	121.00
1	2A	512	G	O4'-C1'-N9	5.24	112.39	108.20
32	2a	1158	C	C6-N1-C2	-5.24	118.20	120.30
32	1a	1027	C	N3-C4-C5	-5.24	119.81	121.90
54	1w	23	A	N1-C6-N6	5.23	121.74	118.60
1	1A	2689	U	P-O3'-C3'	5.22	125.97	119.70
1	1A	2128	C	C2-N1-C1'	5.22	124.54	118.80
1	1A	1174	A	P-O3'-C3'	5.21	125.96	119.70
1	1A	2319	G	O4'-C1'-N9	5.21	112.37	108.20
55	1x	14	A	C4-N9-C1'	5.21	135.67	126.30
55	1x	56	C	N1-C2-O2	5.21	122.02	118.90
32	2a	115	G	P-O3'-C3'	5.21	125.95	119.70
1	1A	943	U	O5'-P-OP2	-5.20	101.02	105.70
1	1A	573	G	OP1-P-O3'	5.20	116.63	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1y	48	C	N3-C2-O2	5.19	125.53	121.90
1	1A	2790	A	C2-N3-C4	5.18	113.19	110.60
32	1a	913	A	P-O3'-C3'	5.18	125.92	119.70
32	2a	1263	C	N3-C4-N4	-5.18	114.38	118.00
32	1a	1000	U	C5-C4-O4	-5.17	122.80	125.90
32	2a	754	C	N3-C2-O2	-5.17	118.28	121.90
1	2A	645	C	N1-C2-O2	5.14	121.98	118.90
32	1a	1029	C	C5-C4-N4	5.13	123.79	120.20
1	1A	1992	G	O4'-C1'-N9	-5.10	104.12	108.20
1	1A	195	A	P-O3'-C3'	5.10	125.82	119.70
55	2x	22	G	N3-C4-N9	-5.10	122.94	126.00
1	1A	2183	C	C6-N1-C2	-5.09	118.26	120.30
55	2x	14	A	C4-C5-N7	-5.09	108.15	110.70
1	2A	898	C	N1-C2-O2	-5.08	115.85	118.90
32	1a	792	A	O4'-C1'-N9	5.07	112.26	108.20
32	1a	1201	A	P-O3'-C3'	5.07	125.79	119.70
57	2y	50	U	C2-N3-C4	5.07	130.04	127.00
1	2A	528	A	OP1-P-O3'	5.06	116.34	105.20
55	1x	22	G	N3-C4-C5	5.06	131.13	128.60
32	1a	1030(C)	G	O4'-C1'-N9	5.06	112.25	108.20
55	2x	22	G	N7-C8-N9	5.06	115.63	113.10
32	2a	1043	C	C2-N1-C1'	5.05	124.36	118.80
1	1A	2327	A	N1-C6-N6	-5.05	115.57	118.60
32	1a	266	G	OP2-P-O3'	5.04	116.30	105.20
1	1A	1814	G	O5'-P-OP2	-5.03	101.17	105.70
1	1A	1064	C	N3-C4-N4	5.03	121.52	118.00
55	1x	22	G	C6-C5-N7	5.01	133.41	130.40
57	2y	64	A	C6-N1-C2	5.01	121.61	118.60

There are no chirality outliers.

There are no planarity outliers.

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%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	253 (93%)	19 (7%)	1 (0%)	34	54
4	1E	202/206 (98%)	187 (93%)	14 (7%)	1 (0%)	29	48
4	2E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	29	48
5	1F	200/210 (95%)	192 (96%)	7 (4%)	1 (0%)	29	48
5	2F	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	15	28
6	1G	179/182 (98%)	159 (89%)	19 (11%)	1 (1%)	25	43
6	2G	179/182 (98%)	150 (84%)	25 (14%)	4 (2%)	6	10
7	1H	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
7	2H	172/180 (96%)	160 (93%)	10 (6%)	2 (1%)	13	24
8	1I	144/148 (97%)	131 (91%)	12 (8%)	1 (1%)	22	39
8	2I	144/148 (97%)	127 (88%)	16 (11%)	1 (1%)	22	39
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	128 (93%)	9 (6%)	1 (1%)	22	39
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	35
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	1P	147/150 (98%)	136 (92%)	8 (5%)	3 (2%)	7	12
11	2P	147/150 (98%)	131 (89%)	13 (9%)	3 (2%)	7	12
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	4 (3%)	1 (1%)	17	31
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	17	31
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	28
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	28
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	14	26
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	14	26
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
21	1Z	148/206 (72%)	129 (87%)	17 (12%)	2 (1%)	11	20
21	2Z	156/206 (76%)	124 (80%)	28 (18%)	4 (3%)	5	8
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
23	11	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	14	26
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	57 (100%)	0	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	1
26	24	67/71 (94%)	50 (75%)	15 (22%)	2 (3%)	4	6
27	15	57/60 (95%)	55 (96%)	2 (4%)	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
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	195 (85%)	25 (11%)	9 (4%)	3	4
33	2b	229/256 (90%)	178 (78%)	42 (18%)	9 (4%)	3	4
34	1c	204/239 (85%)	192 (94%)	11 (5%)	1 (0%)	29	48
34	2c	204/239 (85%)	170 (83%)	32 (16%)	2 (1%)	15	28
35	1d	206/209 (99%)	192 (93%)	13 (6%)	1 (0%)	29	48
35	2d	206/209 (99%)	186 (90%)	20 (10%)	0	100	100
36	1e	146/162 (90%)	129 (88%)	15 (10%)	2 (1%)	11	20
36	2e	146/162 (90%)	131 (90%)	13 (9%)	2 (1%)	11	20
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	22	39
38	2g	153/156 (98%)	133 (87%)	17 (11%)	3 (2%)	7	12
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100	100
40	1i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	19	35
40	2i	125/128 (98%)	105 (84%)	19 (15%)	1 (1%)	19	35
41	1j	95/105 (90%)	84 (88%)	10 (10%)	1 (1%)	14	26
41	2j	94/105 (90%)	77 (82%)	14 (15%)	3 (3%)	4	5
42	1k	112/129 (87%)	103 (92%)	8 (7%)	1 (1%)	17	31
42	2k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	17	31
43	1l	119/132 (90%)	113 (95%)	5 (4%)	1 (1%)	19	35
43	2l	119/132 (90%)	112 (94%)	5 (4%)	2 (2%)	9	16
44	1m	121/126 (96%)	104 (86%)	15 (12%)	2 (2%)	9	16
44	2m	120/126 (95%)	106 (88%)	11 (9%)	3 (2%)	5	8
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	16
46	1o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13	24
46	2o	86/89 (97%)	84 (98%)	1 (1%)	1 (1%)	13	24
47	1p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	73 (91%)	6 (8%)	1 (1%)	12	21
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	90 (93%)	5 (5%)	2 (2%)	7	11
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
51	1t	94/106 (89%)	81 (86%)	12 (13%)	1 (1%)	14	26
51	2t	94/106 (89%)	85 (90%)	8 (8%)	1 (1%)	14	26
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
56	1z	1/3 (33%)	0	1 (100%)	0	100	100
56	2z	1/3 (33%)	1 (100%)	0	0	100	100
All	All	11370/12134 (94%)	10433 (92%)	839 (7%)	98 (1%)	17	31

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	29	LYS
21	1Z	53	ILE
23	11	3	LYS
26	14	53	GLU
26	14	62	ARG
33	1b	22	LYS
35	1d	173	TRP
40	1i	54	ASP
44	1m	67	GLU
44	1m	107	ALA
5	2F	130	ALA
6	2G	126	ASP
26	24	45	GLY
33	2b	17	PHE
43	2l	91	LYS
44	2m	67	GLU
44	2m	106	ASN
46	2o	88	ARG
33	1b	17	PHE

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Mol	Chain	Res	Type
36	1e	85	GLY
5	2F	21	ALA
6	2G	42	GLY
6	2G	43	LEU
6	2G	52	ILE
33	2b	21	ARG
33	2b	123	ALA
38	2g	55	GLY
38	2g	80	VAL
47	2p	52	ASP
48	2q	68	ARG
4	1E	52	LEU
21	1Z	52	SER
26	14	47	GLN
33	1b	126	GLU
38	1g	55	GLY
41	1j	78	ASN
47	1p	52	ASP
9	2N	2	LYS
11	2P	36	LYS
17	2V	79	VAL
21	2Z	52	SER
33	2b	20	GLU
33	2b	74	LYS
34	2c	177	THR
36	2e	97	GLY
51	2t	99	LEU
5	1F	130	ALA
8	1I	10	GLU
10	1O	5	GLN
26	14	63	TYR
33	1b	8	LYS
33	1b	129	GLU
36	1e	86	ALA
43	1l	105	TYR
4	2E	52	LEU
11	2P	45	LEU
33	2b	105	PHE
38	2g	4	ARG
41	2j	75	ILE
41	2j	79	ARG
42	2k	117	ASN

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Mol	Chain	Res	Type
43	2l	105	TYR
48	2q	33	GLY
11	1P	45	LEU
19	1X	2	LYS
26	14	49	PHE
33	1b	124	SER
33	1b	231	GLU
34	1c	80	GLY
46	1o	88	ARG
7	2H	12	PRO
7	2H	126	PRO
8	2I	10	GLU
14	2S	84	GLN
26	24	48	ARG
33	2b	153	ARG
33	2b	213	LEU
44	2m	6	GLY
45	2n	14	PRO
6	1G	43	LEU
11	1P	36	LYS
17	1V	79	VAL
33	1b	16	HIS
51	1t	47	GLY
13	2R	45	ARG
19	2X	93	GLU
21	2Z	146	ILE
33	2b	65	GLY
36	2e	69	VAL
11	2P	122	PRO
41	2j	77	PRO
33	1b	125	PRO
21	2Z	53	ILE
42	1k	49	GLY
3	2D	29	PRO
21	2Z	147	GLY
34	2c	84	ILE
40	2i	41	VAL

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%)	207 (96%)	8 (4%)	34	60
3	2D	215/218 (99%)	204 (95%)	11 (5%)	24	45
4	1E	164/166 (99%)	153 (93%)	11 (7%)	16	31
4	2E	164/166 (99%)	155 (94%)	9 (6%)	21	41
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	15
5	2F	159/166 (96%)	151 (95%)	8 (5%)	24	46
6	1G	143/156 (92%)	132 (92%)	11 (8%)	13	25
6	2G	143/156 (92%)	122 (85%)	21 (15%)	3	5
7	1H	144/148 (97%)	137 (95%)	7 (5%)	25	47
7	2H	144/148 (97%)	129 (90%)	15 (10%)	7	13
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2	4
8	2I	105/124 (85%)	84 (80%)	21 (20%)	1	2
9	1N	118/119 (99%)	113 (96%)	5 (4%)	30	54
9	2N	118/119 (99%)	113 (96%)	5 (4%)	30	54
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	68
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31	56
11	1P	115/116 (99%)	107 (93%)	8 (7%)	15	29
11	2P	115/116 (99%)	104 (90%)	11 (10%)	8	16
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	22	42
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	27	51
13	1R	101/101 (100%)	98 (97%)	3 (3%)	41	68
13	2R	101/101 (100%)	98 (97%)	3 (3%)	41	68
14	1S	86/88 (98%)	80 (93%)	6 (7%)	15	29
14	2S	85/88 (97%)	79 (93%)	6 (7%)	14	28
15	1T	115/127 (91%)	111 (96%)	4 (4%)	36	62
15	2T	113/127 (89%)	104 (92%)	9 (8%)	12	23
16	1U	93/94 (99%)	89 (96%)	4 (4%)	29	53
16	2U	93/94 (99%)	90 (97%)	3 (3%)	39	65
17	1V	80/82 (98%)	77 (96%)	3 (4%)	33	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	2V	80/82 (98%)	69 (86%)	11 (14%)	3	6
18	1W	90/92 (98%)	86 (96%)	4 (4%)	28	52
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	52
19	1X	77/78 (99%)	76 (99%)	1 (1%)	69	87
19	2X	77/78 (99%)	73 (95%)	4 (5%)	23	44
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	19	37
20	2Y	85/91 (93%)	74 (87%)	11 (13%)	4	8
21	1Z	135/179 (75%)	118 (87%)	17 (13%)	4	8
21	2Z	137/179 (76%)	117 (85%)	20 (15%)	3	5
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	62 (95%)	3 (5%)	27	50
23	11	80/83 (96%)	75 (94%)	5 (6%)	18	34
23	21	80/83 (96%)	74 (92%)	6 (8%)	13	26
24	12	65/67 (97%)	59 (91%)	6 (9%)	9	18
24	22	65/67 (97%)	60 (92%)	5 (8%)	13	25
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	37
25	23	50/52 (96%)	47 (94%)	3 (6%)	19	37
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	7
26	24	53/63 (84%)	40 (76%)	13 (24%)	0	1
27	15	50/52 (96%)	48 (96%)	2 (4%)	31	56
27	25	50/52 (96%)	48 (96%)	2 (4%)	31	56
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	10
28	26	50/52 (96%)	42 (84%)	8 (16%)	2	4
29	17	41/42 (98%)	38 (93%)	3 (7%)	14	27
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	15
30	18	54/55 (98%)	48 (89%)	6 (11%)	6	11
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	17
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	69
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	168 (88%)	24 (12%)	4	8
33	2b	187/220 (85%)	155 (83%)	32 (17%)	2	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1c	142/188 (76%)	130 (92%)	12 (8%)	10	21
34	2c	140/188 (74%)	130 (93%)	10 (7%)	14	28
35	1d	169/181 (93%)	156 (92%)	13 (8%)	13	25
35	2d	173/181 (96%)	159 (92%)	14 (8%)	11	23
36	1e	113/123 (92%)	106 (94%)	7 (6%)	18	35
36	2e	114/123 (93%)	104 (91%)	10 (9%)	10	19
37	1f	84/90 (93%)	80 (95%)	4 (5%)	25	48
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	49
38	1g	119/127 (94%)	102 (86%)	17 (14%)	3	6
38	2g	120/127 (94%)	103 (86%)	17 (14%)	3	6
39	1h	114/119 (96%)	106 (93%)	8 (7%)	15	29
39	2h	114/119 (96%)	102 (90%)	12 (10%)	7	13
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	11
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7	14
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	5
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	10
42	1k	82/99 (83%)	71 (87%)	11 (13%)	4	7
42	2k	83/99 (84%)	71 (86%)	12 (14%)	3	6
43	1l	96/108 (89%)	89 (93%)	7 (7%)	14	27
43	2l	96/108 (89%)	88 (92%)	8 (8%)	11	22
44	1m	93/101 (92%)	81 (87%)	12 (13%)	4	8
44	2m	92/101 (91%)	84 (91%)	8 (9%)	10	20
45	1n	49/50 (98%)	47 (96%)	2 (4%)	30	55
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	55
46	1o	78/80 (98%)	74 (95%)	4 (5%)	24	45
46	2o	78/80 (98%)	76 (97%)	2 (3%)	46	72
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	14
47	2p	68/74 (92%)	65 (96%)	3 (4%)	28	52
48	1q	94/97 (97%)	89 (95%)	5 (5%)	22	43
48	2q	94/97 (97%)	88 (94%)	6 (6%)	17	33
49	1r	59/77 (77%)	52 (88%)	7 (12%)	5	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	2r	59/77 (77%)	56 (95%)	3 (5%)	24	45
50	1s	69/80 (86%)	63 (91%)	6 (9%)	10	20
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7	13
51	1t	70/82 (85%)	62 (89%)	8 (11%)	5	11
51	2t	70/82 (85%)	66 (94%)	4 (6%)	20	39
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	40
56	1z	2/2 (100%)	2 (100%)	0	100	100
56	2z	2/2 (100%)	2 (100%)	0	100	100
All	All	9307/10068 (92%)	8550 (92%)	757 (8%)	11	23

All (757) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	12	SER
3	1D	14	ARG
3	1D	32	SER
3	1D	154	LYS
3	1D	175	LEU
3	1D	242	ARG
3	1D	259	THR
3	1D	273	ARG
4	1E	12	THR
4	1E	33	VAL
4	1E	38	THR
4	1E	47	VAL
4	1E	89	ASP
4	1E	90	THR
4	1E	93	VAL
4	1E	113	PHE
4	1E	116	VAL
4	1E	184	VAL
4	1E	188	VAL
5	1F	24	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL

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Mol	Chain	Res	Type
5	1F	106	ARG
5	1F	132	VAL
5	1F	140	LEU
5	1F	144	LYS
5	1F	158	THR
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
5	1F	197	ASP
6	1G	5	VAL
6	1G	7	LEU
6	1G	8	LYS
6	1G	31	VAL
6	1G	36	LYS
6	1G	43	LEU
6	1G	91	ARG
6	1G	115	ARG
6	1G	140	ILE
6	1G	150	ASP
6	1G	159	VAL
7	1H	2	SER
7	1H	13	LYS
7	1H	50	VAL
7	1H	56	SER
7	1H	98	LEU
7	1H	116	GLU
7	1H	129	THR
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	20	ASP
8	1I	40	THR
8	1I	41	GLU
8	1I	42	SER
8	1I	47	LEU
8	1I	50	ARG
8	1I	61	ARG
8	1I	82	ARG
8	1I	87	LYS
8	1I	91	SER
8	1I	92	VAL

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Mol	Chain	Res	Type
8	1I	101	LEU
8	1I	108	THR
8	1I	116	LEU
8	1I	123	LEU
8	1I	129	THR
9	1N	1	MET
9	1N	2	LYS
9	1N	28	THR
9	1N	48	MET
9	1N	83	LYS
10	1O	28	SER
10	1O	96	THR
10	1O	108	GLU
11	1P	3	LEU
11	1P	90	ARG
11	1P	92	GLU
11	1P	95	VAL
11	1P	98	GLU
11	1P	101	VAL
11	1P	147	LEU
11	1P	149	GLU
12	1Q	7	MET
12	1Q	18	LYS
12	1Q	56	ARG
12	1Q	98	LYS
12	1Q	109	VAL
12	1Q	115	MET
13	1R	36	THR
13	1R	42	LYS
13	1R	114	VAL
14	1S	14	VAL
14	1S	15	ARG
14	1S	53	SER
14	1S	69	VAL
14	1S	85	VAL
14	1S	98	VAL
15	1T	28	VAL
15	1T	85	LYS
15	1T	96	ARG
15	1T	128	GLU
16	1U	17	ILE
16	1U	31	SER

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Mol	Chain	Res	Type
16	1U	74	LEU
16	1U	95	LEU
17	1V	38	LEU
17	1V	79	VAL
17	1V	85	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	67	ASP
19	1X	81	VAL
20	1Y	7	VAL
20	1Y	26	LYS
20	1Y	31	LEU
20	1Y	99	CYS
20	1Y	106	LEU
21	1Z	42	VAL
21	1Z	46	LYS
21	1Z	49	ARG
21	1Z	56	VAL
21	1Z	61	LEU
21	1Z	70	LEU
21	1Z	119	GLU
21	1Z	123	ASP
21	1Z	124	ILE
21	1Z	136	PHE
21	1Z	150	LEU
21	1Z	153	SER
21	1Z	154	ASP
21	1Z	157	LEU
21	1Z	161	VAL
21	1Z	170	THR
21	1Z	171	ILE
23	11	11	ARG
23	11	35	THR
23	11	38	SER
23	11	40	ARG
23	11	46	LEU
24	12	19	VAL
24	12	24	LEU
24	12	40	SER
24	12	53	LEU
24	12	55	ARG

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Mol	Chain	Res	Type
24	12	65	ASN
25	13	54	VAL
25	13	55	ARG
25	13	60	GLU
26	14	1	MET
26	14	31	ILE
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
26	14	59	PHE
26	14	63	TYR
26	14	67	TYR
27	15	40	LYS
27	15	57	VAL
28	16	4	GLU
28	16	8	LYS
28	16	9	LEU
28	16	14	THR
28	16	28	ARG
28	16	45	LYS
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
30	18	29	LYS
30	18	31	HIS
30	18	34	TRP
30	18	43	GLN
31	19	7	VAL
33	1b	12	GLU
33	1b	24	TRP
33	1b	28	PHE
33	1b	35	GLU
33	1b	37	ASN
33	1b	39	ILE
33	1b	43	ASP
33	1b	54	THR
33	1b	61	LEU
33	1b	80	ILE
33	1b	81	VAL
33	1b	82	ARG

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Mol	Chain	Res	Type
33	1b	96	ARG
33	1b	102	LEU
33	1b	160	ASP
33	1b	162	ILE
33	1b	185	ILE
33	1b	190	THR
33	1b	208	ILE
33	1b	212	GLN
33	1b	215	LEU
33	1b	222	ILE
33	1b	229	VAL
33	1b	236	TYR
34	1c	3	ASN
34	1c	4	LYS
34	1c	82	GLU
34	1c	101	LEU
34	1c	112	SER
34	1c	119	ARG
34	1c	124	ILE
34	1c	175	LEU
34	1c	190	ARG
34	1c	193	TYR
34	1c	195	VAL
34	1c	207	VAL
35	1d	3	ARG
35	1d	8	VAL
35	1d	11	LEU
35	1d	19	LEU
35	1d	76	ARG
35	1d	91	SER
35	1d	134	ASP
35	1d	140	VAL
35	1d	158	ILE
35	1d	175	SER
35	1d	177	ASP
35	1d	188	LEU
35	1d	193	ASP
36	1e	24	ARG
36	1e	41	VAL
36	1e	53	LEU
36	1e	56	GLN
36	1e	68	GLU

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Mol	Chain	Res	Type
36	1e	75	THR
36	1e	131	ILE
37	1f	45	LEU
37	1f	70	ASP
37	1f	73	ASN
37	1f	75	LEU
38	1g	10	ARG
38	1g	12	LEU
38	1g	21	VAL
38	1g	27	ILE
38	1g	41	ARG
38	1g	50	ILE
38	1g	57	GLU
38	1g	59	LEU
38	1g	61	VAL
38	1g	72	ARG
38	1g	77	SER
38	1g	85	TYR
38	1g	98	SER
38	1g	113	GLU
38	1g	114	ARG
38	1g	115	ARG
38	1g	138	LYS
39	1h	3	THR
39	1h	25	ASP
39	1h	29	SER
39	1h	51	VAL
39	1h	87	SER
39	1h	99	GLU
39	1h	109	ILE
39	1h	112	LEU
40	1i	23	ASN
40	1i	25	LYS
40	1i	27	THR
40	1i	48	GLU
40	1i	53	VAL
40	1i	64	THR
40	1i	88	TYR
40	1i	96	LEU
40	1i	103	THR
40	1i	128	ARG
41	1j	7	LYS

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Mol	Chain	Res	Type
41	1j	17	ASP
41	1j	35	SER
41	1j	38	ILE
41	1j	42	THR
41	1j	43	ARG
41	1j	49	VAL
41	1j	72	VAL
41	1j	81	THR
41	1j	92	THR
42	1k	18	ARG
42	1k	25	TYR
42	1k	31	THR
42	1k	48	ILE
42	1k	80	VAL
42	1k	87	THR
42	1k	96	ARG
42	1k	104	GLN
42	1k	109	VAL
42	1k	114	VAL
42	1k	117	ASN
43	1l	22	SER
43	1l	33	ARG
43	1l	36	VAL
43	1l	58	VAL
43	1l	62	SER
43	1l	83	VAL
43	1l	89	ARG
44	1m	3	ARG
44	1m	4	ILE
44	1m	11	ARG
44	1m	12	ASN
44	1m	17	VAL
44	1m	43	THR
44	1m	49	THR
44	1m	64	TRP
44	1m	94	ARG
44	1m	105	THR
44	1m	106	ASN
44	1m	109	THR
45	1n	13	THR
45	1n	56	VAL
46	1o	24	SER

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Mol	Chain	Res	Type
46	1o	35	ARG
46	1o	62	GLN
46	1o	76	GLU
47	1p	27	LYS
47	1p	43	LYS
47	1p	45	THR
47	1p	54	GLU
47	1p	60	LEU
47	1p	61	SER
47	1p	62	VAL
48	1q	11	VAL
48	1q	36	ILE
48	1q	45	HIS
48	1q	63	ARG
48	1q	66	SER
49	1r	31	LEU
49	1r	36	ASN
49	1r	37	VAL
49	1r	45	SER
49	1r	61	LYS
49	1r	63	GLN
49	1r	76	LEU
50	1s	4	SER
50	1s	5	LEU
50	1s	12	ASP
50	1s	28	LYS
50	1s	41	VAL
50	1s	43	GLU
51	1t	10	LEU
51	1t	23	ARG
51	1t	24	LEU
51	1t	37	SER
51	1t	38	LYS
51	1t	42	GLN
51	1t	43	LEU
51	1t	100	ILE
3	2D	3	VAL
3	2D	22	SER
3	2D	37	LEU
3	2D	61	LEU
3	2D	71	ASP
3	2D	88	ARG

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Mol	Chain	Res	Type
3	2D	171	ASP
3	2D	173	VAL
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
4	2E	12	THR
4	2E	33	VAL
4	2E	38	THR
4	2E	72	VAL
4	2E	90	THR
4	2E	92	THR
4	2E	116	VAL
4	2E	119	ARG
4	2E	145	LYS
5	2F	33	LEU
5	2F	110	LEU
5	2F	119	ARG
5	2F	158	THR
5	2F	162	LEU
5	2F	183	VAL
5	2F	195	ASP
5	2F	197	ASP
6	2G	4	ASP
6	2G	5	VAL
6	2G	7	LEU
6	2G	27	ASN
6	2G	28	VAL
6	2G	31	VAL
6	2G	43	LEU
6	2G	51	ARG
6	2G	60	LEU
6	2G	62	LEU
6	2G	79	ASN
6	2G	91	ARG
6	2G	95	ARG
6	2G	123	ASN
6	2G	133	LEU
6	2G	140	ILE
6	2G	145	THR
6	2G	146	TYR
6	2G	152	LEU
6	2G	162	THR

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Mol	Chain	Res	Type
6	2G	165	THR
7	2H	3	ARG
7	2H	15	VAL
7	2H	16	SER
7	2H	43	VAL
7	2H	49	VAL
7	2H	52	VAL
7	2H	56	SER
7	2H	57	ASP
7	2H	58	GLU
7	2H	70	THR
7	2H	95	ARG
7	2H	111	HIS
7	2H	122	THR
7	2H	127	GLU
7	2H	133	VAL
8	2I	12	LEU
8	2I	14	ASP
8	2I	15	VAL
8	2I	19	VAL
8	2I	38	LEU
8	2I	41	GLU
8	2I	43	ASN
8	2I	44	LEU
8	2I	45	LYS
8	2I	50	ARG
8	2I	51	ILE
8	2I	58	LEU
8	2I	61	ARG
8	2I	72	LEU
8	2I	85	GLU
8	2I	96	ASP
8	2I	101	LEU
8	2I	107	VAL
8	2I	117	GLU
8	2I	123	LEU
8	2I	127	VAL
9	2N	46	VAL
9	2N	48	MET
9	2N	73	THR
9	2N	83	LYS
9	2N	131	GLN

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Mol	Chain	Res	Type
10	2O	66	LYS
10	2O	69	ILE
10	2O	91	LEU
10	2O	112	MET
11	2P	70	GLN
11	2P	90	ARG
11	2P	92	GLU
11	2P	95	VAL
11	2P	98	GLU
11	2P	101	VAL
11	2P	105	LEU
11	2P	131	SER
11	2P	133	SER
11	2P	135	LEU
11	2P	149	GLU
12	2Q	1	MET
12	2Q	12	GLN
12	2Q	18	LYS
12	2Q	21	THR
12	2Q	106	VAL
13	2R	6	SER
13	2R	95	THR
13	2R	114	VAL
14	2S	3	ARG
14	2S	15	ARG
14	2S	49	VAL
14	2S	52	SER
14	2S	63	THR
14	2S	110	LEU
15	2T	17	THR
15	2T	28	VAL
15	2T	40	THR
15	2T	63	VAL
15	2T	72	VAL
15	2T	74	ARG
15	2T	87	ASP
15	2T	89	VAL
15	2T	96	ARG
16	2U	5	LYS
16	2U	74	LEU
16	2U	95	LEU
17	2V	7	THR

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Mol	Chain	Res	Type
17	2V	12	TYR
17	2V	26	ASP
17	2V	39	LEU
17	2V	61	VAL
17	2V	66	ARG
17	2V	71	LEU
17	2V	73	SER
17	2V	79	VAL
17	2V	98	GLU
17	2V	100	ARG
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	67	ASP
19	2X	1	MET
19	2X	57	LEU
19	2X	81	VAL
19	2X	92	LEU
20	2Y	14	LEU
20	2Y	26	LYS
20	2Y	38	ILE
20	2Y	40	GLU
20	2Y	47	LYS
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	90	LEU
20	2Y	97	ARG
20	2Y	98	VAL
20	2Y	99	CYS
21	2Z	16	SER
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	61	LEU
21	2Z	66	SER
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	74	VAL
21	2Z	89	PHE
21	2Z	91	LEU
21	2Z	121	HIS
21	2Z	122	ARG
21	2Z	129	SER

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Mol	Chain	Res	Type
21	2Z	136	PHE
21	2Z	144	LEU
21	2Z	145	GLU
21	2Z	149	SER
21	2Z	154	ASP
21	2Z	171	ILE
21	2Z	174	VAL
22	20	40	GLN
22	20	55	ARG
22	20	68	GLU
23	21	11	ARG
23	21	40	ARG
23	21	46	LEU
23	21	59	THR
23	21	80	LEU
23	21	83	GLU
24	22	38	GLN
24	22	45	SER
24	22	51	ARG
24	22	60	LEU
24	22	70	GLN
25	23	31	LEU
25	23	54	VAL
25	23	59	VAL
26	24	3	GLU
26	24	10	VAL
26	24	27	THR
26	24	33	VAL
26	24	34	GLU
26	24	48	ARG
26	24	50	VAL
26	24	56	VAL
26	24	59	PHE
26	24	61	ARG
26	24	63	TYR
26	24	67	TYR
26	24	68	ARG
27	25	6	VAL
27	25	35	GLU
28	26	7	ILE
28	26	9	LEU
28	26	14	THR

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Mol	Chain	Res	Type
28	26	19	ARG
28	26	20	ASN
28	26	30	THR
28	26	32	ASN
28	26	52	VAL
29	27	1	MET
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	23	VAL
30	28	31	HIS
30	28	34	TRP
30	28	37	SER
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	16	HIS
33	2b	24	TRP
33	2b	35	GLU
33	2b	37	ASN
33	2b	44	LEU
33	2b	48	MET
33	2b	67	THR
33	2b	68	ILE
33	2b	76	GLN
33	2b	83	MET
33	2b	93	VAL
33	2b	95	GLN
33	2b	110	GLN
33	2b	112	VAL
33	2b	115	LEU
33	2b	117	GLU
33	2b	127	ILE
33	2b	160	ASP
33	2b	163	PHE
33	2b	164	VAL
33	2b	168	THR
33	2b	185	ILE
33	2b	187	LEU
33	2b	189	ASP
33	2b	191	ASP

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Mol	Chain	Res	Type
33	2b	198	ASP
33	2b	208	ILE
33	2b	224	GLN
33	2b	230	VAL
34	2c	16	ARG
34	2c	17	ASP
34	2c	26	LYS
34	2c	39	ILE
34	2c	47	LEU
34	2c	91	LEU
34	2c	101	LEU
34	2c	172	ARG
34	2c	190	ARG
34	2c	206	GLU
35	2d	5	ILE
35	2d	28	SER
35	2d	31	CYS
35	2d	34	GLU
35	2d	78	LEU
35	2d	96	LEU
35	2d	119	GLN
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	156	GLU
35	2d	158	ILE
35	2d	162	LEU
35	2d	175	SER
36	2e	10	MET
36	2e	13	ILE
36	2e	18	ARG
36	2e	20	GLN
36	2e	31	LEU
36	2e	38	GLN
36	2e	41	VAL
36	2e	51	VAL
36	2e	71	LEU
36	2e	147	ASP
37	2f	19	LEU
37	2f	63	TYR
37	2f	69	GLU
37	2f	81	ILE

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Mol	Chain	Res	Type
38	2g	9	VAL
38	2g	15	ASP
38	2g	24	THR
38	2g	32	ARG
38	2g	51	GLN
38	2g	52	GLU
38	2g	53	LYS
38	2g	72	ARG
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	94	ARG
38	2g	114	ARG
38	2g	135	VAL
38	2g	144	MET
38	2g	154	TYR
38	2g	155	ARG
39	2h	22	GLU
39	2h	25	ASP
39	2h	29	SER
39	2h	51	VAL
39	2h	52	ASP
39	2h	54	ASP
39	2h	85	ARG
39	2h	112	LEU
39	2h	122	ARG
39	2h	127	LEU
39	2h	133	LEU
39	2h	137	VAL
40	2i	7	THR
40	2i	12	GLU
40	2i	14	VAL
40	2i	20	ARG
40	2i	40	LEU
40	2i	65	VAL
40	2i	88	TYR
40	2i	89	ASN
40	2i	104	ARG
41	2j	11	PHE
41	2j	21	GLN
41	2j	23	ILE
41	2j	42	THR

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Mol	Chain	Res	Type
41	2j	55	LYS
41	2j	71	LEU
41	2j	81	THR
41	2j	84	GLN
42	2k	14	VAL
42	2k	18	ARG
42	2k	48	ILE
42	2k	53	SER
42	2k	62	GLN
42	2k	79	SER
42	2k	81	ASP
42	2k	98	LEU
42	2k	103	LEU
42	2k	105	VAL
42	2k	117	ASN
42	2k	125	PHE
43	2l	18	VAL
43	2l	36	VAL
43	2l	39	VAL
43	2l	40	VAL
43	2l	60	LEU
43	2l	62	SER
43	2l	65	GLU
43	2l	116	SER
44	2m	15	VAL
44	2m	17	VAL
44	2m	32	GLU
44	2m	90	LEU
44	2m	94	ARG
44	2m	103	THR
44	2m	106	ASN
44	2m	117	VAL
45	2n	15	LYS
45	2n	33	VAL
46	2o	35	ARG
46	2o	83	GLU
47	2p	20	VAL
47	2p	43	LYS
47	2p	67	THR
48	2q	26	GLN
48	2q	36	ILE
48	2q	45	HIS

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Mol	Chain	Res	Type
48	2q	63	ARG
48	2q	91	ARG
48	2q	100	LYS
49	2r	31	LEU
49	2r	69	THR
49	2r	82	THR
50	2s	27	GLU
50	2s	37	ARG
50	2s	45	VAL
50	2s	48	THR
50	2s	51	VAL
50	2s	57	HIS
50	2s	77	THR
51	2t	45	GLN
51	2t	46	GLU
51	2t	93	GLU
51	2t	99	LEU
52	2u	6	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	126	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
8	1I	105	HIS
9	1N	8	GLN
10	1O	3	GLN
12	1Q	12	GLN
12	1Q	57	HIS
13	1R	71	GLN
14	1S	68	GLN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	54	HIS
21	1Z	73	GLN
21	1Z	151	HIS
22	10	3	HIS

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Mol	Chain	Res	Type
24	12	46	GLN
25	13	32	GLN
30	18	43	GLN
33	1b	40	HIS
33	1b	78	GLN
33	1b	94	ASN
33	1b	140	HIS
33	1b	212	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	69	HIS
34	1c	162	GLN
34	1c	170	GLN
35	1d	42	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	20	GLN
36	1e	56	GLN
36	1e	78	HIS
36	1e	141	GLN
37	1f	57	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	64	GLN
38	1g	86	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	124	GLN
41	1j	56	HIS
42	1k	99	GLN
43	1l	99	HIS
48	1q	26	GLN
49	1r	63	GLN
50	1s	83	HIS
51	1t	90	GLN
4	2E	48	GLN
4	2E	143	ASN
7	2H	111	HIS
10	2O	3	GLN

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Mol	Chain	Res	Type
10	2O	5	GLN
11	2P	27	HIS
12	2Q	12	GLN
14	2S	38	GLN
15	2T	43	GLN
15	2T	84	GLN
19	2X	31	HIS
21	2Z	151	HIS
22	20	35	ASN
24	22	38	GLN
25	23	32	GLN
31	29	20	HIS
33	2b	135	GLN
33	2b	140	HIS
34	2c	6	HIS
34	2c	139	GLN
34	2c	162	GLN
35	2d	116	GLN
35	2d	119	GLN
35	2d	160	GLN
36	2e	38	GLN
36	2e	78	HIS
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
40	2i	31	GLN
40	2i	34	ASN
40	2i	89	ASN
41	2j	13	HIS
41	2j	62	HIS
42	2k	116	HIS
42	2k	117	ASN
43	2l	99	HIS
44	2m	77	ASN
44	2m	92	HIS
45	2n	49	HIS
47	2p	13	HIS
47	2p	16	HIS
49	2r	63	GLN
50	2s	47	HIS
50	2s	57	HIS
50	2s	69	HIS

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Mol	Chain	Res	Type
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	441 (15%)	30 (1%)
1	2A	2790/2915 (95%)	458 (16%)	25 (0%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	118/121 (97%)	21 (17%)	0
32	1a	1494/1521 (98%)	242 (16%)	0
32	2a	1498/1521 (98%)	275 (18%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	0	0
54	1w	70/76 (92%)	24 (34%)	0
54	2w	67/76 (88%)	23 (34%)	0
55	1x	75/77 (97%)	7 (9%)	0
55	2x	75/77 (97%)	7 (9%)	0
57	1y	71/76 (93%)	27 (38%)	0
57	2y	69/76 (90%)	22 (31%)	0
All	All	9333/9620 (97%)	1558 (16%)	55 (0%)

All (1558) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	14	A
1	1A	15	G
1	1A	27	G
1	1A	34	C
1	1A	45	C
1	1A	58	G
1	1A	61	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

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Mol	Chain	Res	Type
1	1A	119	A
1	1A	120	U
1	1A	139(A)	G
1	1A	154	G
1	1A	154(A)	C
1	1A	173	G
1	1A	174	C
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
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	264	C
1	1A	269	U
1	1A	271(J)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	357	A
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	396	G

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Mol	Chain	Res	Type
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
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	573	G
1	1A	575	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	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(A)	A
1	1A	652(F)	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	764	A
1	1A	765	G
1	1A	775	G

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Mol	Chain	Res	Type
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	811	U
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G
1	1A	880	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	894	C
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A

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Mol	Chain	Res	Type
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1039	G
1	1A	1040	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1057	A
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1065	U
1	1A	1069	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1081	U
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1093	G
1	1A	1094	U
1	1A	1097	U
1	1A	1098	A
1	1A	1099	G
1	1A	1101	U
1	1A	1110	G
1	1A	1111	A

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Mol	Chain	Res	Type
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1135	C
1	1A	1136	G
1	1A	1149	G
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	1220	A
1	1A	1244	G
1	1A	1248	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1276	A
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1320	C
1	1A	1321	A
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1436	G

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Mol	Chain	Res	Type
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1460	A
1	1A	1461	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1539	G
1	1A	1540	U
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1607	C
1	1A	1608	A
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	1722	A
1	1A	1746	G
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A

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Mol	Chain	Res	Type
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1817	G
1	1A	1829	A
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1919	A
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	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1981	A
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	2097	C
1	1A	2102	U
1	1A	2108	C

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Mol	Chain	Res	Type
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2120	G
1	1A	2121	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
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	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2150	U
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2169	A
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2195	C
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G

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Mol	Chain	Res	Type
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2267	A
1	1A	2268	A
1	1A	2269	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2314	C
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2361	A
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G

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Mol	Chain	Res	Type
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	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	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	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2761	G
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2803	C
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A

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Mol	Chain	Res	Type
1	1A	2861	G
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	12	C
2	1B	13	A
2	1B	15	A
2	1B	45	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	110	G
32	1a	5	U
32	1a	6	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	142	G
32	1a	144	G
32	1a	155	C
32	1a	160	A
32	1a	163	C
32	1a	164	U
32	1a	174	C
32	1a	182	U

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Mol	Chain	Res	Type
32	1a	189(C)	C
32	1a	189(E)	U
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	200	G
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	279	A
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	347	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	355	C
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	383	A
32	1a	384	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	424	G
32	1a	429	U
32	1a	439	A
32	1a	441	A
32	1a	442	C

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Mol	Chain	Res	Type
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	483	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	545	C
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	630	G
32	1a	639	G
32	1a	653	A
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	703	G
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	749	C
32	1a	752	G

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Mol	Chain	Res	Type
32	1a	755	G
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	852	G
32	1a	870	U
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	950	U
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1002	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	1022	G

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Mol	Chain	Res	Type
32	1a	1023	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	1034	G
32	1a	1037	C
32	1a	1039	C
32	1a	1040	U
32	1a	1043	C
32	1a	1044	A
32	1a	1051	C
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1127	G
32	1a	1132	C
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1157	A
32	1a	1159	U
32	1a	1174	G
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G

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Mol	Chain	Res	Type
32	1a	1202	G
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1238	A
32	1a	1252	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1275	A
32	1a	1276	G
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1297	C
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1364	U
32	1a	1370	G
32	1a	1371	G
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1452	C
32	1a	1456	G
32	1a	1458	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A

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Mol	Chain	Res	Type
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
54	1w	2	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	9	A
54	1w	14	A
54	1w	15	G
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	36	A
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	66	U
54	1w	68	C
54	1w	69	G
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	14	A
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	59	A
55	1x	61	C
57	1y	5	G
57	1y	6	G
57	1y	9	A
57	1y	14	A
57	1y	19	G

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Mol	Chain	Res	Type
57	1y	20	U
57	1y	21	A
57	1y	27	G
57	1y	35	A
57	1y	36	A
57	1y	40	C
57	1y	44	G
57	1y	45	U
57	1y	46	G7M
57	1y	47	U
57	1y	48	C
57	1y	49	C
57	1y	56	C
57	1y	57	G
57	1y	58	A
57	1y	59	U
57	1y	60	U
57	1y	61	C
57	1y	65	G
57	1y	66	U
57	1y	70	G
57	1y	72	C
1	2A	8	A
1	2A	12	U
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	154	G

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Mol	Chain	Res	Type
1	2A	157	U
1	2A	173	G
1	2A	174	C
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	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	271(J)	C
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	289	A
1	2A	311	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	346	A
1	2A	352	G
1	2A	354	G
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	399	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	435	C

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Mol	Chain	Res	Type
1	2A	442	G
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	479	A
1	2A	480	A
1	2A	481	G
1	2A	494	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	533	G
1	2A	542	C
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	606	U
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	634	C
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G

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Mol	Chain	Res	Type
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	783	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	857	C
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	917	A

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Mol	Chain	Res	Type
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	950	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	999	U
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1114	G
1	2A	1116	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1141	U
1	2A	1142	U
1	2A	1171	G
1	2A	1205	U
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1253	A
1	2A	1256	G

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Mol	Chain	Res	Type
1	2A	1271	G
1	2A	1272	A
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
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	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1416	G
1	2A	1417	C
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
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1505	C
1	2A	1508	A

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Mol	Chain	Res	Type
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1514	U
1	2A	1520	G
1	2A	1526	G
1	2A	1531	C
1	2A	1542	A
1	2A	1545	A
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1743	C
1	2A	1746	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	1816	G
1	2A	1829	A

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Mol	Chain	Res	Type
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1861	G
1	2A	1876	A
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	1931	U
1	2A	1932	A
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
1	2A	1972	A
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	2093	G
1	2A	2099	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2113	U

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Mol	Chain	Res	Type
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2138	C
1	2A	2139	C
1	2A	2140	C
1	2A	2142	C
1	2A	2145	C
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2177	C
1	2A	2178	C
1	2A	2181	G
1	2A	2183	C
1	2A	2185	C
1	2A	2188	C
1	2A	2189	U
1	2A	2198	A

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Mol	Chain	Res	Type
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	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	2406	U
1	2A	2424	C
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2465	C
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A

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Mol	Chain	Res	Type
1	2A	2491	U
1	2A	2494	G
1	2A	2498	C
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2534	A
1	2A	2554	U
1	2A	2555	U
1	2A	2562	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2574	G
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	2630	G
1	2A	2645	G
1	2A	2654	A
1	2A	2679	A
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	2733	A
1	2A	2748	A
1	2A	2751	G
1	2A	2752	C
1	2A	2764	A
1	2A	2765	A

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Mol	Chain	Res	Type
1	2A	2778	A
1	2A	2783	G
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2889	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	9	G
2	2B	12	C
2	2B	13	A
2	2B	17	C
2	2B	33	G
2	2B	40	U
2	2B	41	U
2	2B	45	A
2	2B	53	A
2	2B	61	G
2	2B	73	A
2	2B	75	G
2	2B	85	G
2	2B	89	G
2	2B	91	C
2	2B	106	G
2	2B	110	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	32	A

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Mol	Chain	Res	Type
32	2a	39	G
32	2a	41	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	66	G
32	2a	70	G
32	2a	73	G
32	2a	79	G
32	2a	80	G
32	2a	89	C
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	144	G
32	2a	159	G
32	2a	163	C
32	2a	182	U
32	2a	189(B)	C
32	2a	189(E)	U
32	2a	189(F)	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	231	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	279	A
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	350	G

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Mol	Chain	Res	Type
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	381	C
32	2a	384	G
32	2a	389	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	455	C
32	2a	470	C
32	2a	476	G
32	2a	477	A
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	524	G
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	545	C
32	2a	547	A
32	2a	559	A
32	2a	564	C

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Mol	Chain	Res	Type
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	581	G
32	2a	596	C
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	712	A
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	763	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	859	A
32	2a	874	G

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Mol	Chain	Res	Type
32	2a	887	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	932	C
32	2a	934	C
32	2a	938	A
32	2a	942	G
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	992	U
32	2a	993	G
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1002	G
32	2a	1003	G
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	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030	C

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Mol	Chain	Res	Type
32	2a	1030(A)	G
32	2a	1030(D)	A
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A
32	2a	1036	G
32	2a	1039	C
32	2a	1040	U
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1080	A
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1105	A
32	2a	1108	G
32	2a	1109	C
32	2a	1117	G
32	2a	1124	G
32	2a	1125	U
32	2a	1126	U
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1145	C
32	2a	1146	A
32	2a	1152	A

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Mol	Chain	Res	Type
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1181	G
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	1213	A
32	2a	1215	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1246	C
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1302	U
32	2a	1303	C
32	2a	1316	G
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1359	C

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Mol	Chain	Res	Type
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1378	C
32	2a	1404	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1452	C
32	2a	1460	A
32	2a	1492	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	6	G
54	2w	8	4SU
54	2w	9	A
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	46	G7M
54	2w	48	C
54	2w	50	U
54	2w	51	U
54	2w	58	A
54	2w	62	C
54	2w	64	A
54	2w	65	G
54	2w	68	C
54	2w	69	G
54	2w	70	G

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Mol	Chain	Res	Type
54	2w	74	C
55	2x	9	G
55	2x	18	G
55	2x	19	G
55	2x	20	U
55	2x	21	A
55	2x	47	U
55	2x	69	C
57	2y	2	C
57	2y	8	4SU
57	2y	15	G
57	2y	19	G
57	2y	23	A
57	2y	27	G
57	2y	41	C
57	2y	49	C
57	2y	52	G
57	2y	53	G
57	2y	56	C
57	2y	57	G
57	2y	58	A
57	2y	59	U
57	2y	60	U
57	2y	61	C
57	2y	63	G
57	2y	65	G
57	2y	68	C
57	2y	69	G
57	2y	70	G
57	2y	73	A

All (55) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	90	U
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	685	A
1	1A	746	A

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Mol	Chain	Res	Type
1	1A	974	G
1	1A	1047	G
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1275	A
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1663	C
1	1A	1992	G
1	1A	2126	A
1	1A	2134	A
1	1A	2183	C
1	1A	2238	G
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	229	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	746	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1142(A)	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A

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Mol	Chain	Res	Type
1	2A	1935	G
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	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
32	M2G	2a	966	32	20,27,28	1.42	3 (15%)	22,40,43	0.98	2 (9%)
1	5MC	2A	1942	1	18,22,23	0.98	2 (11%)	26,32,35	1.17	3 (11%)
32	M2G	1a	966	32	20,27,28	1.39	3 (15%)	22,40,43	1.10	3 (13%)
54	PSU	2w	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.78	3 (13%)
1	OMC	1A	1920	1	19,22,23	0.84	0	26,31,34	0.97	1 (3%)
55	8AN	2x	76	56,58,55	19,24,25	1.21	3 (15%)	13,35,38	1.84	2 (15%)
32	5MC	1a	967	32	18,22,23	0.94	2 (11%)	26,32,35	1.10	2 (7%)
54	5MU	1w	54	54	19,22,23	1.29	5 (26%)	28,32,35	2.10	6 (21%)
1	PSU	1A	1911	1	18,21,22	1.34	2 (11%)	22,30,33	1.93	4 (18%)
43	0TD	1l	92	43	7,9,10	4.72	1 (14%)	6,11,13	6.97	3 (50%)
32	UR3	1a	1498	32	19,22,23	0.98	0	26,32,35	1.53	2 (7%)
54	PSU	1w	32	54	18,21,22	1.36	2 (11%)	22,30,33	1.75	3 (13%)
32	5MC	1a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.17	2 (7%)
1	OMG	2A	2251	55,1	18,26,27	0.94	1 (5%)	19,38,41	1.15	3 (15%)
32	MA6	1a	1519	32	19,26,27	0.81	0	18,38,41	1.59	2 (11%)
55	5MU	2x	54	55	19,22,23	1.39	5 (26%)	28,32,35	2.25	6 (21%)
1	OMU	1A	2552	58,1	19,22,23	1.21	2 (10%)	26,31,34	1.70	6 (23%)
1	5MU	2A	1939	58,1	19,22,23	1.40	5 (26%)	28,32,35	2.43	6 (21%)
54	G7M	1w	46	54	20,26,27	1.20	2 (10%)	17,39,42	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	G7M	2y	46	57	20,26,27	1.40	2 (10%)	17,39,42	0.73	1 (5%)
54	PSU	2w	39	54	18,21,22	1.29	2 (11%)	22,30,33	1.96	4 (18%)
57	G7M	1y	46	57	20,26,27	1.32	1 (5%)	17,39,42	0.61	0
32	5MC	1a	1407	32	18,22,23	0.92	1 (5%)	26,32,35	1.15	3 (11%)
55	4SU	1x	8	55	18,21,22	2.05	5 (27%)	26,30,33	1.60	6 (23%)
32	5MC	1a	1404	32	18,22,23	1.06	2 (11%)	26,32,35	1.20	2 (7%)
32	5MC	2a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.22	3 (11%)
1	OMG	1A	2251	55,58,1	18,26,27	0.87	0	19,38,41	1.16	3 (15%)
1	PSU	2A	1917	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
57	PSU	2y	32	57	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
54	MIA	1w	37	54	24,31,32	2.12	3 (12%)	26,44,47	2.89	10 (38%)
54	5MU	2w	54	54	19,22,23	1.35	4 (21%)	28,32,35	1.81	5 (17%)
32	5MC	2a	1407	32	18,22,23	0.93	2 (11%)	26,32,35	1.19	2 (7%)
54	F3N	1w	76	54,1	30,36,37	1.45	5 (16%)	29,51,54	1.26	2 (6%)
1	2MA	2A	2503	58,1	17,25,26	1.01	1 (5%)	17,37,40	1.04	2 (11%)
32	PSU	1a	516	32	18,21,22	1.36	2 (11%)	22,30,33	1.93	5 (22%)
54	PSU	2w	55	54	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
56	FME	2z	1	56	8,9,10	0.96	0	7,9,11	1.60	1 (14%)
1	5MC	1A	1962	1	18,22,23	1.01	2 (11%)	26,32,35	1.21	3 (11%)
32	5MC	2a	967	58,32	18,22,23	0.95	2 (11%)	26,32,35	1.10	2 (7%)
54	MIA	2w	37	54	20,27,32	1.75	3 (15%)	22,39,47	2.00	6 (27%)
1	PSU	1A	1917	1	18,21,22	1.36	3 (16%)	22,30,33	2.07	4 (18%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
32	UR3	2a	1498	32	19,22,23	1.05	1 (5%)	26,32,35	1.41	1 (3%)
32	MA6	1a	1518	32	19,26,27	0.81	0	18,38,41	1.50	2 (11%)
54	G7M	2w	46	54	20,26,27	1.18	1 (5%)	17,39,42	0.78	0
1	5MU	1A	1939	1	19,22,23	1.49	6 (31%)	28,32,35	2.20	5 (17%)
32	MA6	2a	1519	32	19,26,27	0.84	0	18,38,41	1.68	2 (11%)
1	OMC	2A	1920	1	19,22,23	0.82	0	26,31,34	0.82	0
32	4OC	1a	1402	32	20,23,24	0.76	0	26,32,35	1.01	1 (3%)
57	PSU	2y	39	57,42	18,21,22	1.29	2 (11%)	22,30,33	1.98	3 (13%)
1	5MC	1A	1942	1	18,22,23	0.98	2 (11%)	26,32,35	1.23	3 (11%)
32	G7M	2a	527	58,32	20,26,27	1.21	2 (10%)	17,39,42	0.50	0
54	4SU	2w	8	54	18,21,22	1.67	4 (22%)	26,30,33	2.39	5 (19%)
54	PSU	1w	39	54	18,21,22	1.29	2 (11%)	22,30,33	2.07	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	1A	1915	1	19,22,23	1.38	5 (26%)	28,32,35	2.11	8 (28%)
1	PSU	1A	2605	58,1	18,21,22	1.40	2 (11%)	22,30,33	1.92	4 (18%)
1	PSU	2A	2605	1	18,21,22	1.39	3 (16%)	22,30,33	1.92	4 (18%)
55	5MC	2x	32	55	18,22,23	0.96	2 (11%)	26,32,35	1.30	4 (15%)
32	5MC	2a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.17	3 (11%)
32	MA6	2a	1518	32	19,26,27	0.84	0	18,38,41	1.46	2 (11%)
57	MIA	1y	37	57	18,24,32	1.15	2 (11%)	18,35,47	1.27	2 (11%)
57	PSU	1y	39	57	18,21,22	1.40	2 (11%)	22,30,33	1.80	4 (18%)
1	OMU	2A	2552	58,1	19,22,23	1.15	3 (15%)	26,31,34	1.82	6 (23%)
1	5MU	2A	1915	1	19,22,23	1.46	5 (26%)	28,32,35	2.07	7 (25%)
57	MIA	2y	37	57	18,24,32	1.12	2 (11%)	18,35,47	1.25	2 (11%)
54	4SU	1w	8	54	18,21,22	1.83	5 (27%)	26,30,33	1.84	5 (19%)
57	5MU	1y	54	57	19,22,23	1.42	4 (21%)	28,32,35	2.00	7 (25%)
32	G7M	1a	527	58,32	20,26,27	1.22	2 (10%)	17,39,42	0.69	0
55	8AN	1x	76	56,58,55	19,24,25	1.35	3 (15%)	13,35,38	1.91	2 (15%)
55	PSU	2x	55	55	18,21,22	1.36	2 (11%)	22,30,33	1.87	4 (18%)
32	2MG	1a	1207	32	18,26,27	0.91	1 (5%)	16,38,41	1.12	2 (12%)
57	PSU	1y	32	57	18,21,22	1.33	2 (11%)	22,30,33	1.81	4 (18%)
43	0TD	2l	92	43	7,9,10	4.76	1 (14%)	6,11,13	4.12	3 (50%)
54	F3N	2w	76	54,1	30,36,37	1.42	5 (16%)	29,51,54	1.19	1 (3%)
57	PSU	2y	55	57	18,21,22	1.33	2 (11%)	22,30,33	1.88	4 (18%)
55	5MC	1x	32	55	18,22,23	1.01	2 (11%)	26,32,35	1.34	3 (11%)
57	PSU	1y	55	57	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
32	4OC	2a	1402	58,32	20,23,24	0.75	0	26,32,35	1.00	2 (7%)
55	4SU	2x	8	58,55	18,21,22	2.01	6 (33%)	26,30,33	1.53	5 (19%)
1	2MA	1A	2503	58,1	17,25,26	1.00	0	17,37,40	0.98	2 (11%)
57	5MU	2y	54	57	19,22,23	1.41	5 (26%)	28,32,35	1.76	5 (17%)
55	PSU	1x	55	55	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
1	5MC	2A	1962	58,1	18,22,23	1.00	2 (11%)	26,32,35	1.14	2 (7%)
57	4SU	2y	8	57	18,21,22	1.74	4 (22%)	26,30,33	2.23	4 (15%)
54	PSU	1w	55	54	18,21,22	1.41	2 (11%)	22,30,33	1.90	4 (18%)
57	4SU	1y	8	57	18,21,22	1.66	4 (22%)	26,30,33	2.10	5 (19%)
55	5MU	1x	54	55	19,22,23	1.37	4 (21%)	28,32,35	2.03	6 (21%)
32	2MG	2a	1207	32	18,26,27	0.94	1 (5%)	16,38,41	1.11	2 (12%)
1	PSU	2A	1911	1	18,21,22	1.31	2 (11%)	22,30,33	2.01	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	FME	1z	1	56	8,9,10	0.99	0	7,9,11	1.81	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	PSU	2w	32	54	-	1/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
55	8AN	2x	76	56,58,55	-	3/3/25/26	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	1/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	58,1	-	0/9/27/28	0/2/2/2
1	5MU	2A	1939	58,1	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
57	G7M	2y	46	57	-	0/3/25/26	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
57	G7M	1y	46	57	-	1/3/25/26	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
1	OMG	1A	2251	55,58,1	-	1/5/27/28	0/3/3/3
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
57	PSU	2y	32	57	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	5/11/33/34	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	54,1	-	0/15/37/38	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	2A	2503	58,1	-	2/3/25/26	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
56	FME	2z	1	56	-	4/7/9/11	-
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	58,32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
54	G7M	2w	46	54	-	1/3/25/26	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
57	PSU	2y	39	57,42	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	58,32	-	3/3/25/26	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
1	PSU	1A	2605	58,1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
57	MIA	1y	37	57	-	0/3/25/34	0/3/3/3
57	PSU	1y	39	57	-	1/7/25/26	0/2/2/2
1	OMU	2A	2552	58,1	-	0/9/27/28	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
57	MIA	2y	37	57	-	0/3/25/34	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	58,32	-	3/3/25/26	0/3/3/3
55	8AN	1x	76	56,58,55	-	3/3/25/26	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
57	PSU	1y	32	57	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	F3N	2w	76	54,1	-	2/15/37/38	0/4/4/4
57	PSU	2y	55	57	-	2/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
57	PSU	1y	55	57	-	2/7/25/26	0/2/2/2
32	4OC	2a	1402	58,32	-	1/9/29/30	0/2/2/2
55	4SU	2x	8	58,55	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	58,1	-	1/3/25/26	0/3/3/3
57	5MU	2y	54	57	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	58,1	-	2/7/25/26	0/2/2/2
57	4SU	2y	8	57	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
57	4SU	1y	8	57	-	1/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
56	FME	1z	1	56	-	3/7/9/11	-

All (203) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.28	1.69	1.82
43	1l	92	0TD	CB-SB	-12.07	1.69	1.82
54	1w	37	MIA	C13-C14	6.93	1.52	1.32
54	2w	37	MIA	C2-S10	-6.54	1.70	1.75
54	1w	37	MIA	C2-S10	-6.35	1.70	1.75
55	1x	8	4SU	C4-N3	-4.81	1.32	1.37
57	2y	8	4SU	C4-S4	-4.63	1.59	1.68
32	2a	966	M2G	C2-N3	4.61	1.36	1.30
55	2x	8	4SU	C4-N3	-4.55	1.32	1.37
54	2w	8	4SU	C4-S4	-4.53	1.59	1.68
54	2w	76	F3N	CB-CG	-4.48	1.40	1.51
54	1w	8	4SU	C4-S4	-4.41	1.60	1.68
54	1w	76	F3N	CB-CG	-4.41	1.40	1.51
57	2y	46	G7M	C5-C4	4.31	1.47	1.39
55	2x	8	4SU	C4-S4	-4.29	1.60	1.68
57	1y	8	4SU	C4-S4	-4.09	1.60	1.68
57	1y	46	G7M	C5-C4	4.07	1.47	1.39
32	1a	966	M2G	C2-N3	4.06	1.35	1.30
32	1a	527	G7M	C5-C4	3.95	1.47	1.39
57	1y	39	PSU	C6-C5	3.90	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	8	4SU	C2-N3	-3.89	1.31	1.38
54	1w	55	PSU	C6-C5	3.86	1.39	1.35
55	1x	8	4SU	C4-S4	-3.82	1.61	1.68
54	2w	46	G7M	C5-C4	3.70	1.46	1.39
57	2y	32	PSU	C6-C5	3.68	1.39	1.35
54	1w	46	G7M	C5-C4	3.66	1.46	1.39
57	1y	55	PSU	C6-C5	3.65	1.39	1.35
54	1w	76	F3N	O4'-C1'	3.65	1.46	1.41
54	2w	55	PSU	C6-C5	3.61	1.39	1.35
32	2a	527	G7M	C5-C4	3.57	1.46	1.39
32	2a	516	PSU	C6-C5	3.53	1.39	1.35
55	1x	55	PSU	C6-C5	3.52	1.39	1.35
57	1y	32	PSU	C6-C5	3.50	1.39	1.35
54	2w	32	PSU	C6-C5	3.49	1.39	1.35
57	2y	39	PSU	C6-C5	3.49	1.39	1.35
54	1w	8	4SU	C4-N3	-3.49	1.33	1.37
54	2w	39	PSU	C6-C5	3.48	1.39	1.35
55	2x	55	PSU	C6-C5	3.45	1.39	1.35
1	1A	2605	PSU	C6-C5	3.31	1.39	1.35
54	1w	32	PSU	C6-C5	3.24	1.39	1.35
1	2A	1917	PSU	C6-C5	3.21	1.39	1.35
1	1A	1911	PSU	C6-C5	3.15	1.39	1.35
1	1A	1917	PSU	C6-C5	3.15	1.39	1.35
55	2x	8	4SU	C5-C4	-3.13	1.38	1.42
55	1x	8	4SU	C5-C4	-3.09	1.38	1.42
57	2y	55	PSU	C6-C5	3.09	1.38	1.35
1	2A	2605	PSU	C6-C5	3.08	1.38	1.35
1	2A	1911	PSU	C6-C5	3.01	1.38	1.35
1	2A	1942	5MC	C6-C5	3.00	1.39	1.34
1	2A	1915	5MU	C6-C5	2.97	1.39	1.34
32	1a	516	PSU	C6-C5	2.97	1.38	1.35
32	2a	1404	5MC	C6-C5	2.97	1.39	1.34
55	2x	8	4SU	C2-N3	-2.96	1.32	1.38
55	1x	76	8AN	C5-C4	-2.95	1.33	1.40
57	1y	54	5MU	C6-C5	2.92	1.39	1.34
54	2w	76	F3N	O4'-C1'	2.91	1.45	1.41
1	1A	1939	5MU	C6-C5	2.90	1.39	1.34
54	2w	8	4SU	C4-N3	-2.90	1.34	1.37
1	2A	1939	5MU	C6-C5	2.88	1.39	1.34
1	1A	1962	5MC	C6-C5	2.88	1.39	1.34
54	1w	8	4SU	C5-C4	-2.87	1.38	1.42
57	2y	8	4SU	C4-N3	-2.85	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	39	PSU	C6-C5	2.85	1.38	1.35
55	1x	54	5MU	C6-C5	2.85	1.39	1.34
57	2y	54	5MU	C6-C5	2.84	1.39	1.34
32	1a	1407	5MC	C6-C5	2.82	1.39	1.34
55	2x	76	8AN	C5-C4	-2.82	1.33	1.40
32	1a	1404	5MC	C6-C5	2.80	1.39	1.34
55	2x	54	5MU	C6-C5	2.80	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.80	1.33	1.38
32	2a	1400	5MC	C6-C5	2.79	1.39	1.34
54	2w	76	F3N	C5-C4	-2.78	1.33	1.40
32	2a	967	5MC	C6-C5	2.77	1.39	1.34
54	1w	32	PSU	C4-N3	-2.76	1.33	1.38
1	2A	1962	5MC	C6-C5	2.75	1.39	1.34
54	2w	37	MIA	C5-C4	2.75	1.48	1.40
32	1a	1400	5MC	C6-C5	2.74	1.39	1.34
1	1A	1939	5MU	C4-C5	2.73	1.49	1.44
32	1a	966	M2G	C2-N2	2.72	1.40	1.35
54	1w	76	F3N	C5-C4	-2.70	1.33	1.40
57	1y	37	MIA	C5-C4	2.70	1.48	1.40
1	1A	1915	5MU	C6-C5	2.68	1.39	1.34
57	1y	8	4SU	C4-N3	-2.67	1.34	1.37
57	2y	37	MIA	C5-C4	2.65	1.48	1.40
1	2A	1939	5MU	C4-N3	-2.65	1.33	1.38
54	2w	54	5MU	C6-C5	2.64	1.38	1.34
57	1y	37	MIA	C2-N3	2.64	1.36	1.32
1	1A	1939	5MU	C4-N3	-2.64	1.33	1.38
1	1A	1942	5MC	C6-C5	2.64	1.38	1.34
57	2y	37	MIA	C2-N3	2.63	1.36	1.32
1	1A	1917	PSU	C4-N3	-2.63	1.33	1.38
32	1a	516	PSU	C4-N3	-2.63	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.63	1.33	1.38
1	2A	1915	5MU	C4-C5	2.62	1.49	1.44
1	1A	1915	5MU	C4-C5	2.62	1.49	1.44
1	2A	2605	PSU	C4-N3	-2.61	1.34	1.38
54	1w	37	MIA	C5-C4	2.61	1.47	1.40
32	2a	1407	5MC	C6-C5	2.60	1.38	1.34
1	1A	2552	OMU	C4-N3	-2.59	1.33	1.38
55	2x	76	8AN	C6-C5	-2.59	1.33	1.43
57	1y	8	4SU	C2-N1	2.59	1.42	1.38
1	1A	1911	PSU	C4-N3	-2.58	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.58	1.34	1.38
32	1a	967	5MC	C6-C5	2.57	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2251	OMG	C6-N1	-2.57	1.34	1.37
1	2A	1911	PSU	C4-N3	-2.56	1.34	1.38
55	1x	54	5MU	C4-N3	-2.55	1.34	1.38
57	2y	54	5MU	C4-N3	-2.55	1.34	1.38
55	2x	32	5MC	C6-C5	2.53	1.38	1.34
54	2w	76	F3N	C6-C5	-2.53	1.33	1.43
57	1y	54	5MU	C4-C5	2.52	1.49	1.44
55	2x	55	PSU	C4-N3	-2.52	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.52	1.33	1.38
57	2y	8	4SU	C2-N1	2.52	1.42	1.38
55	1x	76	8AN	C6-C5	-2.52	1.33	1.43
57	1y	8	4SU	C5-C4	-2.52	1.39	1.42
54	1w	76	F3N	C6-C5	-2.52	1.33	1.43
54	1w	39	PSU	C4-N3	-2.52	1.34	1.38
55	1x	32	5MC	C6-N1	-2.52	1.33	1.38
55	1x	32	5MC	C6-C5	2.51	1.38	1.34
1	2A	2605	PSU	C2-N3	-2.51	1.33	1.37
57	1y	54	5MU	C2-N1	2.49	1.42	1.38
1	2A	1915	5MU	C2-N1	2.49	1.42	1.38
1	2A	1939	5MU	C2-N1	2.49	1.42	1.38
32	2a	1207	2MG	C6-N1	-2.49	1.34	1.37
54	1w	8	4SU	C2-N1	2.48	1.42	1.38
54	2w	55	PSU	C4-N3	-2.47	1.34	1.38
54	1w	54	5MU	C6-C5	2.47	1.38	1.34
32	2a	966	M2G	C2-N2	2.46	1.39	1.35
55	2x	32	5MC	C6-N1	-2.45	1.33	1.38
32	1a	966	M2G	C6-N1	-2.43	1.34	1.37
55	2x	54	5MU	C4-N3	-2.43	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.42	1.34	1.38
54	2w	8	4SU	C5-C4	-2.41	1.39	1.42
32	2a	966	M2G	C6-N1	-2.41	1.34	1.37
1	1A	1939	5MU	C2-N1	2.40	1.42	1.38
1	1A	1939	5MU	C2-N3	-2.40	1.33	1.38
57	1y	39	PSU	C4-N3	-2.40	1.34	1.38
57	2y	39	PSU	C4-N3	-2.39	1.34	1.38
57	1y	32	PSU	C4-N3	-2.39	1.34	1.38
54	2w	37	MIA	C2-N3	2.38	1.37	1.34
54	2w	54	5MU	C4-N3	-2.37	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.36	1.34	1.38
55	2x	54	5MU	C4-C5	2.36	1.48	1.44
57	1y	55	PSU	C4-N3	-2.35	1.34	1.38
57	2y	46	G7M	C6-N1	-2.35	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1915	5MU	C2-N1	2.34	1.42	1.38
32	2a	1400	5MC	C6-N1	-2.34	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.34	1.34	1.38
1	2A	2552	OMU	C5-C4	2.34	1.48	1.43
1	2A	2503	2MA	C2-N3	2.34	1.36	1.31
54	2w	54	5MU	C2-N1	2.33	1.42	1.38
57	2y	55	PSU	C4-N3	-2.33	1.34	1.38
57	1y	54	5MU	C4-N3	-2.33	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.31	1.34	1.38
32	2a	527	G7M	C6-N1	-2.31	1.34	1.37
57	2y	54	5MU	C2-N1	2.31	1.42	1.38
54	1w	55	PSU	C4-N3	-2.30	1.34	1.38
57	2y	8	4SU	C5-C4	-2.29	1.39	1.42
55	2x	54	5MU	C2-N1	2.29	1.42	1.38
1	2A	1962	5MC	C6-N1	-2.28	1.34	1.38
55	1x	8	4SU	O2-C2	2.28	1.27	1.23
54	1w	8	4SU	C2-N3	-2.27	1.33	1.38
57	2y	32	PSU	C4-N3	-2.27	1.34	1.38
32	2a	516	PSU	C4-N3	-2.27	1.34	1.38
54	2w	32	PSU	C4-N3	-2.25	1.34	1.38
57	2y	54	5MU	C2-N3	-2.25	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.24	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.23	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.21	1.34	1.38
57	2y	54	5MU	C4-C5	2.21	1.48	1.44
1	1A	1915	5MU	C6-N1	-2.20	1.34	1.38
54	2w	39	PSU	C4-N3	-2.19	1.34	1.38
55	1x	54	5MU	C6-N1	-2.18	1.34	1.38
54	1w	54	5MU	C2-N1	2.17	1.41	1.38
54	1w	46	G7M	C6-N1	-2.16	1.34	1.37
1	2A	1915	5MU	C6-N1	-2.16	1.34	1.38
54	1w	54	5MU	C4-N3	-2.16	1.34	1.38
54	1w	76	F3N	C5-N7	-2.16	1.31	1.39
55	1x	54	5MU	C4-C5	2.14	1.48	1.44
1	1A	1939	5MU	C6-N1	-2.13	1.34	1.38
54	2w	76	F3N	C5-N7	-2.13	1.32	1.39
55	2x	76	8AN	C5-N7	-2.12	1.32	1.39
32	1a	967	5MC	C6-N1	-2.11	1.34	1.38
32	2a	1498	UR3	C6-C5	2.10	1.39	1.35
32	1a	1207	2MG	C6-N1	-2.10	1.34	1.37
55	1x	55	PSU	C4-N3	-2.08	1.35	1.38
54	2w	54	5MU	C4-C5	2.08	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	8	4SU	O2-C2	2.07	1.26	1.23
55	2x	54	5MU	C6-N1	-2.06	1.34	1.38
1	1A	2552	OMU	C5-C4	2.06	1.48	1.43
54	1w	54	5MU	C4-C5	2.05	1.48	1.44
55	1x	76	8AN	C5-N7	-2.05	1.32	1.39
1	2A	1939	5MU	C4-C5	2.04	1.48	1.44
32	1a	527	G7M	C6-N1	-2.04	1.34	1.37
1	2A	2552	OMU	C4-N3	-2.04	1.34	1.38
55	2x	8	4SU	C2-N1	2.04	1.41	1.38
54	2w	8	4SU	C2-N1	2.03	1.41	1.38
1	2A	1942	5MC	C6-N1	-2.03	1.34	1.38
54	1w	54	5MU	C6-N1	-2.02	1.34	1.38
1	2A	2552	OMU	C6-C5	2.02	1.39	1.35
1	1A	1917	PSU	C2-N1	-2.01	1.34	1.36
32	2a	967	5MC	C6-N1	-2.01	1.34	1.38

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-16.55	72.51	102.44
43	2l	92	0TD	CSB-SB-CB	-9.11	85.95	102.44
54	1w	37	MIA	C12-C13-C14	-8.62	110.37	127.14
54	2w	8	4SU	C4-N3-C2	-7.57	119.98	127.34
57	2y	8	4SU	C4-N3-C2	-6.59	120.94	127.34
1	1A	1917	PSU	N1-C2-N3	6.49	122.48	115.13
32	1a	1498	UR3	C4-N3-C2	-6.37	118.56	124.56
54	1w	39	PSU	N1-C2-N3	6.37	122.34	115.13
54	2w	8	4SU	C5-C4-N3	6.33	120.56	114.69
57	2y	8	4SU	C5-C4-N3	6.28	120.52	114.69
1	2A	1911	PSU	N1-C2-N3	6.24	122.20	115.13
54	1w	37	MIA	C12-N6-C6	-6.04	113.60	122.55
57	2y	39	PSU	N1-C2-N3	6.03	121.97	115.13
1	2A	1917	PSU	N1-C2-N3	6.03	121.96	115.13
54	2w	39	PSU	N1-C2-N3	6.01	121.94	115.13
1	2A	1939	5MU	C4-N3-C2	-5.98	119.61	127.35
1	1A	1911	PSU	N1-C2-N3	5.97	121.90	115.13
55	1x	55	PSU	N1-C2-N3	5.94	121.86	115.13
1	1A	2605	PSU	N1-C2-N3	5.93	121.85	115.13
1	2A	2605	PSU	N1-C2-N3	5.88	121.80	115.13
57	1y	55	PSU	N1-C2-N3	5.87	121.78	115.13
32	1a	516	PSU	N1-C2-N3	5.85	121.76	115.13
57	2y	32	PSU	N1-C2-N3	5.84	121.75	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	55	PSU	N1-C2-N3	5.82	121.72	115.13
32	2a	1498	UR3	C4-N3-C2	-5.79	119.11	124.56
57	1y	8	4SU	C4-N3-C2	-5.77	121.74	127.34
32	2a	516	PSU	N1-C2-N3	5.76	121.65	115.13
55	2x	55	PSU	N1-C2-N3	5.75	121.65	115.13
55	2x	54	5MU	C4-N3-C2	-5.75	119.91	127.35
57	1y	39	PSU	N1-C2-N3	5.73	121.62	115.13
54	2w	76	F3N	N3-C2-N1	-5.67	119.82	128.68
55	1x	76	8AN	N3-C2-N1	-5.65	119.84	128.68
55	2x	76	8AN	N3-C2-N1	-5.65	119.85	128.68
54	1w	55	PSU	N1-C2-N3	5.62	121.50	115.13
54	2w	32	PSU	N1-C2-N3	5.60	121.47	115.13
54	1w	76	F3N	N3-C2-N1	-5.59	119.94	128.68
1	2A	1939	5MU	O4-C4-C5	-5.59	118.42	124.90
54	1w	32	PSU	N1-C2-N3	5.59	121.46	115.13
1	1A	1939	5MU	C4-N3-C2	-5.50	120.23	127.35
57	2y	55	PSU	N1-C2-N3	5.47	121.33	115.13
55	2x	54	5MU	N3-C2-N1	5.42	122.08	114.89
57	1y	8	4SU	C5-C4-N3	5.41	119.71	114.69
57	1y	32	PSU	N1-C2-N3	5.38	121.23	115.13
54	2w	37	MIA	C12-N6-C6	-5.37	118.25	122.87
1	1A	1939	5MU	C5-C4-N3	5.36	119.89	115.31
1	2A	1939	5MU	C5-C4-N3	5.29	119.83	115.31
1	2A	1939	5MU	N3-C2-N1	5.27	121.89	114.89
54	1w	54	5MU	C4-N3-C2	-5.17	120.65	127.35
1	1A	1915	5MU	C4-N3-C2	-5.16	120.67	127.35
54	1w	8	4SU	C5-C4-N3	5.15	119.47	114.69
1	2A	1915	5MU	C4-N3-C2	-5.14	120.69	127.35
32	1a	1518	MA6	N3-C2-N1	-5.05	120.79	128.68
32	2a	1518	MA6	N3-C2-N1	-5.03	120.82	128.68
54	1w	54	5MU	O4-C4-C5	-4.96	119.15	124.90
55	1x	54	5MU	C4-N3-C2	-4.95	120.94	127.35
32	2a	1519	MA6	N3-C2-N1	-4.95	120.94	128.68
55	1x	54	5MU	N3-C2-N1	4.89	121.39	114.89
1	1A	2552	OMU	N3-C2-N1	4.86	121.34	114.89
57	1y	54	5MU	C4-N3-C2	-4.84	121.09	127.35
32	1a	1519	MA6	N3-C2-N1	-4.84	121.12	128.68
1	2A	1915	5MU	N3-C2-N1	4.83	121.30	114.89
1	2A	2552	OMU	N3-C2-N1	4.82	121.28	114.89
57	1y	54	5MU	N3-C2-N1	4.81	121.28	114.89
1	1A	1915	5MU	N3-C2-N1	4.76	121.20	114.89
1	1A	1939	5MU	C5-C6-N1	-4.74	118.46	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	5MU	N3-C2-N1	4.70	121.14	114.89
54	1w	54	5MU	C5-C4-N3	4.69	119.31	115.31
54	1w	8	4SU	C4-N3-C2	-4.68	122.80	127.34
55	2x	54	5MU	C5-C4-N3	4.67	119.30	115.31
54	1w	37	MIA	C15-C14-C13	-4.65	109.21	122.65
54	1w	54	5MU	N3-C2-N1	4.56	120.95	114.89
54	1w	39	PSU	C4-N3-C2	-4.53	119.82	126.34
1	1A	1915	5MU	C5-C4-N3	4.48	119.13	115.31
1	2A	1915	5MU	C5-C4-N3	4.45	119.11	115.31
55	2x	54	5MU	O4-C4-C5	-4.43	119.76	124.90
57	1y	54	5MU	C5-C4-N3	4.39	119.06	115.31
54	2w	8	4SU	N3-C2-N1	4.39	120.71	114.89
1	2A	1939	5MU	C5-C6-N1	-4.34	118.87	123.34
1	1A	1917	PSU	C4-N3-C2	-4.31	120.13	126.34
1	2A	1911	PSU	C4-N3-C2	-4.27	120.18	126.34
55	2x	32	5MC	C5-C6-N1	-4.25	118.97	123.34
54	2w	39	PSU	C4-N3-C2	-4.24	120.23	126.34
1	1A	1917	PSU	O2-C2-N1	-4.22	118.14	122.79
54	2w	37	MIA	C2-N3-C4	4.20	121.12	115.32
55	1x	54	5MU	O4-C4-C5	-4.20	120.03	124.90
1	1A	2605	PSU	C4-N3-C2	-4.20	120.29	126.34
1	2A	2552	OMU	C4-N3-C2	-4.19	121.05	126.58
1	2A	2552	OMU	O2-C2-N1	-4.19	117.22	122.79
57	2y	54	5MU	C5-C4-N3	4.18	118.88	115.31
54	2w	54	5MU	C5-C4-N3	4.17	118.87	115.31
1	1A	1911	PSU	C4-N3-C2	-4.16	120.34	126.34
1	2A	2605	PSU	C4-N3-C2	-4.14	120.37	126.34
55	1x	54	5MU	C5-C4-N3	4.12	118.83	115.31
57	2y	39	PSU	C4-N3-C2	-4.12	120.41	126.34
54	2w	54	5MU	O4-C4-C5	-4.10	120.15	124.90
32	2a	1400	5MC	C5-C6-N1	-4.10	119.12	123.34
54	1w	37	MIA	C11-S10-C2	-4.09	99.21	102.27
1	1A	1915	5MU	O4-C4-C5	-4.08	120.18	124.90
57	1y	55	PSU	O2-C2-N1	-4.07	118.31	122.79
54	2w	54	5MU	C4-N3-C2	-4.06	122.10	127.35
55	2x	54	5MU	C5-C6-N1	-4.04	119.18	123.34
32	2a	1407	5MC	C5-C6-N1	-4.03	119.19	123.34
55	1x	8	4SU	O2-C2-N1	4.00	128.11	122.79
55	1x	55	PSU	O2-C2-N1	-4.00	118.39	122.79
54	1w	39	PSU	O2-C2-N1	-4.00	118.39	122.79
32	1a	516	PSU	C4-N3-C2	-3.99	120.59	126.34
1	1A	2552	OMU	C4-N3-C2	-3.99	121.32	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1911	PSU	O2-C2-N1	-3.98	118.41	122.79
55	2x	55	PSU	C4-N3-C2	-3.97	120.62	126.34
54	2w	8	4SU	C5-C4-S4	-3.95	119.37	124.47
1	1A	1962	5MC	C5-C6-N1	-3.95	119.28	123.34
54	1w	37	MIA	C16-C14-C13	-3.93	111.28	122.65
55	2x	8	4SU	C5-C4-N3	3.93	118.33	114.69
54	1w	55	PSU	O2-C2-N1	-3.92	118.47	122.79
57	2y	54	5MU	O4-C4-C5	-3.91	120.37	124.90
54	2w	54	5MU	N3-C2-N1	3.89	120.05	114.89
32	1a	1400	5MC	C5-C6-N1	-3.88	119.34	123.34
57	1y	8	4SU	C5-C4-S4	-3.88	119.47	124.47
57	2y	54	5MU	N3-C2-N1	3.87	120.03	114.89
54	1w	37	MIA	C2-N3-C4	3.87	120.65	115.32
1	2A	1917	PSU	C4-N3-C2	-3.86	120.78	126.34
1	2A	1915	5MU	O4-C4-C5	-3.85	120.44	124.90
57	2y	54	5MU	C4-N3-C2	-3.84	122.39	127.35
32	2a	516	PSU	C4-N3-C2	-3.82	120.83	126.34
57	1y	54	5MU	O4-C4-C5	-3.80	120.50	124.90
55	1x	8	4SU	C6-C5-C4	-3.76	116.69	119.95
57	2y	39	PSU	O2-C2-N1	-3.74	118.67	122.79
32	2a	1404	5MC	C5-C6-N1	-3.74	119.49	123.34
1	2A	1915	5MU	C5-C6-N1	-3.73	119.50	123.34
57	2y	8	4SU	C5-C4-S4	-3.72	119.67	124.47
1	1A	1939	5MU	O4-C4-C5	-3.71	120.60	124.90
57	2y	32	PSU	C4-N3-C2	-3.68	121.04	126.34
57	2y	55	PSU	O2-C2-N1	-3.66	118.76	122.79
57	1y	8	4SU	C1'-N1-C2	3.65	124.19	117.57
57	2y	8	4SU	N3-C2-N1	3.65	119.74	114.89
57	1y	32	PSU	O2-C2-N1	-3.65	118.77	122.79
55	1x	55	PSU	C4-N3-C2	-3.65	121.08	126.34
54	2w	55	PSU	C4-N3-C2	-3.64	121.09	126.34
54	1w	32	PSU	C4-N3-C2	-3.63	121.11	126.34
54	2w	32	PSU	C4-N3-C2	-3.60	121.15	126.34
56	2z	1	FME	CA-N-CN	-3.60	117.29	122.82
1	1A	1911	PSU	O2-C2-N1	-3.57	118.86	122.79
32	1a	1519	MA6	C4-C5-N7	-3.56	105.69	109.40
1	2A	1917	PSU	O2-C2-N1	-3.56	118.87	122.79
57	1y	39	PSU	C4-N3-C2	-3.55	121.22	126.34
56	1z	1	FME	CA-N-CN	-3.55	117.36	122.82
32	2a	1519	MA6	C4-C5-N7	-3.54	105.71	109.40
57	1y	55	PSU	C4-N3-C2	-3.54	121.24	126.34
54	2w	39	PSU	O2-C2-N1	-3.53	118.90	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1y	37	MIA	N3-C2-N1	-3.53	123.17	128.68
57	2y	55	PSU	C4-N3-C2	-3.53	121.26	126.34
32	2a	516	PSU	O2-C2-N1	-3.50	118.94	122.79
57	1y	32	PSU	C4-N3-C2	-3.49	121.31	126.34
55	1x	54	5MU	C5-C6-N1	-3.49	119.75	123.34
54	2w	55	PSU	O2-C2-N1	-3.48	118.95	122.79
32	1a	1404	5MC	C5-C6-N1	-3.46	119.78	123.34
55	1x	32	5MC	C5-C6-N1	-3.45	119.79	123.34
57	1y	8	4SU	N3-C2-N1	3.43	119.44	114.89
57	2y	32	PSU	O2-C2-N1	-3.43	119.02	122.79
57	2y	37	MIA	N3-C2-N1	-3.38	123.39	128.68
55	2x	8	4SU	C1'-N1-C2	3.38	123.68	117.57
54	1w	55	PSU	C4-N3-C2	-3.34	121.52	126.34
32	1a	1407	5MC	C5-C6-N1	-3.34	119.91	123.34
1	2A	1942	5MC	C5-C6-N1	-3.33	119.91	123.34
54	2w	32	PSU	O2-C2-N1	-3.32	119.13	122.79
54	1w	54	5MU	C5-C6-N1	-3.32	119.92	123.34
43	2l	92	0TD	OD2-CG-CB	3.29	120.27	113.15
32	2a	967	5MC	C5-C6-N1	-3.27	119.97	123.34
32	1a	516	PSU	O2-C2-N1	-3.26	119.20	122.79
55	2x	8	4SU	C6-C5-C4	-3.22	117.17	119.95
43	1l	92	0TD	OD2-CG-CB	3.18	120.03	113.15
32	1a	967	5MC	C5-C6-N1	-3.18	120.07	123.34
32	1a	1404	5MC	C5-C4-N3	-3.13	118.29	121.67
57	2y	55	PSU	C6-C5-C4	-3.13	116.01	118.20
54	2w	37	MIA	C5-C6-N1	-3.13	118.21	120.81
54	1w	8	4SU	N3-C2-N1	3.12	119.03	114.89
1	1A	2552	OMU	O2-C2-N1	-3.10	118.66	122.79
1	1A	1915	5MU	C5-C6-N1	-3.08	120.17	123.34
55	1x	54	5MU	O2-C2-N1	-3.08	118.69	122.79
54	1w	37	MIA	C5-C6-N1	-3.07	118.26	120.81
54	1w	8	4SU	C5-C4-S4	-3.04	120.55	124.47
54	1w	37	MIA	C2-N1-C6	3.01	122.58	117.19
55	1x	32	5MC	C5-C4-N3	-2.97	118.47	121.67
57	1y	54	5MU	C5-C6-N1	-2.97	120.29	123.34
1	1A	1942	5MC	C5-C6-N1	-2.96	120.29	123.34
1	1A	1915	5MU	C5M-C5-C4	2.96	122.02	118.77
55	1x	8	4SU	C5-C4-N3	2.94	117.42	114.69
1	2A	1939	5MU	O2-C2-N1	-2.93	118.89	122.79
1	2A	1962	5MC	C5-C6-N1	-2.93	120.33	123.34
57	1y	37	MIA	C4-C5-N7	-2.90	106.38	109.40
32	1a	1518	MA6	C4-C5-N7	-2.90	106.38	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	54	5MU	O2-C2-N1	-2.89	118.95	122.79
32	2a	1518	MA6	C4-C5-N7	-2.87	106.41	109.40
1	1A	2605	PSU	O2-C2-N1	-2.86	119.64	122.79
57	2y	37	MIA	C4-C5-N7	-2.86	106.42	109.40
1	2A	2605	PSU	O2-C2-N1	-2.85	119.65	122.79
54	1w	8	4SU	C1'-N1-C2	2.85	122.72	117.57
56	1z	1	FME	CG-CB-CA	-2.84	105.07	112.95
32	1a	1402	4OC	C6-C5-C4	2.78	120.37	116.96
1	1A	1942	5MC	C5-C4-N3	-2.78	118.68	121.67
1	2A	1942	5MC	C5-C4-N3	-2.77	118.69	121.67
54	1w	55	PSU	C6-C5-C4	-2.75	116.27	118.20
1	1A	1915	5MU	O2-C2-N1	-2.74	119.14	122.79
1	1A	1962	5MC	C5-C4-N3	-2.74	118.72	121.67
55	1x	76	8AN	O4'-C1'-C2'	-2.71	102.97	106.93
32	2a	967	5MC	C5-C4-N3	-2.70	118.76	121.67
1	2A	2552	OMU	O4-C4-C5	-2.69	120.43	125.16
32	1a	1407	5MC	C5-C4-N3	-2.65	118.81	121.67
57	2y	54	5MU	C5-C6-N1	-2.65	120.61	123.34
55	1x	8	4SU	C1'-N1-C2	2.65	122.37	117.57
1	2A	2503	2MA	C8-N7-C5	2.64	108.03	102.99
54	1w	54	5MU	O2-C2-N1	-2.63	119.29	122.79
54	2w	54	5MU	C5-C6-N1	-2.63	120.64	123.34
57	1y	39	PSU	O2-C2-N1	-2.62	119.91	122.79
54	2w	37	MIA	C4-C5-N7	-2.60	106.69	109.40
32	1a	1207	2MG	C8-N7-C5	2.59	107.93	102.99
55	2x	76	8AN	O4'-C1'-C2'	-2.59	103.14	106.93
32	2a	1207	2MG	C8-N7-C5	2.59	107.92	102.99
32	2a	1407	5MC	C5-C4-N3	-2.58	118.89	121.67
54	2w	37	MIA	C2-N1-C6	2.57	121.79	117.19
55	2x	32	5MC	C5-C4-N3	-2.57	118.90	121.67
1	1A	2552	OMU	O4-C4-C5	-2.57	120.65	125.16
1	2A	1962	5MC	C5-C4-N3	-2.56	118.91	121.67
54	1w	37	MIA	C4-C5-N7	-2.56	106.73	109.40
32	2a	1404	5MC	C5-C4-N3	-2.56	118.91	121.67
1	2A	2552	OMU	C5-C4-N3	2.54	118.64	114.84
55	2x	55	PSU	O2-C2-N1	-2.53	120.01	122.79
54	2w	8	4SU	O2-C2-N1	-2.53	119.43	122.79
32	1a	516	PSU	O4'-C1'-C2'	2.50	108.67	105.14
1	2A	2251	OMG	C5-C6-N1	2.49	118.34	113.95
1	2A	2503	2MA	C5-C6-N1	2.48	118.30	114.02
54	1w	46	G7M	C3'-C2'-C1'	2.46	104.69	100.98
32	1a	1400	5MC	C5-C4-N3	-2.44	119.04	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2552	OMU	C5-C4-N3	2.44	118.49	114.84
55	2x	8	4SU	O2-C2-N1	2.43	126.01	122.79
54	1w	37	MIA	N3-C2-N1	-2.42	122.54	126.98
1	1A	2552	OMU	C2'-C1'-N1	-2.41	109.55	114.22
1	1A	2251	OMG	C5-C6-N1	2.39	118.18	113.95
32	1a	966	M2G	N1-C2-N2	2.38	120.07	118.04
54	1w	32	PSU	O2-C2-N1	-2.38	120.17	122.79
32	2a	1207	2MG	CM2-N2-C2	-2.38	118.61	123.86
1	2A	2552	OMU	C2'-C1'-N1	-2.37	109.62	114.22
55	2x	55	PSU	C6-C5-C4	-2.37	116.54	118.20
1	1A	2251	OMG	C8-N7-C5	2.37	107.50	102.99
55	1x	8	4SU	S4-C4-N3	-2.35	117.89	120.21
1	2A	2605	PSU	C5-C6-N1	-2.33	118.62	122.11
43	2l	92	0TD	OD1-CG-CB	-2.32	117.57	122.44
55	1x	32	5MC	O2-C2-N3	-2.32	118.56	122.33
32	2a	1400	5MC	C5-C4-N3	-2.31	119.18	121.67
1	1A	1915	5MU	C5M-C5-C6	-2.31	119.76	122.85
1	1A	1962	5MC	CM5-C5-C6	-2.31	119.76	122.85
55	1x	8	4SU	O2-C2-N3	-2.26	117.29	121.50
32	1a	966	M2G	C8-N7-C5	2.26	107.29	102.99
32	2a	966	M2G	C8-N7-C5	2.25	107.28	102.99
54	1w	39	PSU	C5-C6-N1	-2.24	118.74	122.11
57	1y	32	PSU	C6-C5-C4	-2.24	116.63	118.20
1	1A	2605	PSU	C5-C6-N1	-2.24	118.75	122.11
32	1a	1498	UR3	C3U-N3-C4	2.23	121.08	117.89
57	1y	54	5MU	C5M-C5-C4	2.23	121.22	118.77
1	2A	1915	5MU	O2-C2-N1	-2.23	119.83	122.79
32	1a	516	PSU	C5-C6-N1	-2.22	118.77	122.11
1	2A	2251	OMG	C8-N7-C5	2.22	107.21	102.99
1	2A	2251	OMG	O6-C6-C5	-2.21	120.05	124.37
32	1a	966	M2G	C5-C6-N1	2.21	117.85	113.95
54	2w	37	MIA	C11-S10-C2	-2.20	100.62	102.27
1	1A	1911	PSU	C5-C6-N1	-2.20	118.81	122.11
32	1a	1207	2MG	C5-C6-N1	2.20	117.83	113.95
1	1A	2503	2MA	C5-C6-N1	2.17	117.77	114.02
1	1A	2503	2MA	C8-N7-C5	2.17	107.12	102.99
1	1A	1942	5MC	CM5-C5-C6	-2.17	119.95	122.85
55	2x	32	5MC	CM5-C5-C6	-2.16	119.96	122.85
32	1a	967	5MC	C5-C4-N3	-2.15	119.36	121.67
57	2y	46	G7M	C3'-C2'-C1'	2.15	104.21	100.98
1	1A	1920	OMC	O2-C2-N3	-2.11	118.89	122.33
1	1A	2251	OMG	O6-C6-C5	-2.10	120.26	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	76	F3N	O2'-C2'-C3'	-2.10	106.03	111.16
1	2A	1942	5MC	O2-C2-N3	-2.08	118.94	122.33
1	2A	1911	PSU	C5-C6-N1	-2.07	119.00	122.11
55	2x	32	5MC	O2-C2-N3	-2.07	118.96	122.33
57	1y	39	PSU	O4'-C1'-C2'	2.07	108.06	105.14
32	2a	1404	5MC	O2-C2-N3	-2.06	118.97	122.33
32	2a	1402	4OC	CM4-N4-C4	-2.06	118.43	122.45
32	2a	966	M2G	C5-C6-N1	2.06	117.59	113.95
1	1A	1917	PSU	C5-C6-N1	-2.06	119.02	122.11
32	2a	1400	5MC	O2-C2-N3	-2.05	118.99	122.33
1	2A	1915	5MU	C5M-C5-C4	2.05	121.02	118.77
43	1l	92	0TD	OD1-CG-CB	-2.05	118.15	122.44
32	2a	1402	4OC	C6-C5-C4	2.05	119.47	116.96
55	2x	8	4SU	O2-C2-N3	-2.04	117.70	121.50
57	1y	54	5MU	O2-C2-N1	-2.02	120.10	122.79
54	1w	39	PSU	O4'-C1'-C2'	2.01	107.98	105.14
54	2w	39	PSU	O4'-C1'-C2'	2.01	107.98	105.14
32	1a	1407	5MC	O2-C2-N3	-2.01	119.06	122.33

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
55	1x	76	8AN	C3'-C4'-C5'-O5'
57	1y	46	G7M	C4'-C5'-O5'-P
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
57	2y	55	PSU	C2'-C1'-C5-C6
57	2y	55	PSU	O4'-C1'-C5-C6
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
56	1z	1	FME	O1-CN-N-CA
56	1z	1	FME	N-CA-CB-CG
56	2z	1	FME	O1-CN-N-CA
56	2z	1	FME	O-C-CA-CB
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	C3'-C4'-C5'-O5'
55	2x	76	8AN	O4'-C4'-C5'-O5'
55	1x	76	8AN	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
56	2z	1	FME	N-CA-CB-CG
56	1z	1	FME	CB-CG-SD-CE
32	1a	527	G7M	O4'-C4'-C5'-O5'
54	1w	37	MIA	C5-C6-N6-C12
54	1w	46	G7M	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	1w	37	MIA	N1-C6-N6-C12
32	2a	1404	5MC	O4'-C4'-C5'-O5'
32	2a	1404	5MC	C3'-C4'-C5'-O5'
32	2a	527	G7M	C4'-C5'-O5'-P
1	1A	1915	5MU	O4'-C4'-C5'-O5'
55	2x	76	8AN	C4'-C5'-O5'-P
56	2z	1	FME	CB-CG-SD-CE
54	2w	46	G7M	C4'-C5'-O5'-P
54	2w	76	F3N	N-CA-CB-CG
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
54	1w	37	MIA	N6-C12-C13-C14
1	2A	1917	PSU	O4'-C4'-C5'-O5'
1	1A	1911	PSU	O4'-C1'-C5-C4
57	1y	55	PSU	O4'-C1'-C5-C4
1	2A	1962	5MC	C2'-C1'-N1-C6
32	2a	1519	MA6	C4'-C5'-O5'-P
54	2w	76	F3N	C-CA-CB-CG
32	1a	1400	5MC	O4'-C4'-C5'-O5'
57	1y	39	PSU	O4'-C4'-C5'-O5'
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	2503	2MA	C3'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
1	1A	2251	OMG	C1'-C2'-O2'-CM2
55	1x	76	8AN	C4'-C5'-O5'-P
1	1A	2503	2MA	O4'-C4'-C5'-O5'
54	2w	32	PSU	O4'-C4'-C5'-O5'
57	1y	55	PSU	O4'-C1'-C5-C6
43	2l	92	0TD	CG-CB-SB-CSB
1	1A	1920	OMC	C2'-C1'-N1-C2
57	1y	8	4SU	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C2'-C1'-N1-C2
32	1a	527	G7M	C4'-C5'-O5'-P

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 2784 ligands modelled in this entry, 2782 are monoatomic - leaving 2 for Mogul analysis.

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.57	159 (5%) 24 25	14, 30, 79, 88	0
1	2A	2789/2915 (95%)	0.55	142 (5%) 28 29	26, 48, 76, 86	0
2	1B	120/121 (99%)	0.15	0 100 100	24, 42, 54, 75	0
2	2B	120/121 (99%)	0.10	1 (0%) 86 87	47, 60, 68, 72	0
3	1D	275/276 (99%)	0.66	1 (0%) 92 93	14, 31, 43, 63	0
3	2D	275/276 (99%)	0.75	0 100 100	25, 41, 51, 68	0
4	1E	204/206 (99%)	0.50	2 (0%) 82 84	14, 35, 54, 63	0
4	2E	204/206 (99%)	0.47	5 (2%) 57 61	29, 49, 60, 66	0
5	1F	202/210 (96%)	0.37	2 (0%) 82 84	14, 37, 56, 68	0
5	2F	202/210 (96%)	0.49	4 (1%) 65 68	28, 54, 64, 68	0
6	1G	181/182 (99%)	0.34	2 (1%) 80 82	33, 49, 61, 71	0
6	2G	181/182 (99%)	0.50	4 (2%) 62 65	50, 61, 68, 73	0
7	1H	174/180 (96%)	0.34	0 100 100	33, 47, 55, 60	0
7	2H	174/180 (96%)	2.37	99 (56%) 0 0	56, 67, 73, 75	0
8	1I	146/148 (98%)	0.37	4 (2%) 54 58	37, 59, 66, 69	0
8	2I	146/148 (98%)	0.71	14 (9%) 8 7	44, 60, 68, 71	0
9	1N	140/140 (100%)	0.46	0 100 100	19, 34, 50, 59	0
9	2N	140/140 (100%)	0.66	7 (5%) 28 30	38, 53, 63, 72	0
10	1O	122/122 (100%)	0.44	0 100 100	24, 35, 49, 55	0
10	2O	122/122 (100%)	0.47	2 (1%) 72 74	37, 48, 60, 63	0
11	1P	149/150 (99%)	0.39	2 (1%) 77 79	15, 39, 58, 64	0
11	2P	149/150 (99%)	1.19	27 (18%) 1 1	28, 54, 67, 71	0
12	1Q	141/141 (100%)	0.43	1 (0%) 87 89	19, 35, 47, 60	0
12	2Q	141/141 (100%)	0.80	13 (9%) 9 9	35, 52, 62, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.36	0 100 100	22, 31, 39, 48	0
13	2R	118/118 (100%)	0.41	0 100 100	34, 44, 53, 60	0
14	1S	110/112 (98%)	0.34	0 100 100	30, 40, 51, 54	0
14	2S	110/112 (98%)	0.78	7 (6%) 19 20	47, 56, 63, 68	0
15	1T	131/146 (89%)	0.26	1 (0%) 86 87	27, 39, 57, 65	0
15	2T	131/146 (89%)	0.47	3 (2%) 60 63	39, 51, 61, 65	0
16	1U	116/118 (98%)	0.43	0 100 100	17, 26, 42, 51	0
16	2U	116/118 (98%)	0.69	5 (4%) 35 38	35, 50, 61, 66	0
17	1V	101/101 (100%)	0.31	1 (0%) 82 84	19, 36, 50, 57	0
17	2V	101/101 (100%)	0.46	3 (2%) 50 53	36, 57, 63, 71	0
18	1W	112/113 (99%)	0.45	1 (0%) 84 86	17, 27, 43, 67	0
18	2W	112/113 (99%)	0.65	2 (1%) 68 71	30, 41, 56, 82	0
19	1X	95/96 (98%)	0.62	0 100 100	21, 31, 51, 68	0
19	2X	95/96 (98%)	0.58	2 (2%) 63 66	36, 49, 61, 71	0
20	1Y	107/110 (97%)	0.37	0 100 100	28, 43, 57, 66	0
20	2Y	107/110 (97%)	0.60	4 (3%) 41 45	48, 59, 67, 72	0
21	1Z	154/206 (74%)	0.49	6 (3%) 39 42	35, 52, 69, 72	0
21	2Z	160/206 (77%)	1.12	30 (18%) 1 1	47, 64, 72, 75	0
22	10	83/85 (97%)	0.42	0 100 100	20, 30, 41, 53	0
22	20	83/85 (97%)	0.78	6 (7%) 15 16	34, 50, 58, 64	0
23	11	97/98 (98%)	0.34	1 (1%) 82 84	21, 38, 58, 62	0
23	21	97/98 (98%)	0.58	3 (3%) 49 52	32, 45, 60, 66	0
24	12	70/72 (97%)	0.52	0 100 100	27, 39, 52, 63	0
24	22	70/72 (97%)	0.36	0 100 100	47, 56, 63, 66	0
25	13	59/60 (98%)	0.33	0 100 100	17, 31, 52, 60	0
25	23	59/60 (98%)	0.94	5 (8%) 10 10	43, 54, 63, 66	0
26	14	69/71 (97%)	0.45	5 (7%) 15 16	42, 60, 71, 75	0
26	24	69/71 (97%)	0.90	11 (15%) 1 1	60, 67, 73, 79	0
27	15	59/60 (98%)	0.48	1 (1%) 70 72	15, 30, 57, 62	0
27	25	59/60 (98%)	0.51	0 100 100	27, 43, 61, 65	0
28	16	53/54 (98%)	0.24	0 100 100	26, 35, 44, 50	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.75	5 (9%) 8 8	39, 49, 55, 58	0
29	17	48/49 (97%)	0.62	0 100 100	15, 21, 43, 50	0
29	27	48/49 (97%)	0.84	2 (4%) 36 39	27, 35, 55, 61	0
30	18	64/65 (98%)	0.41	0 100 100	21, 27, 35, 46	0
30	28	64/65 (98%)	1.08	8 (12%) 3 3	38, 45, 51, 54	0
31	19	37/37 (100%)	0.46	0 100 100	26, 34, 42, 50	0
31	29	37/37 (100%)	1.24	6 (16%) 1 1	45, 55, 60, 62	0
32	1a	1488/1521 (97%)	0.52	77 (5%) 27 29	27, 55, 75, 87	0
32	2a	1491/1521 (98%)	0.65	115 (7%) 13 13	40, 62, 76, 87	0
33	1b	231/256 (90%)	0.95	39 (16%) 1 1	50, 63, 70, 78	0
33	2b	231/256 (90%)	1.39	65 (28%) 0 0	58, 67, 72, 77	0
34	1c	206/239 (86%)	0.96	20 (9%) 7 7	49, 58, 66, 73	0
34	2c	206/239 (86%)	1.65	65 (31%) 0 0	59, 66, 72, 76	0
35	1d	208/209 (99%)	0.55	4 (1%) 66 69	43, 57, 64, 67	0
35	2d	208/209 (99%)	0.52	2 (0%) 82 84	47, 57, 64, 72	0
36	1e	148/162 (91%)	0.60	7 (4%) 31 33	40, 53, 60, 64	0
36	2e	148/162 (91%)	0.83	15 (10%) 7 6	50, 60, 65, 68	0
37	1f	100/101 (99%)	0.27	0 100 100	46, 55, 61, 62	0
37	2f	100/101 (99%)	0.29	0 100 100	47, 56, 62, 64	0
38	1g	155/156 (99%)	0.79	14 (9%) 9 9	49, 58, 68, 76	0
38	2g	155/156 (99%)	1.16	30 (19%) 1 1	54, 65, 70, 76	0
39	1h	137/138 (99%)	0.48	4 (2%) 51 55	45, 55, 61, 63	0
39	2h	137/138 (99%)	0.77	12 (8%) 10 10	51, 61, 66, 71	0
40	1i	127/128 (99%)	1.58	35 (27%) 0 0	44, 63, 69, 71	0
40	2i	127/128 (99%)	2.47	73 (57%) 0 0	57, 67, 72, 73	0
41	1j	97/105 (92%)	1.33	20 (20%) 1 0	45, 62, 69, 73	0
41	2j	96/105 (91%)	2.08	47 (48%) 0 0	58, 68, 72, 73	0
42	1k	114/129 (88%)	0.61	8 (7%) 16 16	32, 54, 62, 69	0
42	2k	114/129 (88%)	0.52	5 (4%) 34 37	48, 60, 66, 70	0
43	1l	121/132 (91%)	0.46	1 (0%) 86 87	33, 44, 54, 60	0
43	2l	121/132 (91%)	0.67	7 (5%) 23 24	44, 53, 61, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.45	5 (4%) 37 40	46, 57, 63, 68	0
44	2m	122/126 (96%)	0.84	17 (13%) 2 2	56, 64, 69, 72	0
45	1n	60/61 (98%)	1.30	13 (21%) 0 0	50, 55, 62, 62	0
45	2n	60/61 (98%)	2.71	39 (65%) 0 0	60, 67, 70, 73	0
46	1o	88/89 (98%)	0.44	2 (2%) 60 63	40, 53, 62, 68	0
46	2o	88/89 (98%)	0.50	2 (2%) 60 63	48, 58, 64, 67	0
47	1p	82/88 (93%)	1.00	10 (12%) 4 3	46, 58, 64, 69	0
47	2p	82/88 (93%)	0.56	3 (3%) 41 45	49, 57, 64, 67	0
48	1q	99/105 (94%)	0.58	8 (8%) 12 12	43, 54, 63, 67	0
48	2q	99/105 (94%)	0.77	5 (5%) 28 29	51, 57, 64, 68	0
49	1r	68/88 (77%)	0.42	0 100 100	46, 54, 63, 66	0
49	2r	68/88 (77%)	0.29	0 100 100	49, 57, 65, 69	0
50	1s	83/93 (89%)	0.64	4 (4%) 30 32	49, 58, 66, 70	0
50	2s	83/93 (89%)	1.08	14 (16%) 1 1	60, 66, 71, 73	0
51	1t	96/106 (90%)	1.54	30 (31%) 0 0	50, 58, 65, 73	0
51	2t	96/106 (90%)	1.24	19 (19%) 1 1	46, 57, 68, 75	0
52	1u	23/27 (85%)	1.50	5 (21%) 0 0	50, 54, 58, 60	0
52	2u	23/27 (85%)	2.18	14 (60%) 0 0	62, 65, 69, 73	0
53	1v	13/24 (54%)	1.58	4 (30%) 0 0	38, 42, 76, 78	0
53	2v	13/24 (54%)	1.87	6 (46%) 0 0	52, 59, 79, 87	0
54	1w	66/76 (86%)	0.89	8 (12%) 4 4	22, 68, 79, 83	0
54	2w	64/76 (84%)	1.19	9 (14%) 2 2	37, 75, 81, 85	0
55	1x	72/77 (93%)	0.32	1 (1%) 75 77	19, 51, 68, 75	0
55	2x	72/77 (93%)	0.26	0 100 100	35, 61, 70, 80	0
56	1z	2/3 (66%)	0.54	0 100 100	18, 18, 18, 19	0
56	2z	2/3 (66%)	1.09	0 100 100	31, 31, 31, 32	0
57	1y	67/76 (88%)	4.72	66 (98%) 0 0	54, 80, 85, 86	0
57	2y	66/76 (86%)	4.74	65 (98%) 0 0	62, 82, 86, 87	0
All	All	20875/21754 (95%)	0.69	1623 (7%) 13 13	14, 52, 72, 88	0

All (1623) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
54	2w	71	G	11.9
57	2y	36	A	11.1
1	2A	2115	G	9.3
1	2A	2146	C	9.3
57	1y	35	A	9.3
57	1y	19	G	9.2
57	1y	5	G	9.0
57	1y	34	G	8.9
40	2i	14	VAL	8.9
44	1m	124	PRO	8.8
1	1A	2146	C	8.7
1	2A	2147	G	8.5
1	2A	2127	G	8.5
57	2y	57	G	8.4
1	1A	2145	C	8.4
57	1y	38	A	8.3
1	1A	2160	G	8.2
54	1w	70	G	8.2
26	24	51	ASP	8.1
1	1A	2129	C	8.1
57	1y	36	A	7.8
1	2A	2128	C	7.7
1	2A	2160	G	7.7
1	1A	2159	G	7.7
57	2y	29	G	7.7
26	24	50	VAL	7.6
1	1A	2181	G	7.5
57	2y	35	A	7.4
21	2Z	155	LEU	7.4
1	1A	2147	G	7.3
1	2A	2167	U	7.3
44	2m	124	PRO	7.3
32	2a	1030(B)	C	7.3
1	2A	2116	G	7.2
1	1A	2161	C	7.2
1	2A	2145	C	7.2
1	1A	2175	C	7.2
57	2y	74	C	7.2
1	2A	2113	U	7.2
33	1b	228	GLY	7.2
1	2A	2142	C	7.1
57	2y	34	G	7.0
1	2A	2141	G	7.0

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Mol	Chain	Res	Type	RSRZ
51	1t	95	ALA	7.0
1	1A	2131	G	7.0
38	2g	80	VAL	7.0
57	2y	63	G	6.9
57	1y	1	G	6.9
40	2i	65	VAL	6.9
1	1A	2115	G	6.7
57	2y	1	G	6.7
1	2A	2123	G	6.7
1	1A	2140	C	6.7
57	2y	62	C	6.7
1	1A	2112	G	6.6
57	1y	57	G	6.6
1	2A	883	G	6.6
1	2A	2117	A	6.5
1	2A	2168	G	6.5
57	1y	71	G	6.5
33	1b	233	SER	6.5
33	2b	127	ILE	6.5
7	2H	35	VAL	6.5
34	2c	87	LEU	6.4
1	2A	2162	G	6.4
1	1A	1095	A	6.4
53	2v	12	A	6.4
57	1y	21	A	6.4
44	2m	123	ALA	6.3
1	1A	2113	U	6.3
40	2i	67	GLY	6.3
38	1g	81	GLY	6.3
57	2y	52	G	6.3
1	2A	2110	G	6.3
7	2H	105	LEU	6.3
33	2b	81	VAL	6.3
1	1A	2162	G	6.3
57	1y	24	G	6.2
57	2y	28	G	6.2
57	1y	13	C	6.2
1	2A	2139	C	6.1
1	1A	2130	U	6.1
1	2A	2138	C	6.1
1	2A	2161	C	6.1
1	1A	2110	G	6.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2181	G	6.1
41	1j	18	ALA	6.1
1	2A	2112	G	6.1
32	2a	1030(A)	G	6.1
40	2i	80	GLY	6.1
21	2Z	149	SER	6.1
1	1A	2178	C	6.1
45	2n	25	VAL	6.0
1	2A	2126	A	6.0
32	1a	1028	C	6.0
32	2a	1033	G	6.0
32	2a	1034	G	6.0
57	1y	53	G	6.0
1	1A	2127	G	5.9
40	2i	109	VAL	5.9
1	2A	2120	G	5.9
1	2A	2154	G	5.9
57	2y	33	U	5.9
1	2A	2174	C	5.9
1	1A	2133	G	5.9
57	1y	30	G	5.9
57	2y	53	G	5.9
1	1A	2174	C	5.9
1	2A	2159	G	5.9
1	1A	1076	C	5.9
1	2A	2143	C	5.9
1	1A	2166	G	5.8
38	2g	156	TRP	5.8
1	2A	888	C	5.8
1	1A	2132	U	5.8
57	1y	70	G	5.8
57	2y	19	G	5.8
57	2y	15	G	5.8
54	2w	70	G	5.7
1	2A	2170	A	5.7
38	2g	154	TYR	5.7
41	2j	40	LEU	5.7
1	1A	2116	G	5.7
32	1a	1001(A)	G	5.7
57	2y	12	U	5.7
40	2i	76	ALA	5.7
1	2A	2169	A	5.7

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Mol	Chain	Res	Type	RSRZ
57	1y	75	C	5.6
1	2A	2133	G	5.6
1	2A	2166	G	5.6
1	2A	2129	C	5.6
1	1A	2120	G	5.6
1	2A	2121	G	5.6
1	2A	2125	G	5.5
57	1y	74	C	5.5
40	2i	102	LEU	5.5
40	2i	108	VAL	5.5
32	1a	1036	G	5.5
32	1a	1029	C	5.5
41	2j	72	VAL	5.5
57	1y	20	U	5.5
1	2A	2100	G	5.5
45	2n	42	ILE	5.5
57	1y	2	C	5.5
57	2y	65	G	5.5
1	2A	2189	U	5.4
57	2y	18	G	5.4
57	2y	38	A	5.4
1	1A	2111	C	5.4
7	2H	44	VAL	5.4
57	1y	58	A	5.4
1	2A	2188	C	5.4
1	2A	2104	G	5.4
54	1w	71	G	5.4
1	2A	2152	G	5.4
34	2c	160	ALA	5.4
1	1A	2108	C	5.3
57	2y	58	A	5.3
1	1A	2109	U	5.3
32	2a	1031	G	5.3
45	2n	24	CYS	5.3
57	2y	56	C	5.3
21	2Z	170	THR	5.3
1	1A	2141	G	5.3
1	2A	2103	C	5.3
54	2w	72	C	5.3
42	1k	14	VAL	5.3
1	1A	1096	A	5.3
1	2A	885	C	5.3

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Mol	Chain	Res	Type	RSRZ
57	1y	3	C	5.3
57	1y	52	G	5.3
32	1a	1257	U	5.2
53	1v	12	A	5.2
57	1y	4	C	5.2
57	1y	56	C	5.2
1	2A	2144	U	5.2
57	2y	75	C	5.2
57	2y	14	A	5.2
1	2A	884	C	5.2
34	2c	92	ALA	5.2
57	1y	29	G	5.2
1	1A	2180	U	5.1
1	2A	2179	C	5.1
7	2H	24	VAL	5.1
33	2b	34	ALA	5.1
40	1i	19	LEU	5.1
26	24	63	TYR	5.1
38	2g	79	ARG	5.1
1	2A	2106	G	5.1
57	2y	44	G	5.1
1	2A	652(B)	A	5.1
32	2a	1286	A	5.1
57	2y	24	G	5.1
1	1A	2114	A	5.1
41	2j	96	ILE	5.1
7	2H	48	GLY	5.1
38	2g	82	GLY	5.1
41	2j	75	ILE	5.1
1	1A	2117	A	5.0
1	2A	2135	A	5.0
1	2A	2182	G	5.0
7	2H	99	VAL	5.0
7	2H	72	ILE	5.0
1	1A	2143	C	5.0
57	2y	67	C	5.0
1	1A	2168	G	5.0
53	1v	13	A	5.0
57	2y	21	A	5.0
1	1A	2123	G	5.0
1	2A	2149	G	5.0
57	2y	30	G	5.0

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Mol	Chain	Res	Type	RSRZ
34	2c	193	TYR	5.0
1	1A	1064	C	5.0
1	1A	1059	G	5.0
1	1A	2128	C	5.0
1	1A	2188	C	5.0
32	2a	1027	C	5.0
32	2a	1150	U	4.9
1	1A	2170	A	4.9
57	2y	26	A	4.9
41	2j	20	ALA	4.9
45	2n	43	CYS	4.9
1	1A	2106	G	4.9
1	1A	2165	G	4.9
45	2n	26	ARG	4.9
7	2H	96	ALA	4.9
57	2y	45	U	4.9
1	1A	2142	C	4.9
40	1i	14	VAL	4.9
34	2c	75	VAL	4.8
45	2n	38	GLY	4.8
32	1a	1003	G	4.8
45	2n	34	TYR	4.8
1	2A	2177	C	4.8
18	2W	112	GLY	4.8
32	2a	1030	C	4.8
57	2y	42	C	4.8
7	2H	102	ALA	4.8
7	2H	113	VAL	4.8
57	2y	31	A	4.8
1	2A	2109	U	4.8
57	1y	25	C	4.8
57	1y	22	G	4.7
1	1A	884	C	4.7
34	2c	157	ILE	4.7
7	2H	106	THR	4.7
1	1A	2169	A	4.7
32	2a	1001(A)	G	4.7
32	2a	1036	G	4.7
57	1y	63	G	4.7
57	1y	62	C	4.7
57	2y	25	C	4.7
1	2A	2158	A	4.7

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Mol	Chain	Res	Type	RSRZ
32	2a	1287	A	4.7
52	1u	2	GLY	4.7
1	1A	2144	U	4.7
1	2A	2122	U	4.7
45	2n	55	GLY	4.7
1	1A	896	A	4.7
7	2H	121	ILE	4.7
57	1y	18	G	4.7
57	1y	28	G	4.7
1	2A	2105	C	4.7
1	2A	2175	C	4.7
7	2H	103	LEU	4.7
1	1A	2158	A	4.6
1	2A	229	A	4.6
34	2c	124	ILE	4.7
40	2i	10	ARG	4.6
57	2y	64	A	4.6
32	2a	1032	G	4.6
40	2i	105	ASP	4.6
1	2A	2114	A	4.6
34	2c	145	GLY	4.6
1	1A	2148	G	4.6
33	1b	229	VAL	4.6
45	2n	39	LEU	4.6
57	2y	43	C	4.6
40	2i	66	ARG	4.6
1	1A	2171	A	4.6
1	1A	2164	C	4.6
1	1A	2182	G	4.6
7	2H	98	LEU	4.6
50	2s	82	GLY	4.6
1	2A	2111	C	4.6
57	1y	67	C	4.6
57	2y	66	U	4.6
57	1y	27	G	4.6
45	2n	37	PHE	4.6
14	2S	20	ARG	4.5
21	2Z	153	SER	4.5
32	2a	1024	G	4.5
40	2i	5	TYR	4.5
1	1A	2118	U	4.5
57	1y	61	C	4.5

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Mol	Chain	Res	Type	RSRZ
38	1g	156	TRP	4.5
1	2A	2148	G	4.5
40	1i	84	ALA	4.5
7	2H	6	ARG	4.5
32	1a	1001	A	4.5
57	1y	48	C	4.5
32	1a	1031	G	4.5
1	1A	1066	U	4.5
32	1a	1030(B)	C	4.5
45	2n	61	TRP	4.4
1	2A	2183	C	4.4
33	2b	231	GLU	4.4
1	2A	2165	G	4.4
40	2i	75	ASP	4.4
1	1A	2135	A	4.4
1	2A	2134	A	4.4
32	2a	91	C	4.4
1	2A	2124	G	4.4
1	2A	2155	G	4.4
32	1a	1032	G	4.4
54	1w	44	G	4.4
52	2u	17	THR	4.4
32	2a	1249	C	4.4
57	1y	33	U	4.4
57	1y	42	C	4.4
57	2y	73	A	4.4
1	2A	1026	U	4.4
41	2j	67	THR	4.4
32	2a	1035	A	4.3
32	2a	1029	C	4.3
1	2A	2118	U	4.3
57	1y	50	U	4.3
1	1A	2139	C	4.3
7	2H	73	ALA	4.3
41	2j	38	ILE	4.3
32	1a	1532	U	4.3
57	2y	5	G	4.3
1	1A	2179	C	4.3
32	2a	1532	U	4.3
38	1g	79	ARG	4.3
1	1A	1077	A	4.3
41	2j	74	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
57	2y	61	C	4.3
21	2Z	58	VAL	4.3
1	2A	652(U)	G	4.3
1	1A	1072	C	4.2
57	2y	51	U	4.2
45	2n	13	THR	4.2
1	1A	1063	G	4.2
34	2c	41	GLY	4.2
45	2n	2	ALA	4.2
40	2i	9	ARG	4.2
1	2A	2156	G	4.2
32	2a	1023	G	4.2
6	2G	29	TRP	4.2
7	2H	128	PRO	4.2
40	1i	31	GLN	4.2
1	1A	1175	U	4.2
1	1A	888	C	4.2
1	1A	1092	C	4.2
7	2H	115	VAL	4.2
14	2S	5	THR	4.2
40	2i	72	GLY	4.2
7	2H	34	GLU	4.2
57	1y	51	U	4.2
54	1w	72	C	4.2
1	2A	2153	G	4.2
1	1A	885	C	4.2
57	1y	31	A	4.2
12	2Q	33	GLY	4.1
51	1t	47	GLY	4.1
1	1A	897	C	4.1
48	1q	36	ILE	4.1
7	2H	76	VAL	4.1
45	2n	10	ALA	4.1
38	2g	32	ARG	4.1
1	2A	887	A	4.1
1	1A	2157	G	4.1
32	2a	1002	G	4.1
32	2a	1021	G	4.1
23	2l	2	SER	4.1
44	2m	68	GLY	4.1
57	2y	11	C	4.1
45	1n	2	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2164	C	4.1
1	1A	2102	U	4.1
57	2y	23	A	4.1
33	2b	165	VAL	4.1
41	2j	44	VAL	4.1
34	1c	193	TYR	4.1
1	1A	1509	C	4.1
1	2A	1041	C	4.1
1	2A	2108	C	4.1
57	2y	41	C	4.1
57	2y	72	C	4.1
45	2n	51	GLY	4.1
7	2H	92	ILE	4.0
1	2A	1170	G	4.0
32	1a	1030(A)	G	4.0
32	1a	204	U	4.0
32	2a	1257	U	4.0
20	2Y	1	MET	4.0
1	1A	2105	C	4.0
1	1A	1065	U	4.0
40	1i	49	PRO	4.0
7	2H	93	GLY	4.0
43	2l	55	VAL	4.0
1	1A	2177	C	4.0
1	2A	2802	G	4.0
40	2i	63	ILE	4.0
1	1A	2104	G	4.0
1	1A	2149	G	4.0
1	2A	896	A	4.0
57	1y	23	A	4.0
21	2Z	148	ASP	4.0
34	1c	180	ALA	4.0
44	1m	123	ALA	4.0
33	2b	33	TYR	4.0
25	23	54	VAL	4.0
34	2c	154	SER	4.0
1	1A	2103	C	3.9
1	1A	2185	C	3.9
32	2a	1039	C	3.9
33	2b	44	LEU	3.9
1	1A	2121	G	3.9
32	1a	78	G	3.9

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Mol	Chain	Res	Type	RSRZ
57	1y	44	G	3.9
57	1y	47	U	3.9
34	1c	41	GLY	3.9
34	1c	81	GLY	3.9
53	2v	24	A	3.9
32	2a	1022	G	3.9
32	2a	1030(C)	G	3.9
52	2u	14	TRP	3.9
51	1t	45	GLN	3.9
57	1y	69	G	3.9
57	2y	71	G	3.9
34	2c	182	ILE	3.9
51	1t	67	ALA	3.9
1	2A	2171	A	3.9
1	2A	2190	G	3.9
33	2b	17	PHE	3.9
45	2n	7	ILE	3.9
1	1A	2167	U	3.9
1	2A	2180	U	3.9
7	2H	16	SER	3.9
32	2a	1149	C	3.9
7	2H	79	VAL	3.9
45	2n	12	ARG	3.9
32	1a	1286	A	3.8
32	2a	1447	A	3.8
52	2u	16	GLY	3.8
17	2V	72	VAL	3.8
33	2b	136	VAL	3.8
32	1a	1030(D)	A	3.8
1	1A	2154	G	3.8
1	2A	2151	G	3.8
57	1y	65	G	3.8
1	2A	897	C	3.8
11	2P	91	PHE	3.8
40	1i	52	ALA	3.8
1	1A	1094	U	3.8
32	2a	1026	G	3.8
45	2n	35	ARG	3.8
57	2y	68	C	3.8
41	2j	27	ALA	3.8
38	2g	4	ARG	3.8
40	1i	117	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
40	2i	28	VAL	3.8
1	1A	2152	G	3.8
1	1A	2187	G	3.8
1	2A	2101	G	3.8
1	2A	2140	C	3.8
1	1A	2119	A	3.8
7	2H	49	VAL	3.8
21	2Z	141	VAL	3.8
33	2b	124	SER	3.8
33	2b	207	ALA	3.8
1	1A	2101	G	3.8
32	2a	1040	U	3.8
51	1t	79	ARG	3.8
57	1y	15	G	3.8
1	1A	229	A	3.8
1	1A	887	A	3.8
32	2a	1005	A	3.8
33	2b	122	PHE	3.7
41	1j	47	PHE	3.7
7	2H	74	ASN	3.7
32	2a	1007	C	3.7
57	2y	4	C	3.7
32	2a	1154	G	3.7
7	2H	71	LEU	3.7
32	1a	1531	A	3.7
57	2y	76	A	3.7
1	2A	2804	C	3.7
44	2m	120	LYS	3.7
26	14	54	GLY	3.7
57	1y	64	A	3.7
33	2b	214	ILE	3.7
34	2c	8	ILE	3.7
1	2A	2102	U	3.7
32	1a	1446	U	3.7
40	2i	125	TYR	3.7
40	2i	56	LEU	3.7
1	2A	1114	G	3.7
7	2H	171	LEU	3.7
1	1A	1082	U	3.7
32	2a	80	G	3.7
33	2b	121	LEU	3.7
34	2c	60	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
40	2i	15	ALA	3.7
57	1y	49	C	3.7
57	2y	47	U	3.6
1	1A	1057	A	3.6
1	2A	892	G	3.6
50	2s	80	TYR	3.6
41	2j	34	VAL	3.6
32	1a	1030(C)	G	3.6
32	1a	1034	G	3.6
7	2H	51	ARG	3.6
1	2A	2107	C	3.6
1	2A	2136	C	3.6
34	2c	159	GLY	3.6
57	2y	13	C	3.6
33	2b	51	LEU	3.6
40	2i	62	TYR	3.6
34	2c	195	VAL	3.6
32	2a	216	G	3.6
1	2A	645	C	3.6
33	2b	216	SER	3.6
7	2H	45	VAL	3.6
7	2H	52	VAL	3.6
32	2a	204	U	3.6
32	2a	1446	U	3.6
32	2a	1116	C	3.6
1	1A	1084	A	3.6
1	1A	2176	A	3.6
40	1i	81	ILE	3.6
1	2A	2172	U	3.6
57	1y	66	U	3.6
32	1a	999	C	3.6
26	14	63	TYR	3.6
34	2c	100	ALA	3.6
38	1g	80	VAL	3.6
41	2j	66	ARG	3.5
32	2a	1452	C	3.5
38	2g	121	ALA	3.5
1	1A	2151	G	3.5
11	2P	101	VAL	3.5
32	1a	104	G	3.5
32	2a	79	G	3.5
32	2a	1156	G	3.5

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Mol	Chain	Res	Type	RSRZ
57	1y	10	G	3.5
7	2H	8	PRO	3.5
1	1A	2189	U	3.5
35	2d	117	ALA	3.5
40	2i	4	TYR	3.5
1	2A	2157	G	3.5
57	1y	45	U	3.5
4	1E	195	LEU	3.5
30	28	18	ALA	3.5
32	1a	1035	A	3.5
32	2a	1157	A	3.5
40	1i	76	ALA	3.5
40	2i	61	ALA	3.5
44	2m	72	ALA	3.5
50	2s	50	ALA	3.5
7	2H	25	LYS	3.5
1	1A	1093	G	3.5
57	1y	59	U	3.5
34	2c	33	LEU	3.5
40	2i	7	THR	3.5
1	1A	1069	A	3.5
32	2a	1030(D)	A	3.5
31	29	16	VAL	3.5
7	2H	21	PRO	3.5
45	2n	14	PRO	3.5
1	2A	2137	C	3.5
57	2y	2	C	3.5
57	1y	12	U	3.5
34	2c	178	LEU	3.5
40	2i	8	GLY	3.5
1	1A	893	C	3.5
34	2c	39	ILE	3.5
1	2A	2130	U	3.5
40	2i	103	THR	3.5
1	1A	2125	G	3.5
32	1a	1023	G	3.5
51	1t	38	LYS	3.5
53	2v	13	A	3.4
7	2H	100	GLY	3.4
32	1a	1033	G	3.4
32	2a	1370	G	3.4
32	2a	1531	A	3.4

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Mol	Chain	Res	Type	RSRZ
41	2j	98	ILE	3.4
1	1A	1060	U	3.4
33	2b	215	LEU	3.4
33	1b	133	LYS	3.4
1	2A	274	G	3.4
1	1A	1078	U	3.4
11	2P	148	LEU	3.4
38	2g	40	ALA	3.4
41	2j	18	ALA	3.4
38	2g	81	GLY	3.4
40	2i	115	GLY	3.4
40	2i	90	PRO	3.4
33	1b	236	TYR	3.4
38	2g	12	LEU	3.4
40	2i	114	TYR	3.4
45	2n	53	LEU	3.4
1	1A	1099	G	3.4
11	1P	143	GLY	3.4
11	2P	28	GLY	3.4
32	2a	1250	A	3.4
40	2i	82	ALA	3.4
7	2H	10	PRO	3.4
33	1b	232	PRO	3.4
40	2i	49	PRO	3.4
1	1A	271(K)	U	3.4
38	1g	85	TYR	3.4
7	2H	165	ALA	3.4
50	2s	13	ASP	3.4
57	1y	68	C	3.4
33	1b	227	GLY	3.4
40	2i	73	GLN	3.4
32	2a	1130	A	3.4
1	1A	889	C	3.4
1	2A	275	G	3.4
7	2H	169	VAL	3.4
45	2n	11	LYS	3.4
57	2y	27	G	3.4
34	1c	14	ILE	3.3
36	2e	13	ILE	3.3
21	2Z	159	PRO	3.3
7	2H	95	ARG	3.3
33	1b	81	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
34	2c	86	VAL	3.3
50	2s	45	VAL	3.3
41	2j	25	GLU	3.3
30	28	19	SER	3.3
21	2Z	171	ILE	3.3
38	2g	30	ILE	3.3
45	2n	44	LEU	3.3
32	1a	1025	U	3.3
40	1i	15	ALA	3.3
41	2j	15	THR	3.3
52	2u	21	TYR	3.3
40	1i	113	LYS	3.3
41	2j	65	LEU	3.3
51	1t	13	LEU	3.3
52	2u	5	ASP	3.3
57	1y	6	G	3.3
28	26	42	TRP	3.3
34	2c	184	TYR	3.3
21	2Z	144	LEU	3.3
26	24	68	ARG	3.3
57	2y	40	C	3.3
40	2i	45	ALA	3.3
1	1A	1058	G	3.3
1	2A	2184	G	3.3
32	1a	1024	G	3.3
26	24	66	SER	3.3
17	2V	92	THR	3.3
52	2u	13	ILE	3.3
7	2H	82	GLY	3.3
45	1n	51	GLY	3.3
57	2y	6	G	3.3
34	2c	196	LEU	3.3
32	1a	1040	U	3.3
9	2N	10	GLU	3.3
32	1a	1037	C	3.3
53	1v	14	A	3.3
53	2v	15	A	3.3
33	2b	92	TYR	3.3
1	1A	2155	G	3.2
7	2H	29	PRO	3.2
40	1i	98	PRO	3.2
43	2l	93	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
11	2P	118	GLY	3.2
51	1t	22	ARG	3.2
57	2y	59	U	3.2
32	1a	171	A	3.2
32	2a	1008	C	3.2
33	2b	75	LYS	3.2
51	1t	14	LYS	3.2
57	1y	72	C	3.2
41	2j	39	PRO	3.2
22	20	62	LEU	3.2
21	2Z	152	ALA	3.2
33	1b	18	GLY	3.2
38	2g	5	ARG	3.2
32	2a	998	G	3.2
32	2a	1202	G	3.2
32	2a	1006	C	3.2
32	2a	1028	C	3.2
12	2Q	114	ALA	3.2
1	1A	2100	G	3.2
57	2y	22	G	3.2
1	1A	2107	C	3.2
41	2j	69	ASN	3.2
51	1t	9	ASN	3.2
7	2H	167	GLU	3.2
1	1A	2172	U	3.2
33	2b	201	ILE	3.2
1	1A	2163	C	3.2
30	28	23	VAL	3.2
34	1c	86	VAL	3.2
1	2A	2119	A	3.2
32	1a	162	A	3.2
50	2s	30	LEU	3.2
11	2P	140	ALA	3.2
51	1t	76	ALA	3.2
1	1A	2122	U	3.2
7	2H	91	GLY	3.2
34	2c	96	GLY	3.2
1	2A	2191	G	3.2
7	2H	107	VAL	3.2
32	1a	1026	G	3.2
1	1A	1067	A	3.2
21	2Z	4	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
7	2H	123	PHE	3.2
41	1j	38	ILE	3.2
51	2t	41	ILE	3.2
57	2y	50	U	3.2
38	2g	9	VAL	3.2
1	2A	898	C	3.1
32	2a	1283	G	3.1
34	2c	57	ILE	3.1
39	2h	58	TYR	3.1
40	2i	33	PHE	3.1
1	1A	2184	G	3.1
51	2t	57	ARG	3.1
7	2H	145	ALA	3.1
47	1p	60	LEU	3.1
7	2H	132	ARG	3.1
51	1t	100	ILE	3.1
33	2b	232	PRO	3.1
52	2u	23	PRO	3.1
32	1a	1041	A	3.1
53	2v	14	A	3.1
57	1y	73	A	3.1
54	2w	31	A	3.1
5	1F	21	ALA	3.1
21	1Z	165	VAL	3.1
34	2c	198	VAL	3.1
51	1t	69	GLY	3.1
34	2c	20	SER	3.1
7	2H	126	PRO	3.1
7	2H	148	ILE	3.1
32	2a	90	U	3.1
36	2e	10	MET	3.1
40	2i	18	PHE	3.1
41	2j	47	PHE	3.1
7	2H	32	GLU	3.1
41	2j	29	ARG	3.1
1	2A	2173	A	3.1
7	2H	31	GLY	3.1
7	2H	33	LEU	3.1
40	1i	100	GLY	3.1
41	1j	34	VAL	3.1
16	2U	2	PRO	3.1
21	2Z	145	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	2A	889	C	3.1
7	2H	66	GLY	3.1
40	2i	27	THR	3.1
1	1A	2126	A	3.0
1	2A	2176	A	3.0
7	2H	133	VAL	3.1
40	2i	17	VAL	3.1
41	1j	62	HIS	3.1
41	2j	19	SER	3.1
1	1A	882	G	3.0
1	1A	1087	G	3.0
4	2E	77	ILE	3.0
32	2a	1224	G	3.0
40	2i	74	ILE	3.0
7	2H	20	ALA	3.0
38	2g	22	LEU	3.0
36	2e	34	VAL	3.0
1	1A	278	A	3.0
32	2a	1041	A	3.0
1	1A	1097	U	3.0
33	2b	32	ILE	3.0
45	2n	36	PHE	3.0
20	2Y	55	TYR	3.0
40	2i	36	TYR	3.0
1	1A	892	G	3.0
1	1A	1074	G	3.0
8	2I	43	ASN	3.0
11	2P	93	GLY	3.0
32	1a	102	G	3.0
40	1i	8	GLY	3.0
40	2i	121	ARG	3.0
51	1t	64	ASP	3.0
1	2A	894	C	3.0
28	26	52	VAL	3.0
33	1b	136	VAL	3.0
57	2y	49	C	3.0
1	1A	1054	A	3.0
54	2w	47	U	3.0
43	2l	64	TYR	3.0
1	2A	2131	G	3.0
32	2a	1003	G	3.0
1	1A	1070	A	3.0

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Mol	Chain	Res	Type	RSRZ
21	2Z	69	THR	3.0
40	1i	45	ALA	3.0
40	2i	122	ALA	3.0
51	2t	72	LEU	3.0
52	1u	17	THR	3.0
1	2A	895	U	3.0
32	1a	841	U	3.0
44	1m	25	ILE	3.0
6	1G	146	TYR	3.0
40	1i	5	TYR	3.0
57	1y	14	A	3.0
41	2j	88	LEU	3.0
7	2H	125	VAL	3.0
8	2I	13	GLY	3.0
38	2g	78	ARG	3.0
41	2j	31	GLY	3.0
32	1a	216	G	3.0
1	1A	886	C	3.0
1	1A	2138	C	3.0
4	2E	176	ILE	3.0
32	2a	980	C	3.0
11	2P	115	LEU	3.0
21	2Z	157	LEU	3.0
34	1c	65	ALA	3.0
36	2e	12	LEU	3.0
40	1i	82	ALA	3.0
12	2Q	19	GLY	3.0
52	2u	10	ARG	3.0
41	2j	24	VAL	2.9
1	1A	1075	C	2.9
7	2H	36	PRO	2.9
36	2e	146	ALA	2.9
40	2i	43	ALA	2.9
41	2j	32	ALA	2.9
42	1k	15	ALA	2.9
46	2o	31	LEU	2.9
7	2H	19	VAL	2.9
21	1Z	141	VAL	2.9
33	2b	95	GLN	2.9
32	1a	1030	C	2.9
1	1A	1056	G	2.9
7	2H	7	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
33	2b	123	ALA	2.9
40	1i	106	ALA	2.9
41	1j	16	LEU	2.9
41	2j	12	ASP	2.9
33	2b	132	LYS	2.9
45	1n	61	TRP	2.9
33	2b	211	ILE	2.9
45	2n	46	GLU	2.9
44	2m	119	GLY	2.9
8	1I	40	THR	2.9
32	1a	150	C	2.9
39	1h	133	LEU	2.9
39	2h	112	LEU	2.9
41	1j	17	ASP	2.9
51	1t	43	LEU	2.9
40	2i	93	ARG	2.9
45	2n	31	ARG	2.9
1	1A	890	A	2.9
32	2a	1248	A	2.9
33	1b	216	SER	2.9
33	1b	105	PHE	2.9
50	2s	63	THR	2.9
34	2c	21	ARG	2.9
40	2i	128	ARG	2.9
52	1u	18	TYR	2.9
52	2u	22	ARG	2.9
21	2Z	139	VAL	2.9
32	2a	1057	G	2.9
1	2A	1113	U	2.9
28	26	20	ASN	2.9
7	2H	39	PRO	2.9
33	2b	131	PRO	2.9
7	2H	70	THR	2.9
39	1h	39	LEU	2.9
41	1j	46	ARG	2.9
45	2n	3	ARG	2.9
51	1t	17	ARG	2.9
1	2A	652(T)	C	2.9
33	2b	48	MET	2.9
40	1i	65	VAL	2.9
7	2H	166	GLY	2.9
22	20	65	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
32	1a	1447	A	2.9
51	1t	80	ARG	2.9
4	2E	52	LEU	2.9
1	2A	2163	C	2.8
7	2H	78	GLY	2.8
8	1I	136	VAL	2.8
31	29	29	ASN	2.8
32	2a	1018	C	2.8
40	2i	91	ASP	2.8
50	2s	68	GLY	2.8
57	1y	60	U	2.8
1	2A	882	G	2.8
8	2I	100	ALA	2.8
33	2b	29	ALA	2.8
11	2P	138	LEU	2.8
57	2y	69	G	2.8
47	2p	59	TRP	2.8
33	2b	37	ASN	2.8
12	2Q	32	TYR	2.8
36	1e	10	MET	2.8
40	2i	57	GLY	2.8
1	1A	2137	C	2.8
38	2g	147	ALA	2.8
40	2i	13	ALA	2.8
51	2t	16	HIS	2.8
7	2H	159	GLU	2.8
40	1i	99	LEU	2.8
1	1A	1176	G	2.8
39	2h	122	ARG	2.8
52	1u	14	TRP	2.8
23	11	2	SER	2.8
26	24	45	GLY	2.8
48	2q	33	GLY	2.8
54	1w	69	G	2.8
32	2a	1122	U	2.8
36	2e	11	ILE	2.8
52	1u	11	GLY	2.8
7	2H	37	VAL	2.8
32	2a	1009	G	2.8
32	2a	1220	G	2.8
33	1b	165	VAL	2.8
7	2H	30	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
45	1n	7	ILE	2.8
8	2I	93	THR	2.8
11	2P	96	THR	2.8
12	1Q	59	ARG	2.8
32	1a	1137	C	2.8
54	2w	4	C	2.8
34	1c	205	GLY	2.8
7	2H	17	VAL	2.8
34	2c	18	TRP	2.8
45	1n	56	VAL	2.8
1	1A	2153	G	2.8
1	1A	2156	G	2.8
12	2Q	6	ARG	2.8
32	2a	202	U	2.8
33	2b	228	GLY	2.8
36	2e	20	GLN	2.8
51	1t	32	ALA	2.8
1	2A	2178	C	2.8
30	28	60	LEU	2.8
11	2P	139	LYS	2.8
41	1j	41	PRO	2.8
45	2n	23	ARG	2.8
45	2n	18	VAL	2.8
54	1w	14	A	2.8
41	1j	20	ALA	2.8
47	1p	7	ALA	2.8
51	2t	9	ASN	2.8
1	2A	2186	G	2.8
1	1A	2136	C	2.8
57	2y	3	C	2.8
7	2H	69	ARG	2.8
7	2H	65	HIS	2.8
33	2b	19	HIS	2.8
40	2i	12	GLU	2.7
47	1p	66	PRO	2.8
21	2Z	96	VAL	2.7
26	24	18	CYS	2.7
51	2t	47	GLY	2.7
32	1a	1021	G	2.7
32	2a	1385	G	2.7
11	2P	95	VAL	2.7
43	2l	39	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
33	2b	185	ILE	2.7
39	2h	65	TYR	2.7
42	1k	74	ALA	2.7
4	2E	63	LEU	2.7
32	1a	1285	A	2.7
32	2a	1014	A	2.7
7	2H	124	GLU	2.7
11	2P	92	GLU	2.7
51	1t	18	GLN	2.7
1	2A	1040	C	2.7
8	2I	1	MET	2.7
21	1Z	1	MET	2.7
57	2y	10	G	2.7
40	1i	26	VAL	2.7
11	2P	103	ALA	2.7
51	2t	12	ALA	2.7
32	1a	1027	C	2.7
7	2H	141	VAL	2.7
9	2N	9	VAL	2.7
29	27	46	VAL	2.7
1	2A	881	G	2.7
32	1a	927	G	2.7
1	2A	2150	U	2.7
5	2F	115	ALA	2.7
33	1b	123	ALA	2.7
44	2m	121	LYS	2.7
40	2i	88	TYR	2.7
1	1A	1098	A	2.7
57	2y	7	A	2.7
38	2g	31	MET	2.7
48	2q	85	VAL	2.7
41	2j	21	GLN	2.7
1	1A	895	U	2.7
34	1c	15	THR	2.7
34	2c	177	THR	2.7
36	2e	54	ALA	2.7
51	1t	40	ALA	2.7
32	2a	1133	G	2.7
33	2b	152	PHE	2.7
41	2j	11	PHE	2.7
44	2m	70	LEU	2.7
34	2c	83	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
7	2H	108	GLY	2.7
40	2i	70	LYS	2.7
47	1p	48	TRP	2.7
4	1E	68	ALA	2.7
32	1a	194	C	2.7
38	2g	24	THR	2.7
26	24	59	PHE	2.7
40	1i	79	LEU	2.7
41	2j	85	LEU	2.7
33	2b	133	LYS	2.7
54	2w	44	G	2.7
34	2c	142	MET	2.7
12	2Q	109	VAL	2.6
21	2Z	126	VAL	2.6
33	2b	71	VAL	2.6
34	2c	138	VAL	2.6
34	1c	83	ARG	2.6
1	2A	277	C	2.6
33	1b	213	LEU	2.6
34	2c	155	GLY	2.6
31	29	30	PRO	2.6
33	1b	234	PRO	2.6
1	2A	1042	G	2.6
32	1a	1002	G	2.6
40	2i	107	ARG	2.6
7	2H	111	HIS	2.6
32	1a	197	A	2.6
32	2a	1349	A	2.6
33	2b	85	ALA	2.6
12	2Q	17	LEU	2.6
34	1c	32	LEU	2.6
35	2d	23	GLY	2.6
11	2P	102	ARG	2.6
32	1a	79	G	2.6
1	1A	1083	U	2.6
57	1y	7	A	2.6
34	1c	128	PHE	2.6
32	1a	163	C	2.6
32	2a	1037	C	2.6
44	2m	87	TYR	2.6
47	1p	58	TYR	2.6
7	2H	80	SER	2.6

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Mol	Chain	Res	Type	RSRZ
26	14	66	SER	2.6
7	2H	142	GLY	2.6
15	2T	37	GLY	2.6
33	1b	15	VAL	2.6
33	2b	14	GLY	2.6
34	2c	189	ALA	2.6
40	2i	52	ALA	2.6
46	2o	60	VAL	2.6
1	1A	2186	G	2.6
1	2A	2793	G	2.6
21	2Z	154	ASP	2.6
32	1a	93	G	2.6
32	2a	1323	G	2.6
41	2j	71	LEU	2.6
45	2n	6	LEU	2.6
16	2U	88	ILE	2.6
33	1b	211	ILE	2.6
38	2g	119	ARG	2.6
22	20	45	PHE	2.6
32	2a	999	C	2.6
41	2j	68	HIS	2.6
36	1e	51	VAL	2.6
38	1g	21	VAL	2.6
40	1i	121	ARG	2.6
52	2u	24	ARG	2.6
33	2b	98	LEU	2.6
1	1A	2190	G	2.6
32	2a	1115	C	2.6
42	2k	25	TYR	2.6
6	2G	49	ASP	2.6
42	1k	64	ALA	2.6
7	2H	43	VAL	2.6
33	2b	112	VAL	2.6
45	1n	13	THR	2.6
7	2H	112	PRO	2.6
33	1b	187	LEU	2.6
41	1j	85	LEU	2.6
32	1a	170	U	2.6
36	2e	84	PHE	2.6
45	2n	16	PHE	2.6
40	2i	124	GLN	2.6
44	2m	64	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
32	2a	1142	G	2.6
41	2j	36	GLY	2.6
38	2g	2	ALA	2.5
47	1p	62	VAL	2.5
12	2Q	113	GLN	2.5
41	2j	6	ILE	2.5
36	1e	42	GLY	2.5
47	1p	59	TRP	2.5
7	2H	18	GLU	2.5
51	2t	31	SER	2.5
1	1A	2134	A	2.5
32	1a	220	G	2.5
32	1a	998	G	2.5
38	1g	154	TYR	2.5
34	2c	163	ALA	2.5
40	2i	106	ALA	2.5
44	1m	109	THR	2.5
51	2t	59	ALA	2.5
32	2a	1153	C	2.5
32	2a	1260	C	2.5
40	2i	31	GLN	2.5
57	2y	60	U	2.5
21	1Z	146	ILE	2.5
21	2Z	93	ASP	2.5
21	2Z	147	GLY	2.5
26	24	49	PHE	2.5
52	2u	11	GLY	2.5
7	2H	129	THR	2.5
32	1a	149	A	2.5
34	2c	48	TYR	2.5
52	2u	8	THR	2.5
1	1A	2124	G	2.5
14	2S	56	LEU	2.5
32	2a	1068	G	2.5
39	2h	39	LEU	2.5
32	1a	202	U	2.5
5	1F	16	GLY	2.5
39	1h	6	ILE	2.5
50	1s	38	SER	2.5
7	2H	40	GLU	2.5
34	1c	23	TYR	2.5
38	1g	54	THR	2.5

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Mol	Chain	Res	Type	RSRZ
42	2k	68	ALA	2.5
7	2H	94	TYR	2.5
9	2N	72	TYR	2.5
47	2p	58	TYR	2.5
1	1A	2173	A	2.5
8	2I	75	LEU	2.5
27	15	60	VAL	2.5
32	2a	1180	A	2.5
39	2h	133	LEU	2.5
42	2k	47	VAL	2.5
48	1q	31	LEU	2.5
1	2A	2132	U	2.5
32	2a	1358	U	2.5
57	1y	11	C	2.5
57	1y	41	C	2.5
32	1a	138	G	2.5
33	2b	146	GLN	2.5
34	2c	80	GLY	2.5
34	2c	188	LEU	2.5
40	1i	28	VAL	2.5
40	2i	39	GLY	2.5
43	1l	14	GLY	2.5
51	2t	62	LEU	2.5
41	2j	13	HIS	2.5
32	2a	1324	A	2.5
32	2a	1374	A	2.5
34	2c	152	ILE	2.5
38	2g	27	ILE	2.5
1	1A	879	G	2.5
33	2b	120	ALA	2.5
33	2b	113	HIS	2.5
34	2c	91	LEU	2.5
48	1q	98	LEU	2.5
7	2H	127	GLU	2.5
50	2s	35	SER	2.5
54	2w	45	U	2.5
21	2Z	133	ILE	2.5
34	2c	45	LYS	2.5
57	1y	26	A	2.5
1	1A	1100	C	2.5
32	1a	1352	C	2.5
8	2I	59	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
34	2c	109	PRO	2.5
41	2j	91	PRO	2.5
7	2H	88	LEU	2.4
33	2b	115	LEU	2.4
45	2n	40	CYS	2.4
38	2g	6	ARG	2.4
7	2H	131	VAL	2.4
26	14	50	VAL	2.4
33	2b	15	VAL	2.4
40	2i	11	LYS	2.4
1	2A	272(A)	U	2.4
32	1a	101	A	2.4
32	2a	1004	A	2.4
32	2a	1288	A	2.4
1	2A	886	C	2.4
32	2a	175	C	2.4
32	2a	187	C	2.4
32	2a	217	C	2.4
34	2c	205	GLY	2.4
42	2k	117	ASN	2.4
44	2m	100	GLY	2.4
45	1n	14	PRO	2.4
38	2g	117	ALA	2.4
1	1A	1068	G	2.4
33	2b	118	LEU	2.4
33	2b	164	VAL	2.4
36	2e	32	VAL	2.4
43	2l	18	VAL	2.4
21	2Z	8	TYR	2.4
38	2g	85	TYR	2.4
7	2H	47	GLU	2.4
25	23	30	ARG	2.4
32	1a	161	A	2.4
21	2Z	151	HIS	2.4
30	28	55	ALA	2.4
32	1a	100	C	2.4
32	1a	174	C	2.4
33	2b	16	HIS	2.4
19	2X	95	LEU	2.4
51	1t	99	LEU	2.4
33	2b	230	VAL	2.4
32	2a	1185	G	2.4

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Mol	Chain	Res	Type	RSRZ
33	2b	236	TYR	2.4
33	1b	127	ILE	2.4
34	2c	186	PHE	2.4
51	2t	55	ILE	2.4
8	2I	57	ARG	2.4
41	2j	10	GLY	2.4
4	2E	53	PRO	2.4
1	2A	6	A	2.4
30	28	17	THR	2.4
1	2A	652(V)	C	2.4
32	1a	1007	C	2.4
57	2y	48	C	2.4
34	2c	47	LEU	2.4
48	1q	66	SER	2.4
40	1i	112	LYS	2.4
50	2s	52	TYR	2.4
33	2b	83	MET	2.4
51	1t	63	ILE	2.4
1	2A	2792	G	2.4
38	2g	7	ALA	2.4
2	2B	90	A	2.4
32	1a	1157	A	2.4
50	1s	4	SER	2.4
40	2i	120	ARG	2.4
7	2H	135	GLY	2.4
38	1g	84	ASN	2.4
33	1b	134	GLU	2.4
48	2q	36	ILE	2.4
45	2n	15	LYS	2.4
8	2I	94	ALA	2.4
40	2i	46	ALA	2.4
41	2j	73	ASP	2.4
51	1t	12	ALA	2.4
1	2A	11	G	2.4
32	2a	1184	G	2.4
40	2i	104	ARG	2.4
5	2F	174	VAL	2.4
7	2H	28	GLY	2.4
22	20	42	GLY	2.4
25	23	56	VAL	2.4
32	2a	1001	A	2.4
35	1d	198	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
41	1j	36	GLY	2.4
21	1Z	104	PHE	2.4
51	1t	16	HIS	2.4
45	2n	30	ALA	2.4
34	2c	165	THR	2.4
41	1j	100	THR	2.4
11	2P	123	LEU	2.4
31	29	13	LYS	2.3
20	2Y	42	VAL	2.3
45	2n	56	VAL	2.3
1	1A	1026	U	2.3
1	2A	1043	C	2.3
1	2A	1118	C	2.3
54	1w	3	C	2.3
11	2P	122	PRO	2.3
11	2P	110	TYR	2.3
38	1g	25	ALA	2.3
38	2g	46	ALA	2.3
41	1j	26	ALA	2.3
40	1i	80	GLY	2.3
51	1t	72	LEU	2.3
31	29	20	HIS	2.3
32	2a	198	G	2.3
32	2a	1117	G	2.3
40	2i	42	ARG	2.3
1	2A	2185	C	2.3
32	1a	201	C	2.3
33	2b	105	PHE	2.3
7	2H	164	TYR	2.3
47	1p	39	TYR	2.3
41	2j	48	THR	2.3
45	2n	22	THR	2.3
40	2i	30	GLY	2.3
12	2Q	37	LEU	2.3
33	1b	221	LEU	2.3
38	2g	16	LEU	2.3
41	2j	8	LEU	2.3
33	2b	220	ASP	2.3
1	1A	1081	U	2.3
11	2P	137	LYS	2.3
1	2A	614(B)	G	2.3
33	1b	208	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
33	2b	70	PHE	2.3
45	1n	16	PHE	2.3
1	1A	1073	A	2.3
5	2F	111	ALA	2.3
38	1g	24	THR	2.3
10	2O	108	GLU	2.3
29	27	47	ARG	2.3
38	1g	12	LEU	2.3
33	2b	139	LYS	2.3
11	2P	75	ILE	2.3
21	2Z	57	ILE	2.3
33	1b	185	ILE	2.3
8	2I	11	ASN	2.3
33	2b	204	ASN	2.3
26	24	52	THR	2.3
33	1b	114	ARG	2.3
33	1b	117	GLU	2.3
33	2b	168	THR	2.3
40	2i	69	GLY	2.3
44	2m	99	ARG	2.3
51	1t	59	ALA	2.3
1	1A	2207	G	2.3
1	2A	1117	G	2.3
32	2a	1179	A	2.3
40	1i	114	TYR	2.3
34	2c	101	LEU	2.3
46	1o	57	LEU	2.3
44	2m	92	HIS	2.3
51	2t	73	HIS	2.3
36	1e	96	PRO	2.3
39	1h	67	PRO	2.3
48	1q	28	PRO	2.3
32	1a	1000	U	2.3
15	1T	38	ASN	2.3
11	2P	116	GLY	2.3
40	2i	24	GLY	2.3
48	2q	59	ILE	2.3
21	2Z	156	LYS	2.3
36	1e	21	ALA	2.3
45	2n	4	LYS	2.3
1	2A	2801(A)	A	2.3
32	1a	191	G	2.3

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Mol	Chain	Res	Type	RSRZ
32	2a	97	G	2.3
32	2a	1143	G	2.3
57	1y	76	A	2.3
7	2H	114	VAL	2.3
34	2c	190	ARG	2.3
41	2j	86	MET	2.3
18	1W	112	GLY	2.3
34	2c	134	ILE	2.3
40	2i	126	SER	2.3
16	2U	35	ALA	2.3
36	2e	132	ALA	2.3
25	23	60	GLU	2.3
40	1i	4	TYR	2.3
1	1A	1847	A	2.2
32	2a	1092	A	2.2
41	1j	70	ARG	2.2
1	2A	1183	G	2.2
32	2a	1155	G	2.2
34	2c	102	ASN	2.2
34	2c	49	SER	2.2
5	2F	198	ALA	2.2
39	2h	83	ILE	2.2
7	2H	12	PRO	2.2
32	2a	1284	C	2.2
51	2t	26	ASN	2.2
1	1A	529	A	2.2
11	2P	109	GLY	2.2
8	2I	3	VAL	2.2
32	2a	1151	A	2.2
36	1e	23	GLY	2.2
44	2m	7	VAL	2.2
40	2i	55	ALA	2.2
34	2c	15	THR	2.2
33	2b	111	ARG	2.2
34	2c	42	LEU	2.2
51	2t	13	LEU	2.2
9	2N	8	GLN	2.2
26	24	67	TYR	2.2
40	1i	88	TYR	2.2
45	2n	54	PRO	2.2
33	1b	78	GLN	2.2
1	2A	2099	U	2.2

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Mol	Chain	Res	Type	RSRZ
32	2a	969	A	2.2
12	2Q	66	ILE	2.2
33	1b	137	ARG	2.2
42	1k	72	ALA	2.2
43	2l	30	ALA	2.2
45	2n	45	ARG	2.2
40	2i	37	PHE	2.2
41	2j	81	THR	2.2
41	1j	90	LEU	2.2
51	2t	99	LEU	2.2
8	1l	41	GLU	2.2
34	2c	63	ASN	2.2
1	2A	1116	C	2.2
15	2T	111	ARG	2.2
32	2a	1114	C	2.2
36	2e	33	VAL	2.2
1	2A	652(A)	A	2.2
15	2T	59	THR	2.2
35	1d	70	ILE	2.2
1	1A	1062	G	2.2
1	2A	1533	G	2.2
22	20	52	GLY	2.2
34	2c	43	LEU	2.2
39	2h	36	LEU	2.2
40	1i	24	GLY	2.2
42	1k	103	LEU	2.2
45	2n	50	LYS	2.2
51	1t	84	LEU	2.2
32	2a	1353	G	2.2
7	2H	23	ARG	2.2
25	23	29	ARG	2.2
40	2i	111	ARG	2.2
33	2b	150	SER	2.2
12	2Q	1	MET	2.2
33	2b	219	VAL	2.2
34	1c	66	VAL	2.2
35	1d	133	VAL	2.2
40	2i	53	VAL	2.2
48	2q	23	VAL	2.2
54	1w	20	U	2.2
12	2Q	121	ALA	2.2
34	1c	113	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
41	2j	26	ALA	2.2
3	1D	50	THR	2.2
8	1I	43	ASN	2.2
44	2m	106	ASN	2.2
7	2H	54	ARG	2.2
26	14	55	ARG	2.2
1	2A	2319	G	2.2
7	2H	84	SER	2.2
32	1a	1138	G	2.2
32	2a	1371	G	2.2
33	1b	231	GLU	2.2
34	1c	206	GLU	2.2
39	2h	94	TYR	2.2
57	2y	70	G	2.2
40	1i	58	HIS	2.2
1	2A	271(K)	U	2.2
34	2c	141	VAL	2.2
41	1j	94	VAL	2.2
45	1n	18	VAL	2.2
50	1s	58	VAL	2.2
18	2W	5	ALA	2.2
42	1k	97	ALA	2.2
46	1o	30	ALA	2.2
1	1A	1079	C	2.2
20	2Y	44	ILE	2.2
36	1e	135	THR	2.2
57	1y	43	C	2.2
33	1b	21	ARG	2.2
34	2c	164	ARG	2.2
41	1j	39	PRO	2.2
8	2I	38	LEU	2.2
33	1b	118	LEU	2.2
28	26	13	CYS	2.2
31	29	14	CYS	2.2
21	2Z	166	SER	2.2
1	1A	1091	G	2.1
21	2Z	51	ALA	2.1
30	28	24	ALA	2.1
32	2a	1017	G	2.1
33	1b	230	VAL	2.1
17	1V	70	ILE	2.1
28	26	14	THR	2.1

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Mol	Chain	Res	Type	RSRZ
51	1t	86	ARG	2.1
36	2e	89	ILE	2.1
51	2t	63	ILE	2.1
51	2t	101	GLY	2.1
38	1g	43	PHE	2.1
40	2i	98	PRO	2.1
40	1i	85	LEU	2.1
34	1c	184	TYR	2.1
14	2S	12	PHE	2.1
32	1a	199	G	2.1
34	2c	72	LYS	2.1
38	2g	36	LYS	2.1
1	2A	2803	C	2.1
35	1d	152	SER	2.1
41	2j	9	ARG	2.1
45	1n	12	ARG	2.1
52	2u	15	ARG	2.1
7	2H	46	GLU	2.1
34	2c	82	GLU	2.1
1	1A	2150	U	2.1
11	2P	125	VAL	2.1
12	2Q	28	ALA	2.1
16	2U	21	ALA	2.1
41	1j	44	VAL	2.1
21	1Z	167	PRO	2.1
33	2b	135	GLN	2.1
34	1c	39	ILE	2.1
39	2h	101	PRO	2.1
50	1s	40	ILE	2.1
50	2s	49	ILE	2.1
22	20	57	PHE	2.1
6	1G	139	LEU	2.1
6	2G	152	LEU	2.1
34	1c	101	LEU	2.1
1	1A	1055	G	2.1
7	2H	2	SER	2.1
11	2P	94	GLU	2.1
36	2e	24	ARG	2.1
45	1n	41	ARG	2.1
51	1t	70	SER	2.1
51	2t	74	LYS	2.1
1	1A	899	A	2.1

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Mol	Chain	Res	Type	RSRZ
34	2c	207	VAL	2.1
39	2h	19	VAL	2.1
42	2k	74	ALA	2.1
38	1g	120	ILE	2.1
7	2H	104	GLU	2.1
8	2I	12	LEU	2.1
8	2I	82	ARG	2.1
11	2P	85	LEU	2.1
21	2Z	61	LEU	2.1
30	28	57	ARG	2.1
33	1b	121	LEU	2.1
34	2c	156	ARG	2.1
41	2j	90	LEU	2.1
50	2s	10	PHE	2.1
7	2H	22	GLY	2.1
32	1a	146	G	2.1
32	2a	71	C	2.1
54	2w	29	G	2.1
55	1x	67	C	2.1
33	2b	45	GLN	2.1
33	2b	110	GLN	2.1
9	2N	102	ALA	2.1
11	2P	58	THR	2.1
14	2S	14	VAL	2.1
33	1b	120	ALA	2.1
14	2S	3	ARG	2.1
19	2X	69	TYR	2.1
44	2m	49	THR	2.1
48	1q	32	TYR	2.1
53	1v	15	A	2.1
40	1i	20	ARG	2.1
41	1j	9	ARG	2.1
33	1b	222	ILE	2.1
34	1c	45	LYS	2.1
34	2c	199	LYS	2.1
11	2P	130	PHE	2.1
41	2j	62	HIS	2.1
48	1q	27	PHE	2.1
1	1A	1080	C	2.1
33	1b	52	GLU	2.1
33	1b	59	GLU	2.1
1	1A	2805	G	2.1

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Mol	Chain	Res	Type	RSRZ
32	1a	105	G	2.1
32	1a	1009	G	2.1
32	2a	485	G	2.1
33	2b	144	ARG	2.1
33	2b	7	VAL	2.1
40	1i	27	THR	2.1
40	2i	123	PRO	2.1
48	1q	7	THR	2.1
14	2S	92	TYR	2.1
32	2a	1280	A	2.1
34	2c	94	LEU	2.1
34	2c	204	LEU	2.1
36	2e	123	LEU	2.1
43	2l	62	SER	2.1
47	1p	11	SER	2.1
47	1p	78	GLY	2.1
23	2l	69	LYS	2.1
6	2G	163	ALA	2.0
7	2H	55	PRO	2.0
9	2N	92	ALA	2.0
16	2U	68	ALA	2.0
32	1a	221	C	2.0
1	1A	1101	U	2.0
9	2N	46	VAL	2.0
32	2a	164	U	2.0
11	1P	99	LEU	2.0
32	1a	344	A	2.0
40	1i	50	LEU	2.0
41	2j	63	PHE	2.0
10	2O	76	ALA	2.0
34	2c	53	ALA	2.0
45	1n	59	ALA	2.0
1	1A	2183	C	2.0
32	1a	1038	C	2.0
32	2a	1020	U	2.0
32	2a	1141	C	2.0
42	1k	78	GLN	2.0
40	2i	99	LEU	2.0
32	1a	1187	G	2.0
32	2a	1061	G	2.0
1	1A	1086	A	2.0
39	2h	9	MET	2.0

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Mol	Chain	Res	Type	RSRZ
44	1m	2	ALA	2.0
33	1b	19	HIS	2.0
44	2m	122	LYS	2.0
45	1n	15	LYS	2.0
21	2Z	128	VAL	2.0
40	2i	71	SER	2.0
50	2s	67	VAL	2.0
50	2s	81	ARG	2.0
51	1t	23	ARG	2.0
52	2u	9	ARG	2.0
7	2H	9	ILE	2.0
32	1a	1006	C	2.0
32	2a	1326	C	2.0
17	2V	94	LEU	2.0
23	21	73	LEU	2.0
33	1b	41	ILE	2.0
51	2t	100	ILE	2.0
57	1y	40	C	2.0
47	2p	60	LEU	2.0
38	2g	26	PHE	2.0
32	1a	1287	A	2.0
32	2a	145	G	2.0
32	2a	1016	A	2.0
32	2a	1186	G	2.0
32	2a	1221	G	2.0
53	2v	23	A	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	4SU	2y	8	20/21	0.44	0.35	76,88,95,107	0
57	G7M	2y	46	24/25	0.62	0.36	76,84,87,99	0
57	MIA	2y	37	22/30	0.65	0.51	71,77,91,104	0
57	PSU	2y	32	20/21	0.67	0.44	73,79,83,89	0
57	MIA	1y	37	22/30	0.68	0.49	69,78,88,96	0
57	PSU	1y	55	20/21	0.68	0.57	79,84,91,100	0
54	G7M	2w	46	24/25	0.68	0.25	64,76,88,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	4SU	1y	8	20/21	0.70	0.29	76,80,94,101	0
57	G7M	1y	46	24/25	0.71	0.29	64,78,86,92	0
57	5MU	2y	54	21/22	0.73	0.45	67,76,83,95	0
57	5MU	1y	54	21/22	0.74	0.46	74,80,86,95	0
57	PSU	1y	39	20/21	0.77	0.47	70,81,84,85	0
57	PSU	2y	55	20/21	0.80	0.46	74,80,85,87	0
57	PSU	2y	39	20/21	0.80	0.46	74,80,87,90	0
57	PSU	1y	32	20/21	0.81	0.42	70,76,88,96	0
54	G7M	1w	46	24/25	0.82	0.18	66,70,84,96	0
54	4SU	2w	8	20/21	0.84	0.17	67,74,82,83	0
54	4SU	1w	8	20/21	0.86	0.18	56,70,78,81	0
54	PSU	2w	32	20/21	0.86	0.27	52,65,81,85	0
54	PSU	2w	55	20/21	0.88	0.17	58,68,76,77	0
54	5MU	2w	54	21/22	0.89	0.17	56,63,68,71	0
54	MIA	2w	37	25/30	0.89	0.22	52,60,67,87	0
43	0TD	2l	92	10/11	0.90	0.22	47,51,57,72	0
55	4SU	2x	8	20/21	0.90	0.17	57,62,65,71	0
55	PSU	2x	55	20/21	0.90	0.17	55,59,68,73	0
32	M2G	2a	966	25/26	0.91	0.25	45,56,64,76	0
54	PSU	1w	55	20/21	0.91	0.20	40,60,66,67	0
55	5MU	2x	54	21/22	0.91	0.22	59,65,69,71	0
32	2MG	1a	1207	24/25	0.92	0.17	48,56,59,63	0
43	0TD	1l	92	10/11	0.92	0.17	39,42,47,58	0
32	5MC	2a	967	21/22	0.92	0.22	51,56,64,66	0
32	2MG	2a	1207	24/25	0.92	0.18	59,68,70,71	0
1	OMC	2A	1920	21/22	0.93	0.18	48,51,56,63	0
54	PSU	2w	39	20/21	0.93	0.26	47,62,68,68	0
32	PSU	2a	516	20/21	0.93	0.19	47,58,63,64	0
32	G7M	2a	527	24/25	0.93	0.18	47,53,58,61	0
55	PSU	1x	55	20/21	0.93	0.19	45,51,64,67	0
55	4SU	1x	8	20/21	0.93	0.18	49,54,59,60	0
54	MIA	1w	37	29/30	0.93	0.23	35,44,52,76	0
32	4OC	2a	1402	22/23	0.94	0.16	47,50,54,56	0
32	5MC	2a	1404	21/22	0.94	0.18	42,48,51,52	0
1	5MU	1A	1915	21/22	0.94	0.19	34,41,45,50	0
32	M2G	1a	966	25/26	0.94	0.19	33,42,46,50	0
55	5MC	2x	32	21/22	0.94	0.17	51,58,64,70	0
1	PSU	2A	1911	20/21	0.94	0.16	42,50,54,57	0
1	5MU	2A	1915	21/22	0.94	0.15	50,58,62,64	0
32	5MC	1a	967	21/22	0.94	0.22	37,43,48,53	0
54	PSU	1w	32	20/21	0.94	0.22	46,52,59,63	0
56	FME	1z	1	10/11	0.94	0.17	19,23,25,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	5MC	2a	1407	21/22	0.95	0.19	36,43,50,52	0
32	MA6	2a	1518	24/25	0.95	0.20	42,48,53,53	0
54	PSU	1w	39	20/21	0.95	0.20	30,52,60,67	0
32	MA6	1a	1519	24/25	0.95	0.20	31,36,42,49	0
1	PSU	2A	1917	20/21	0.95	0.14	43,55,58,58	0
55	5MC	1x	32	21/22	0.95	0.18	34,42,49,55	0
1	5MC	2A	1942	21/22	0.95	0.18	44,49,56,57	0
32	5MC	2a	1400	21/22	0.95	0.22	48,55,60,63	0
1	OMU	2A	2552	21/22	0.95	0.23	27,36,43,46	0
55	5MU	1x	54	21/22	0.95	0.20	52,56,62,68	0
56	FME	2z	1	10/11	0.95	0.19	29,35,42,48	0
32	5MC	1a	1404	21/22	0.96	0.20	26,32,38,39	0
32	MA6	2a	1519	24/25	0.96	0.22	42,50,53,55	0
32	G7M	1a	527	24/25	0.96	0.21	33,39,46,48	0
55	8AN	1x	76	22/23	0.96	0.21	14,18,23,33	0
1	5MC	2A	1962	21/22	0.96	0.20	24,38,43,48	0
54	5MU	1w	54	21/22	0.96	0.16	34,50,54,57	0
1	PSU	1A	1917	20/21	0.96	0.16	33,39,43,45	0
32	5MC	1a	1400	21/22	0.96	0.19	36,43,46,48	0
55	8AN	2x	76	22/23	0.96	0.20	24,35,41,42	0
54	F3N	2w	76	33/34	0.96	0.21	26,33,36,38	0
32	4OC	1a	1402	22/23	0.96	0.20	30,38,42,46	0
32	UR3	2a	1498	21/22	0.96	0.21	46,49,53,53	0
1	5MC	1A	1962	21/22	0.97	0.21	23,28,32,36	0
32	PSU	1a	516	20/21	0.97	0.14	38,46,50,50	0
1	PSU	2A	2605	20/21	0.97	0.18	24,30,35,35	0
1	PSU	1A	1911	20/21	0.97	0.18	33,42,46,48	0
32	UR3	1a	1498	21/22	0.97	0.21	29,35,39,40	0
32	MA6	1a	1518	24/25	0.97	0.20	28,35,37,41	0
54	F3N	1w	76	33/34	0.97	0.22	13,19,21,25	0
1	OMC	1A	1920	21/22	0.97	0.20	26,39,44,47	0
1	5MU	1A	1939	21/22	0.97	0.21	15,22,28,30	0
1	5MC	1A	1942	21/22	0.97	0.20	29,36,40,47	0
1	2MA	1A	2503	23/24	0.98	0.23	12,14,17,18	0
1	OMG	2A	2251	24/25	0.98	0.21	25,32,38,43	0
1	2MA	2A	2503	23/24	0.98	0.20	23,29,32,34	0
1	OMU	1A	2552	21/22	0.98	0.19	17,24,27,28	0
1	PSU	1A	2605	20/21	0.98	0.21	15,20,24,24	0
32	5MC	1a	1407	21/22	0.98	0.19	27,35,39,42	0
1	5MU	2A	1939	21/22	0.98	0.19	24,30,34,35	0
1	OMG	1A	2251	24/25	0.98	0.20	15,20,22,24	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1799	1/1	0.06	0.29	68,68,68,68	0
58	MG	2a	1773	1/1	0.18	0.17	59,59,59,59	0
58	MG	2A	3788	1/1	0.24	0.28	60,60,60,60	0
58	MG	1a	1782	1/1	0.29	0.17	57,57,57,57	0
58	MG	1U	209	1/1	0.31	0.49	59,59,59,59	0
58	MG	18	109	1/1	0.34	0.27	58,58,58,58	0
58	MG	1A	3981	1/1	0.35	0.29	54,54,54,54	0
58	MG	2A	3067	1/1	0.46	0.14	58,58,58,58	0
58	MG	2A	3342	1/1	0.47	0.16	70,70,70,70	0
58	MG	1a	1672	1/1	0.47	0.28	55,55,55,55	0
58	MG	1B	229	1/1	0.47	0.15	66,66,66,66	0
58	MG	2B	211	1/1	0.49	0.26	77,77,77,77	0
58	MG	1A	3069	1/1	0.52	0.20	55,55,55,55	0
58	MG	1A	3961	1/1	0.52	0.12	51,51,51,51	0
58	MG	1A	3889	1/1	0.53	0.11	39,39,39,39	0
58	MG	1A	3939	1/1	0.53	0.12	51,51,51,51	0
58	MG	1a	1774	1/1	0.53	0.10	59,59,59,59	0
58	MG	1A	3414	1/1	0.53	0.28	68,68,68,68	0
58	MG	10	107	1/1	0.53	0.30	54,54,54,54	0
58	MG	1A	3959	1/1	0.54	0.12	48,48,48,48	0
58	MG	2a	1781	1/1	0.54	0.18	56,56,56,56	0
58	MG	1A	3947	1/1	0.55	0.06	46,46,46,46	0
58	MG	2A	3051	1/1	0.57	0.35	65,65,65,65	0
58	MG	2a	1641	1/1	0.57	0.18	54,54,54,54	0
58	MG	1A	3796	1/1	0.58	0.16	44,44,44,44	0
58	MG	1Y	203	1/1	0.58	0.20	66,66,66,66	0
58	MG	2A	3355	1/1	0.58	0.33	61,61,61,61	0
58	MG	1A	3651	1/1	0.58	0.15	63,63,63,63	0
58	MG	1A	4033	1/1	0.59	0.13	42,42,42,42	0
58	MG	1A	4026	1/1	0.61	0.12	49,49,49,49	0
58	MG	2A	3104	1/1	0.61	0.16	52,52,52,52	0
58	MG	1A	3405	1/1	0.61	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3335	1/1	0.61	0.25	52,52,52,52	0
58	MG	2A	3698	1/1	0.61	0.12	55,55,55,55	0
58	MG	2A	3338	1/1	0.62	0.19	68,68,68,68	0
58	MG	2a	1646	1/1	0.62	0.17	66,66,66,66	0
58	MG	1a	1805	1/1	0.62	0.25	56,56,56,56	0
58	MG	1A	4072	1/1	0.62	0.17	47,47,47,47	0
58	MG	1A	3637	1/1	0.63	0.15	38,38,38,38	0
58	MG	1A	3602	1/1	0.63	0.24	52,52,52,52	0
58	MG	2A	3835	1/1	0.63	0.11	63,63,63,63	0
58	MG	2A	3627	1/1	0.63	0.14	53,53,53,53	0
58	MG	1a	1770	1/1	0.64	0.27	72,72,72,72	0
58	MG	1A	3798	1/1	0.64	0.13	67,67,67,67	0
58	MG	1A	4054	1/1	0.64	0.12	42,42,42,42	0
58	MG	1A	3254	1/1	0.64	0.15	63,63,63,63	0
58	MG	1a	1766	1/1	0.64	0.15	68,68,68,68	0
58	MG	2A	3486	1/1	0.65	0.17	56,56,56,56	0
58	MG	1a	1744	1/1	0.65	0.17	64,64,64,64	0
58	MG	1A	4032	1/1	0.65	0.21	57,57,57,57	0
58	MG	2a	1680	1/1	0.65	0.21	54,54,54,54	0
58	MG	2A	3192	1/1	0.65	0.23	48,48,48,48	0
58	MG	2A	3399	1/1	0.65	0.17	58,58,58,58	0
58	MG	2v	101	1/1	0.65	0.29	75,75,75,75	0
58	MG	1A	4024	1/1	0.66	0.13	47,47,47,47	0
58	MG	1A	3861	1/1	0.66	0.13	65,65,65,65	0
58	MG	1a	1636	1/1	0.66	0.19	67,67,67,67	0
58	MG	2A	3204	1/1	0.66	0.19	66,66,66,66	0
58	MG	1l	201	1/1	0.66	0.15	62,62,62,62	0
58	MG	1A	3988	1/1	0.66	0.15	56,56,56,56	0
58	MG	2A	3353	1/1	0.66	0.25	60,60,60,60	0
58	MG	2A	3136	1/1	0.67	0.32	50,50,50,50	0
58	MG	2A	3268	1/1	0.67	0.26	65,65,65,65	0
58	MG	2A	3313	1/1	0.67	0.20	61,61,61,61	0
58	MG	1A	3927	1/1	0.67	0.14	59,59,59,59	0
58	MG	1A	3946	1/1	0.68	0.17	46,46,46,46	0
58	MG	2A	3829	1/1	0.68	0.20	31,31,31,31	0
58	MG	2E	301	1/1	0.69	0.20	52,52,52,52	0
58	MG	1w	108	1/1	0.69	0.13	67,67,67,67	0
58	MG	2A	3187	1/1	0.69	0.28	61,61,61,61	0
58	MG	2A	3283	1/1	0.69	0.22	49,49,49,49	0
58	MG	2a	1713	1/1	0.69	0.14	58,58,58,58	0
58	MG	2a	1721	1/1	0.69	0.10	67,67,67,67	0
58	MG	1A	3791	1/1	0.69	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3317	1/1	0.69	0.18	57,57,57,57	0
58	MG	2A	3327	1/1	0.69	0.36	65,65,65,65	0
58	MG	1A	3755	1/1	0.70	0.19	57,57,57,57	0
58	MG	1E	311	1/1	0.70	0.18	54,54,54,54	0
58	MG	2A	3745	1/1	0.70	0.11	67,67,67,67	0
58	MG	2a	1601	1/1	0.70	0.20	59,59,59,59	0
58	MG	2A	3290	1/1	0.70	0.14	62,62,62,62	0
58	MG	1A	3173	1/1	0.70	0.16	57,57,57,57	0
58	MG	1A	4030	1/1	0.71	0.19	50,50,50,50	0
58	MG	1a	1696	1/1	0.71	0.25	57,57,57,57	0
58	MG	1A	3966	1/1	0.71	0.12	43,43,43,43	0
58	MG	2a	1758	1/1	0.71	0.17	62,62,62,62	0
58	MG	2A	3152	1/1	0.71	0.18	56,56,56,56	0
58	MG	2A	3031	1/1	0.71	0.21	59,59,59,59	0
58	MG	1a	1662	1/1	0.71	0.10	50,50,50,50	0
58	MG	1A	3467	1/1	0.72	0.18	60,60,60,60	0
58	MG	25	102	1/1	0.72	0.34	57,57,57,57	0
58	MG	2a	1741	1/1	0.72	0.21	69,69,69,69	0
58	MG	2a	1752	1/1	0.72	0.09	69,69,69,69	0
58	MG	2A	3562	1/1	0.72	0.30	44,44,44,44	0
58	MG	2A	3595	1/1	0.72	0.25	73,73,73,73	0
58	MG	2A	3190	1/1	0.72	0.31	62,62,62,62	0
58	MG	2A	3128	1/1	0.72	0.55	63,63,63,63	0
58	MG	1A	4028	1/1	0.73	0.16	46,46,46,46	0
58	MG	2a	1642	1/1	0.73	0.18	54,54,54,54	0
58	MG	1A	4065	1/1	0.73	0.14	48,48,48,48	0
58	MG	2A	3734	1/1	0.73	0.15	47,47,47,47	0
58	MG	2A	3254	1/1	0.73	0.40	61,61,61,61	0
58	MG	1A	3673	1/1	0.73	0.12	33,33,33,33	0
58	MG	1A	3978	1/1	0.73	0.27	64,64,64,64	0
58	MG	2A	3158	1/1	0.73	0.14	64,64,64,64	0
58	MG	2A	3065	1/1	0.73	0.25	51,51,51,51	0
58	MG	2A	3511	1/1	0.73	0.15	63,63,63,63	0
58	MG	2A	3316	1/1	0.73	0.16	58,58,58,58	0
58	MG	1A	3954	1/1	0.73	0.18	61,61,61,61	0
58	MG	2A	3443	1/1	0.74	0.42	58,58,58,58	0
58	MG	1A	3538	1/1	0.74	0.23	40,40,40,40	0
58	MG	1A	3745	1/1	0.74	0.08	47,47,47,47	0
58	MG	1A	3980	1/1	0.74	0.12	48,48,48,48	0
58	MG	2A	3191	1/1	0.74	0.34	69,69,69,69	0
58	MG	2A	3624	1/1	0.74	0.16	62,62,62,62	0
58	MG	2X	101	1/1	0.74	0.21	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3293	1/1	0.74	0.15	50,50,50,50	0
58	MG	1A	3950	1/1	0.74	0.08	41,41,41,41	0
58	MG	2a	1626	1/1	0.74	0.18	65,65,65,65	0
58	MG	2a	1832	1/1	0.74	0.13	64,64,64,64	0
58	MG	1P	204	1/1	0.74	0.31	46,46,46,46	0
58	MG	1A	3074	1/1	0.75	0.41	54,54,54,54	0
58	MG	2A	3195	1/1	0.75	0.19	65,65,65,65	0
58	MG	2A	3605	1/1	0.75	0.24	34,34,34,34	0
58	MG	1a	1793	1/1	0.75	0.18	71,71,71,71	0
58	MG	1A	3499	1/1	0.75	0.23	39,39,39,39	0
58	MG	2A	3630	1/1	0.75	0.28	50,50,50,50	0
58	MG	1A	3103	1/1	0.75	0.12	53,53,53,53	0
58	MG	2A	3719	1/1	0.75	0.23	43,43,43,43	0
58	MG	2a	1712	1/1	0.75	0.12	61,61,61,61	0
58	MG	1A	3554	1/1	0.75	0.12	51,51,51,51	0
58	MG	2A	3356	1/1	0.75	0.29	57,57,57,57	0
58	MG	1A	3410	1/1	0.75	0.28	49,49,49,49	0
58	MG	2A	3799	1/1	0.75	0.16	55,55,55,55	0
58	MG	1A	3278	1/1	0.75	0.20	39,39,39,39	0
58	MG	1A	3420	1/1	0.75	0.23	38,38,38,38	0
58	MG	2A	3495	1/1	0.75	0.17	46,46,46,46	0
58	MG	1A	3996	1/1	0.75	0.14	46,46,46,46	0
58	MG	2E	307	1/1	0.75	0.12	53,53,53,53	0
58	MG	1A	4040	1/1	0.76	0.11	37,37,37,37	0
58	MG	1a	1706	1/1	0.76	0.25	54,54,54,54	0
58	MG	2A	3006	1/1	0.76	0.14	47,47,47,47	0
58	MG	1A	3784	1/1	0.76	0.18	34,34,34,34	0
58	MG	1A	3991	1/1	0.76	0.14	29,29,29,29	0
58	MG	1A	3318	1/1	0.76	0.31	45,45,45,45	0
58	MG	2A	3215	1/1	0.76	0.39	62,62,62,62	0
58	MG	2A	3357	1/1	0.76	0.16	58,58,58,58	0
58	MG	1B	212	1/1	0.76	0.21	51,51,51,51	0
58	MG	2A	3101	1/1	0.76	0.17	53,53,53,53	0
58	MG	2A	3823	1/1	0.76	0.08	67,67,67,67	0
58	MG	2A	3824	1/1	0.76	0.14	52,52,52,52	0
58	MG	1B	227	1/1	0.76	0.21	41,41,41,41	0
58	MG	1A	4010	1/1	0.76	0.17	53,53,53,53	0
58	MG	2a	1760	1/1	0.76	0.10	56,56,56,56	0
58	MG	2a	1765	1/1	0.76	0.10	61,61,61,61	0
58	MG	2B	206	1/1	0.76	0.19	57,57,57,57	0
58	MG	1A	3131	1/1	0.76	0.19	41,41,41,41	0
58	MG	1a	1674	1/1	0.76	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2l	201	1/1	0.76	0.13	61,61,61,61	0
58	MG	1a	1811	1/1	0.76	0.14	63,63,63,63	0
58	MG	2A	3310	1/1	0.77	0.16	57,57,57,57	0
58	MG	1A	3851	1/1	0.77	0.17	59,59,59,59	0
58	MG	2A	3074	1/1	0.77	0.17	53,53,53,53	0
58	MG	1A	3855	1/1	0.77	0.21	51,51,51,51	0
58	MG	1A	3187	1/1	0.77	0.12	62,62,62,62	0
58	MG	2A	3212	1/1	0.77	0.17	64,64,64,64	0
58	MG	1A	4039	1/1	0.77	0.09	45,45,45,45	0
58	MG	2a	1748	1/1	0.77	0.13	58,58,58,58	0
58	MG	1a	1658	1/1	0.77	0.13	55,55,55,55	0
58	MG	2A	3260	1/1	0.77	0.24	45,45,45,45	0
58	MG	1A	3365	1/1	0.77	0.17	52,52,52,52	0
58	MG	1A	3713	1/1	0.77	0.20	34,34,34,34	0
58	MG	2A	3396	1/1	0.77	0.18	52,52,52,52	0
58	MG	2a	1608	1/1	0.77	0.20	57,57,57,57	0
58	MG	2a	1616	1/1	0.77	0.20	59,59,59,59	0
58	MG	1A	3938	1/1	0.77	0.14	54,54,54,54	0
58	MG	1a	1794	1/1	0.77	0.08	56,56,56,56	0
58	MG	2x	101	1/1	0.77	0.31	51,51,51,51	0
58	MG	1A	3312	1/1	0.78	0.24	58,58,58,58	0
58	MG	2A	3084	1/1	0.78	0.23	38,38,38,38	0
58	MG	26	101	1/1	0.78	0.23	53,53,53,53	0
58	MG	1a	1689	1/1	0.78	0.17	51,51,51,51	0
58	MG	2A	3351	1/1	0.78	0.45	66,66,66,66	0
58	MG	1A	3951	1/1	0.78	0.43	62,62,62,62	0
58	MG	18	101	1/1	0.78	0.16	40,40,40,40	0
58	MG	2A	3717	1/1	0.78	0.32	47,47,47,47	0
58	MG	18	107	1/1	0.78	0.15	55,55,55,55	0
58	MG	1a	1745	1/1	0.78	0.14	54,54,54,54	0
58	MG	2a	1667	1/1	0.78	0.24	70,70,70,70	0
58	MG	2A	3360	1/1	0.78	0.23	61,61,61,61	0
58	MG	2a	1704	1/1	0.78	0.17	60,60,60,60	0
58	MG	2A	3375	1/1	0.78	0.11	43,43,43,43	0
58	MG	2A	3789	1/1	0.78	0.20	33,33,33,33	0
58	MG	2A	3793	1/1	0.78	0.13	47,47,47,47	0
58	MG	2A	3394	1/1	0.78	0.15	59,59,59,59	0
58	MG	1A	3794	1/1	0.78	0.08	39,39,39,39	0
58	MG	2A	3159	1/1	0.78	0.16	46,46,46,46	0
58	MG	2a	1757	1/1	0.78	0.20	79,79,79,79	0
58	MG	2A	3166	1/1	0.78	0.24	56,56,56,56	0
58	MG	2a	1759	1/1	0.78	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3463	1/1	0.78	0.42	44,44,44,44	0
58	MG	2A	3843	1/1	0.78	0.21	54,54,54,54	0
58	MG	1A	3924	1/1	0.78	0.19	31,31,31,31	0
58	MG	2B	207	1/1	0.78	0.19	57,57,57,57	0
58	MG	2a	1826	1/1	0.78	0.17	59,59,59,59	0
58	MG	2B	210	1/1	0.78	0.21	67,67,67,67	0
58	MG	1A	4041	1/1	0.78	0.15	30,30,30,30	0
58	MG	1A	3960	1/1	0.78	0.31	52,52,52,52	0
58	MG	1A	3454	1/1	0.78	0.28	48,48,48,48	0
58	MG	2x	104	1/1	0.78	0.26	61,61,61,61	0
58	MG	2A	3450	1/1	0.79	0.28	56,56,56,56	0
58	MG	1a	1743	1/1	0.79	0.16	35,35,35,35	0
58	MG	2A	3100	1/1	0.79	0.14	53,53,53,53	0
58	MG	1a	1646	1/1	0.79	0.12	45,45,45,45	0
58	MG	2A	3497	1/1	0.79	0.15	42,42,42,42	0
58	MG	1A	3691	1/1	0.79	0.16	40,40,40,40	0
58	MG	2A	3861	1/1	0.79	0.21	37,37,37,37	0
58	MG	2A	3124	1/1	0.79	0.31	44,44,44,44	0
58	MG	1A	3617	1/1	0.79	0.12	26,26,26,26	0
58	MG	2A	3343	1/1	0.79	0.13	57,57,57,57	0
58	MG	1A	4002	1/1	0.79	0.17	41,41,41,41	0
58	MG	1A	3929	1/1	0.79	0.13	41,41,41,41	0
58	MG	2A	3259	1/1	0.79	0.16	39,39,39,39	0
58	MG	2A	3681	1/1	0.79	0.23	55,55,55,55	0
58	MG	1A	3719	1/1	0.79	0.23	50,50,50,50	0
58	MG	1A	3720	1/1	0.79	0.14	51,51,51,51	0
58	MG	2A	3270	1/1	0.79	0.23	71,71,71,71	0
58	MG	2a	1800	1/1	0.79	0.18	61,61,61,61	0
58	MG	2A	3163	1/1	0.79	0.11	52,52,52,52	0
58	MG	2a	1612	1/1	0.79	0.18	46,46,46,46	0
58	MG	2A	3286	1/1	0.79	0.26	55,55,55,55	0
58	MG	1A	3646	1/1	0.79	0.14	35,35,35,35	0
58	MG	2w	104	1/1	0.79	0.18	65,65,65,65	0
58	MG	2A	3178	1/1	0.79	0.22	41,41,41,41	0
58	MG	1a	1737	1/1	0.79	0.35	68,68,68,68	0
58	MG	2a	1618	1/1	0.80	0.30	63,63,63,63	0
58	MG	1A	3663	1/1	0.80	0.20	40,40,40,40	0
58	MG	1A	3841	1/1	0.80	0.35	67,67,67,67	0
58	MG	2A	3080	1/1	0.80	0.18	43,43,43,43	0
58	MG	2A	3816	1/1	0.80	0.13	53,53,53,53	0
58	MG	1a	1625	1/1	0.80	0.15	55,55,55,55	0
58	MG	2a	1678	1/1	0.80	0.32	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1709	1/1	0.80	0.13	55,55,55,55	0
58	MG	1a	1713	1/1	0.80	0.26	57,57,57,57	0
58	MG	2A	3830	1/1	0.80	0.11	49,49,49,49	0
58	MG	2A	3512	1/1	0.80	0.14	45,45,45,45	0
58	MG	1A	3417	1/1	0.80	0.15	52,52,52,52	0
58	MG	2A	3568	1/1	0.80	0.15	37,37,37,37	0
58	MG	2A	3865	1/1	0.80	0.18	52,52,52,52	0
58	MG	2A	3867	1/1	0.80	0.22	46,46,46,46	0
58	MG	1a	1808	1/1	0.80	0.16	48,48,48,48	0
58	MG	1a	1740	1/1	0.80	0.13	64,64,64,64	0
58	MG	1S	203	1/1	0.80	0.18	55,55,55,55	0
58	MG	1A	3384	1/1	0.80	0.28	37,37,37,37	0
58	MG	1A	3435	1/1	0.80	0.17	43,43,43,43	0
58	MG	2a	1772	1/1	0.80	0.15	55,55,55,55	0
58	MG	1a	1759	1/1	0.80	0.13	62,62,62,62	0
58	MG	2P	201	1/1	0.80	0.20	53,53,53,53	0
58	MG	2A	3282	1/1	0.80	0.20	51,51,51,51	0
58	MG	2a	1811	1/1	0.80	0.25	69,69,69,69	0
58	MG	2A	3703	1/1	0.80	0.21	63,63,63,63	0
58	MG	1A	3543	1/1	0.80	0.12	58,58,58,58	0
58	MG	2A	3060	1/1	0.80	0.12	49,49,49,49	0
58	MG	2A	3173	1/1	0.80	0.14	61,61,61,61	0
58	MG	2a	1610	1/1	0.80	0.14	53,53,53,53	0
58	MG	1A	3238	1/1	0.80	0.24	59,59,59,59	0
58	MG	2A	3307	1/1	0.80	0.24	51,51,51,51	0
58	MG	1A	3362	1/1	0.81	0.16	53,53,53,53	0
58	MG	1D	312	1/1	0.81	0.20	29,29,29,29	0
58	MG	2a	1625	1/1	0.81	0.23	50,50,50,50	0
58	MG	1A	3363	1/1	0.81	0.27	51,51,51,51	0
58	MG	1A	4011	1/1	0.81	0.12	25,25,25,25	0
58	MG	2A	3768	1/1	0.81	0.26	42,42,42,42	0
58	MG	2A	3213	1/1	0.81	0.12	50,50,50,50	0
58	MG	2a	1659	1/1	0.81	0.12	69,69,69,69	0
58	MG	2a	1665	1/1	0.81	0.16	54,54,54,54	0
58	MG	1A	3436	1/1	0.81	0.21	41,41,41,41	0
58	MG	2a	1671	1/1	0.81	0.16	50,50,50,50	0
58	MG	2A	3227	1/1	0.81	0.21	54,54,54,54	0
58	MG	1A	4025	1/1	0.81	0.28	59,59,59,59	0
58	MG	2a	1701	1/1	0.81	0.28	58,58,58,58	0
58	MG	1A	3952	1/1	0.81	0.12	43,43,43,43	0
58	MG	1A	3306	1/1	0.81	0.37	59,59,59,59	0
58	MG	2A	3423	1/1	0.81	0.32	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3956	1/1	0.81	0.14	54,54,54,54	0
58	MG	2a	1729	1/1	0.81	0.16	55,55,55,55	0
58	MG	1A	3459	1/1	0.81	0.16	43,43,43,43	0
58	MG	1A	3229	1/1	0.81	0.20	37,37,37,37	0
58	MG	1A	3479	1/1	0.81	0.14	49,49,49,49	0
58	MG	2A	3488	1/1	0.81	0.18	43,43,43,43	0
58	MG	1A	3385	1/1	0.81	0.21	45,45,45,45	0
58	MG	1A	3315	1/1	0.81	0.29	53,53,53,53	0
58	MG	1A	3266	1/1	0.81	0.15	46,46,46,46	0
58	MG	1A	3548	1/1	0.81	0.31	52,52,52,52	0
58	MG	1A	3319	1/1	0.81	0.24	50,50,50,50	0
58	MG	1A	4092	1/1	0.81	0.12	41,41,41,41	0
58	MG	1A	3595	1/1	0.81	0.21	33,33,33,33	0
58	MG	2A	3176	1/1	0.81	0.16	50,50,50,50	0
58	MG	2a	1803	1/1	0.81	0.08	65,65,65,65	0
58	MG	1B	224	1/1	0.81	0.25	53,53,53,53	0
58	MG	2A	3334	1/1	0.81	0.22	50,50,50,50	0
58	MG	1a	1703	1/1	0.81	0.18	45,45,45,45	0
58	MG	1A	3175	1/1	0.81	0.22	50,50,50,50	0
58	MG	2q	201	1/1	0.81	0.43	56,56,56,56	0
58	MG	2A	3682	1/1	0.81	0.20	57,57,57,57	0
58	MG	2A	3040	1/1	0.81	0.11	58,58,58,58	0
58	MG	2w	105	1/1	0.81	0.09	60,60,60,60	0
58	MG	2A	3349	1/1	0.81	0.36	46,46,46,46	0
58	MG	2x	103	1/1	0.81	0.17	50,50,50,50	0
58	MG	2A	3709	1/1	0.81	0.12	66,66,66,66	0
58	MG	2A	3127	1/1	0.82	0.22	41,41,41,41	0
58	MG	1a	1619	1/1	0.82	0.17	45,45,45,45	0
58	MG	2A	3560	1/1	0.82	0.14	37,37,37,37	0
58	MG	2A	3130	1/1	0.82	0.14	41,41,41,41	0
58	MG	2A	3242	1/1	0.82	0.22	61,61,61,61	0
58	MG	1w	101	1/1	0.82	0.32	67,67,67,67	0
58	MG	1A	3332	1/1	0.82	0.17	57,57,57,57	0
58	MG	1A	3205	1/1	0.82	0.17	48,48,48,48	0
58	MG	2A	3265	1/1	0.82	0.22	53,53,53,53	0
58	MG	2A	3871	1/1	0.82	0.25	51,51,51,51	0
58	MG	2a	1724	1/1	0.82	0.21	60,60,60,60	0
58	MG	1A	3220	1/1	0.82	0.29	45,45,45,45	0
58	MG	2A	3667	1/1	0.82	0.27	64,64,64,64	0
58	MG	2A	3676	1/1	0.82	0.25	42,42,42,42	0
58	MG	1A	3556	1/1	0.82	0.15	39,39,39,39	0
58	MG	2B	220	1/1	0.82	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3371	1/1	0.82	0.20	40,40,40,40	0
58	MG	1R	204	1/1	0.82	0.32	42,42,42,42	0
58	MG	2A	3702	1/1	0.82	0.13	51,51,51,51	0
58	MG	1A	4064	1/1	0.82	0.10	36,36,36,36	0
58	MG	2a	1767	1/1	0.82	0.20	73,73,73,73	0
58	MG	1A	3661	1/1	0.82	0.24	38,38,38,38	0
58	MG	1A	3569	1/1	0.82	0.23	47,47,47,47	0
58	MG	2A	3409	1/1	0.82	0.16	56,56,56,56	0
58	MG	2a	1606	1/1	0.82	0.17	56,56,56,56	0
58	MG	2A	3186	1/1	0.82	0.24	33,33,33,33	0
58	MG	1A	3501	1/1	0.82	0.25	59,59,59,59	0
58	MG	14	101	1/1	0.82	0.10	51,51,51,51	0
58	MG	1A	3006	1/1	0.82	0.21	48,48,48,48	0
58	MG	1A	3995	1/1	0.82	0.12	27,27,27,27	0
58	MG	2l	204	1/1	0.82	0.12	54,54,54,54	0
58	MG	1A	3608	1/1	0.82	0.12	51,51,51,51	0
58	MG	2A	3796	1/1	0.82	0.18	52,52,52,52	0
58	MG	2w	102	1/1	0.82	0.92	57,57,57,57	0
58	MG	2a	1637	1/1	0.82	0.11	61,61,61,61	0
58	MG	1a	1723	1/1	0.82	0.27	55,55,55,55	0
58	MG	2A	3806	1/1	0.82	0.12	37,37,37,37	0
58	MG	2A	3807	1/1	0.82	0.15	37,37,37,37	0
58	MG	1a	1734	1/1	0.82	0.18	39,39,39,39	0
58	MG	2A	3583	1/1	0.83	0.16	41,41,41,41	0
58	MG	2A	3832	1/1	0.83	0.18	47,47,47,47	0
58	MG	2A	3266	1/1	0.83	0.14	42,42,42,42	0
58	MG	2A	3836	1/1	0.83	0.08	50,50,50,50	0
58	MG	2a	1687	1/1	0.83	0.16	52,52,52,52	0
58	MG	1B	231	1/1	0.83	0.11	68,68,68,68	0
58	MG	2A	3619	1/1	0.83	0.10	47,47,47,47	0
58	MG	1A	3466	1/1	0.83	0.28	60,60,60,60	0
58	MG	2A	3280	1/1	0.83	0.61	57,57,57,57	0
58	MG	1A	3725	1/1	0.83	0.12	51,51,51,51	0
58	MG	1A	4081	1/1	0.83	0.15	27,27,27,27	0
58	MG	2A	3670	1/1	0.83	0.15	59,59,59,59	0
58	MG	2A	3388	1/1	0.83	0.15	53,53,53,53	0
58	MG	1a	1624	1/1	0.83	0.21	49,49,49,49	0
58	MG	2A	3011	1/1	0.83	0.16	41,41,41,41	0
58	MG	1a	1773	1/1	0.83	0.09	58,58,58,58	0
58	MG	2A	3298	1/1	0.83	0.27	53,53,53,53	0
58	MG	2A	3210	1/1	0.83	0.27	46,46,46,46	0
58	MG	1A	3875	1/1	0.83	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3042	1/1	0.83	0.44	42,42,42,42	0
58	MG	1a	1627	1/1	0.83	0.15	52,52,52,52	0
58	MG	2A	3721	1/1	0.83	0.11	38,38,38,38	0
58	MG	2A	3467	1/1	0.83	0.17	47,47,47,47	0
58	MG	2a	1775	1/1	0.83	0.20	51,51,51,51	0
58	MG	2A	3477	1/1	0.83	0.18	57,57,57,57	0
58	MG	2A	3222	1/1	0.83	0.40	50,50,50,50	0
58	MG	1B	208	1/1	0.83	0.11	64,64,64,64	0
58	MG	1A	3742	1/1	0.83	0.10	32,32,32,32	0
58	MG	2a	1617	1/1	0.83	0.13	54,54,54,54	0
58	MG	2a	1829	1/1	0.83	0.22	53,53,53,53	0
58	MG	2A	3251	1/1	0.83	0.17	61,61,61,61	0
58	MG	2A	3498	1/1	0.83	0.14	65,65,65,65	0
58	MG	1A	3565	1/1	0.83	0.09	57,57,57,57	0
58	MG	2a	1627	1/1	0.83	0.27	53,53,53,53	0
58	MG	2q	203	1/1	0.83	0.16	66,66,66,66	0
58	MG	2t	201	1/1	0.83	0.11	44,44,44,44	0
58	MG	1a	1802	1/1	0.83	0.11	58,58,58,58	0
58	MG	2A	3519	1/1	0.83	0.33	52,52,52,52	0
58	MG	1A	3080	1/1	0.83	0.40	52,52,52,52	0
58	MG	2A	3262	1/1	0.83	0.26	42,42,42,42	0
58	MG	2a	1655	1/1	0.83	0.11	53,53,53,53	0
58	MG	1A	3248	1/1	0.83	0.29	43,43,43,43	0
58	MG	2A	3571	1/1	0.83	0.18	36,36,36,36	0
58	MG	1A	3734	1/1	0.84	0.16	48,48,48,48	0
58	MG	2a	1661	1/1	0.84	0.19	52,52,52,52	0
58	MG	1A	3536	1/1	0.84	0.23	55,55,55,55	0
58	MG	1a	1678	1/1	0.84	0.25	40,40,40,40	0
58	MG	1B	237	1/1	0.84	0.12	36,36,36,36	0
58	MG	1A	4038	1/1	0.84	0.11	35,35,35,35	0
58	MG	1A	3211	1/1	0.84	0.19	59,59,59,59	0
58	MG	2A	3848	1/1	0.84	0.09	53,53,53,53	0
58	MG	2a	1688	1/1	0.84	0.10	60,60,60,60	0
58	MG	2a	1689	1/1	0.84	0.14	60,60,60,60	0
58	MG	2A	3855	1/1	0.84	0.53	71,71,71,71	0
58	MG	1N	202	1/1	0.84	0.20	38,38,38,38	0
58	MG	2A	3863	1/1	0.84	0.16	54,54,54,54	0
58	MG	1O	203	1/1	0.84	0.18	55,55,55,55	0
58	MG	1A	3949	1/1	0.84	0.19	36,36,36,36	0
58	MG	2a	1722	1/1	0.84	0.11	66,66,66,66	0
58	MG	1A	3860	1/1	0.84	0.20	29,29,29,29	0
58	MG	2B	203	1/1	0.84	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1733	1/1	0.84	0.12	54,54,54,54	0
58	MG	2B	205	1/1	0.84	0.12	46,46,46,46	0
58	MG	1A	4044	1/1	0.84	0.07	48,48,48,48	0
58	MG	2A	3223	1/1	0.84	0.10	55,55,55,55	0
58	MG	2A	3224	1/1	0.84	0.12	52,52,52,52	0
58	MG	1A	3020	1/1	0.84	0.22	37,37,37,37	0
58	MG	2B	214	1/1	0.84	0.15	41,41,41,41	0
58	MG	1A	4055	1/1	0.84	0.38	61,61,61,61	0
58	MG	2A	3250	1/1	0.84	0.20	63,63,63,63	0
58	MG	1A	3862	1/1	0.84	0.14	63,63,63,63	0
58	MG	1A	3469	1/1	0.84	0.14	51,51,51,51	0
58	MG	1A	3887	1/1	0.84	0.10	54,54,54,54	0
58	MG	1A	4080	1/1	0.84	0.17	29,29,29,29	0
58	MG	2A	3112	1/1	0.84	0.10	56,56,56,56	0
58	MG	2a	1793	1/1	0.84	0.16	53,53,53,53	0
58	MG	1A	4022	1/1	0.84	0.10	60,60,60,60	0
58	MG	2A	3434	1/1	0.84	0.24	50,50,50,50	0
58	MG	1a	1605	1/1	0.84	0.11	42,42,42,42	0
58	MG	2a	1817	1/1	0.84	0.15	60,60,60,60	0
58	MG	1A	4089	1/1	0.84	0.19	45,45,45,45	0
58	MG	2A	3758	1/1	0.84	0.12	55,55,55,55	0
58	MG	2a	1613	1/1	0.84	0.14	62,62,62,62	0
58	MG	1a	1622	1/1	0.84	0.22	54,54,54,54	0
58	MG	1A	3083	1/1	0.84	0.22	39,39,39,39	0
58	MG	2n	101	1/1	0.84	0.11	61,61,61,61	0
58	MG	1A	4096	1/1	0.84	0.12	52,52,52,52	0
58	MG	2a	1622	1/1	0.84	0.24	76,76,76,76	0
58	MG	1A	3378	1/1	0.84	0.14	36,36,36,36	0
58	MG	1a	1798	1/1	0.84	0.11	65,65,65,65	0
58	MG	1a	1629	1/1	0.84	0.20	50,50,50,50	0
58	MG	1A	3359	1/1	0.84	0.19	48,48,48,48	0
58	MG	1B	215	1/1	0.84	0.19	39,39,39,39	0
58	MG	1A	3567	1/1	0.84	0.35	55,55,55,55	0
58	MG	1A	3836	1/1	0.84	0.16	48,48,48,48	0
58	MG	1a	1671	1/1	0.84	0.17	52,52,52,52	0
58	MG	1A	3613	1/1	0.85	0.20	16,16,16,16	0
58	MG	1A	3294	1/1	0.85	0.15	38,38,38,38	0
58	MG	1A	3633	1/1	0.85	0.12	53,53,53,53	0
58	MG	1a	1681	1/1	0.85	0.16	56,56,56,56	0
58	MG	2A	3473	1/1	0.85	0.27	66,66,66,66	0
58	MG	2A	3162	1/1	0.85	0.34	63,63,63,63	0
58	MG	1T	202	1/1	0.85	0.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3487	1/1	0.85	0.16	58,58,58,58	0
58	MG	2a	1666	1/1	0.85	0.10	60,60,60,60	0
58	MG	1A	3810	1/1	0.85	0.16	46,46,46,46	0
58	MG	2A	3813	1/1	0.85	0.10	52,52,52,52	0
58	MG	2A	3288	1/1	0.85	0.18	61,61,61,61	0
58	MG	1a	1699	1/1	0.85	0.17	49,49,49,49	0
58	MG	1V	204	1/1	0.85	0.22	40,40,40,40	0
58	MG	2A	3505	1/1	0.85	0.12	55,55,55,55	0
58	MG	1x	102	1/1	0.85	0.23	52,52,52,52	0
58	MG	2A	3301	1/1	0.85	0.24	56,56,56,56	0
58	MG	1x	105	1/1	0.85	0.14	53,53,53,53	0
58	MG	2a	1705	1/1	0.85	0.22	48,48,48,48	0
58	MG	1A	3532	1/1	0.85	0.15	37,37,37,37	0
58	MG	1A	3122	1/1	0.85	0.22	30,30,30,30	0
58	MG	1A	3730	1/1	0.85	0.12	59,59,59,59	0
58	MG	1A	3272	1/1	0.85	0.31	37,37,37,37	0
58	MG	1A	3397	1/1	0.85	0.26	45,45,45,45	0
58	MG	2A	3203	1/1	0.85	0.19	57,57,57,57	0
58	MG	1A	3139	1/1	0.85	0.11	50,50,50,50	0
58	MG	2A	3611	1/1	0.85	0.12	63,63,63,63	0
58	MG	2A	3617	1/1	0.85	0.15	23,23,23,23	0
58	MG	2B	202	1/1	0.85	0.17	52,52,52,52	0
58	MG	1A	3667	1/1	0.85	0.16	18,18,18,18	0
58	MG	2A	3621	1/1	0.85	0.21	46,46,46,46	0
58	MG	1A	3868	1/1	0.85	0.23	40,40,40,40	0
58	MG	1A	3772	1/1	0.85	0.14	26,26,26,26	0
58	MG	2a	1764	1/1	0.85	0.12	53,53,53,53	0
58	MG	2A	3073	1/1	0.85	0.17	39,39,39,39	0
58	MG	2A	3632	1/1	0.85	0.10	42,42,42,42	0
58	MG	2A	3641	1/1	0.85	0.13	35,35,35,35	0
58	MG	2A	3660	1/1	0.85	0.07	66,66,66,66	0
58	MG	1B	226	1/1	0.85	0.20	54,54,54,54	0
58	MG	2E	303	1/1	0.85	0.12	59,59,59,59	0
58	MG	2E	306	1/1	0.85	0.15	29,29,29,29	0
58	MG	1A	3779	1/1	0.85	0.07	59,59,59,59	0
58	MG	2F	303	1/1	0.85	0.16	48,48,48,48	0
58	MG	1a	1764	1/1	0.85	0.12	61,61,61,61	0
58	MG	1A	4035	1/1	0.85	0.15	40,40,40,40	0
58	MG	1A	3783	1/1	0.85	0.19	54,54,54,54	0
58	MG	2A	3684	1/1	0.85	0.12	53,53,53,53	0
58	MG	2A	3697	1/1	0.85	0.15	53,53,53,53	0
58	MG	2d	301	1/1	0.85	0.28	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3246	1/1	0.85	0.24	64,64,64,64	0
58	MG	2A	3247	1/1	0.85	0.14	68,68,68,68	0
58	MG	1A	3373	1/1	0.85	0.15	43,43,43,43	0
58	MG	2A	3704	1/1	0.85	0.17	69,69,69,69	0
58	MG	1A	3789	1/1	0.85	0.11	38,38,38,38	0
58	MG	2A	3710	1/1	0.85	0.26	55,55,55,55	0
58	MG	1A	3987	1/1	0.85	0.22	58,58,58,58	0
58	MG	1A	3681	1/1	0.85	0.13	15,15,15,15	0
58	MG	1a	1669	1/1	0.85	0.14	57,57,57,57	0
58	MG	1A	3989	1/1	0.85	0.22	46,46,46,46	0
58	MG	2A	3135	1/1	0.85	0.13	25,25,25,25	0
58	MG	2A	3747	1/1	0.85	0.14	57,57,57,57	0
58	MG	2a	1628	1/1	0.85	0.34	57,57,57,57	0
58	MG	1A	3775	1/1	0.86	0.17	39,39,39,39	0
58	MG	1a	1704	1/1	0.86	0.22	60,60,60,60	0
58	MG	2a	1609	1/1	0.86	0.25	51,51,51,51	0
58	MG	1A	3777	1/1	0.86	0.17	18,18,18,18	0
58	MG	2a	1611	1/1	0.86	0.18	64,64,64,64	0
58	MG	1A	3151	1/1	0.86	0.20	30,30,30,30	0
58	MG	2A	3656	1/1	0.86	0.23	54,54,54,54	0
58	MG	2A	3090	1/1	0.86	0.12	61,61,61,61	0
58	MG	1a	1712	1/1	0.86	0.17	51,51,51,51	0
58	MG	2A	3305	1/1	0.86	0.18	58,58,58,58	0
58	MG	2a	1619	1/1	0.86	0.15	54,54,54,54	0
58	MG	2a	1621	1/1	0.86	0.16	58,58,58,58	0
58	MG	2A	3673	1/1	0.86	0.14	61,61,61,61	0
58	MG	1R	202	1/1	0.86	0.15	26,26,26,26	0
58	MG	1A	3275	1/1	0.86	0.16	44,44,44,44	0
58	MG	1A	3208	1/1	0.86	0.15	44,44,44,44	0
58	MG	1a	1736	1/1	0.86	0.14	46,46,46,46	0
58	MG	1A	3443	1/1	0.86	0.13	51,51,51,51	0
58	MG	2a	1640	1/1	0.86	0.21	48,48,48,48	0
58	MG	2A	3320	1/1	0.86	0.31	48,48,48,48	0
58	MG	1T	204	1/1	0.86	0.14	40,40,40,40	0
58	MG	1A	3552	1/1	0.86	0.18	51,51,51,51	0
58	MG	2A	3335	1/1	0.86	0.24	44,44,44,44	0
58	MG	2a	1657	1/1	0.86	0.13	68,68,68,68	0
58	MG	2A	3131	1/1	0.86	0.09	48,48,48,48	0
58	MG	1A	3256	1/1	0.86	0.25	45,45,45,45	0
58	MG	2a	1664	1/1	0.86	0.13	59,59,59,59	0
58	MG	1A	3674	1/1	0.86	0.14	26,26,26,26	0
58	MG	1a	1755	1/1	0.86	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	10	105	1/1	0.86	0.21	47,47,47,47	0
58	MG	1A	3327	1/1	0.86	0.24	35,35,35,35	0
58	MG	2A	3743	1/1	0.86	0.22	46,46,46,46	0
58	MG	11	104	1/1	0.86	0.10	31,31,31,31	0
58	MG	1A	3460	1/1	0.86	0.21	46,46,46,46	0
58	MG	1A	3700	1/1	0.86	0.15	54,54,54,54	0
58	MG	1A	3296	1/1	0.86	0.20	46,46,46,46	0
58	MG	2a	1690	1/1	0.86	0.19	50,50,50,50	0
58	MG	2a	1692	1/1	0.86	0.18	48,48,48,48	0
58	MG	2A	3780	1/1	0.86	0.16	45,45,45,45	0
58	MG	1a	1775	1/1	0.86	0.14	65,65,65,65	0
58	MG	2A	3374	1/1	0.86	0.21	45,45,45,45	0
58	MG	1A	3846	1/1	0.86	0.16	46,46,46,46	0
58	MG	2A	3383	1/1	0.86	0.11	61,61,61,61	0
58	MG	2a	1717	1/1	0.86	0.28	57,57,57,57	0
58	MG	1A	3297	1/1	0.86	0.11	51,51,51,51	0
58	MG	1a	1606	1/1	0.86	0.16	47,47,47,47	0
58	MG	1a	1796	1/1	0.86	0.18	46,46,46,46	0
58	MG	1A	3404	1/1	0.86	0.16	41,41,41,41	0
58	MG	2A	3408	1/1	0.86	0.29	53,53,53,53	0
58	MG	2a	1738	1/1	0.86	0.11	62,62,62,62	0
58	MG	2A	3821	1/1	0.86	0.16	31,31,31,31	0
58	MG	1A	3337	1/1	0.86	0.21	49,49,49,49	0
58	MG	2a	1750	1/1	0.86	0.08	51,51,51,51	0
58	MG	1A	3727	1/1	0.86	0.17	39,39,39,39	0
58	MG	2a	1756	1/1	0.86	0.13	65,65,65,65	0
58	MG	1A	3604	1/1	0.86	0.20	42,42,42,42	0
58	MG	1a	1807	1/1	0.86	0.07	51,51,51,51	0
58	MG	1A	3492	1/1	0.86	0.17	43,43,43,43	0
58	MG	2A	3460	1/1	0.86	0.23	51,51,51,51	0
58	MG	1A	3301	1/1	0.86	0.43	54,54,54,54	0
58	MG	1a	1813	1/1	0.86	0.14	53,53,53,53	0
58	MG	1f	202	1/1	0.86	0.28	58,58,58,58	0
58	MG	2A	3851	1/1	0.86	0.14	43,43,43,43	0
58	MG	2A	3216	1/1	0.86	0.20	37,37,37,37	0
58	MG	2A	3484	1/1	0.86	0.14	49,49,49,49	0
58	MG	2A	3220	1/1	0.86	0.17	51,51,51,51	0
58	MG	2a	1788	1/1	0.86	0.17	57,57,57,57	0
58	MG	2a	1790	1/1	0.86	0.25	59,59,59,59	0
58	MG	1A	4097	1/1	0.86	0.19	49,49,49,49	0
58	MG	1A	3884	1/1	0.86	0.17	38,38,38,38	0
58	MG	2A	3494	1/1	0.86	0.13	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1805	1/1	0.86	0.22	56,56,56,56	0
58	MG	1a	1650	1/1	0.86	0.16	49,49,49,49	0
58	MG	2a	1816	1/1	0.86	0.23	56,56,56,56	0
58	MG	1A	3360	1/1	0.86	0.21	65,65,65,65	0
58	MG	1A	3998	1/1	0.86	0.12	43,43,43,43	0
58	MG	2A	3001	1/1	0.86	0.38	51,51,51,51	0
58	MG	2A	3004	1/1	0.86	0.36	35,35,35,35	0
58	MG	1A	3746	1/1	0.86	0.14	42,42,42,42	0
58	MG	1A	3899	1/1	0.86	0.18	40,40,40,40	0
58	MG	1A	3509	1/1	0.86	0.18	55,55,55,55	0
58	MG	1A	4017	1/1	0.86	0.07	38,38,38,38	0
58	MG	1B	230	1/1	0.86	0.14	75,75,75,75	0
58	MG	2A	3044	1/1	0.86	0.23	51,51,51,51	0
58	MG	1A	4021	1/1	0.86	0.12	65,65,65,65	0
58	MG	2A	3054	1/1	0.86	0.14	49,49,49,49	0
58	MG	1A	3760	1/1	0.86	0.14	47,47,47,47	0
58	MG	2w	103	1/1	0.86	0.14	54,54,54,54	0
58	MG	2A	3063	1/1	0.86	0.29	50,50,50,50	0
58	MG	2A	3064	1/1	0.86	0.19	56,56,56,56	0
58	MG	1A	3019	1/1	0.86	0.26	36,36,36,36	0
58	MG	1A	3932	1/1	0.86	0.18	22,22,22,22	0
58	MG	2A	3285	1/1	0.86	0.39	61,61,61,61	0
58	MG	1A	3766	1/1	0.87	0.18	19,19,19,19	0
58	MG	2A	3442	1/1	0.87	0.10	55,55,55,55	0
58	MG	2A	3106	1/1	0.87	0.10	42,42,42,42	0
58	MG	2A	3759	1/1	0.87	0.18	51,51,51,51	0
58	MG	1a	1797	1/1	0.87	0.16	44,44,44,44	0
58	MG	2A	3457	1/1	0.87	0.26	44,44,44,44	0
58	MG	1A	4042	1/1	0.87	0.15	32,32,32,32	0
58	MG	2A	3462	1/1	0.87	0.28	44,44,44,44	0
58	MG	1A	3323	1/1	0.87	0.13	32,32,32,32	0
58	MG	1A	4048	1/1	0.87	0.22	19,19,19,19	0
58	MG	2A	3468	1/1	0.87	0.34	50,50,50,50	0
58	MG	1A	3156	1/1	0.87	0.18	38,38,38,38	0
58	MG	2A	3271	1/1	0.87	0.23	54,54,54,54	0
58	MG	2A	3481	1/1	0.87	0.20	54,54,54,54	0
58	MG	1A	3498	1/1	0.87	0.23	44,44,44,44	0
58	MG	1a	1690	1/1	0.87	0.26	45,45,45,45	0
58	MG	1A	4059	1/1	0.87	0.18	43,43,43,43	0
58	MG	2A	3140	1/1	0.87	0.19	34,34,34,34	0
58	MG	2A	3490	1/1	0.87	0.24	69,69,69,69	0
58	MG	1a	1812	1/1	0.87	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3898	1/1	0.87	0.19	30,30,30,30	0
58	MG	1e	202	1/1	0.87	0.15	42,42,42,42	0
58	MG	1A	3676	1/1	0.87	0.12	25,25,25,25	0
58	MG	2A	3841	1/1	0.87	0.33	64,64,64,64	0
58	MG	2A	3295	1/1	0.87	0.22	57,57,57,57	0
58	MG	2a	1720	1/1	0.87	0.10	51,51,51,51	0
58	MG	2A	3507	1/1	0.87	0.13	56,56,56,56	0
58	MG	1A	3910	1/1	0.87	0.11	46,46,46,46	0
58	MG	1A	3217	1/1	0.87	0.22	49,49,49,49	0
58	MG	2a	1728	1/1	0.87	0.19	47,47,47,47	0
58	MG	1A	3086	1/1	0.87	0.35	27,27,27,27	0
58	MG	1A	3092	1/1	0.87	0.18	47,47,47,47	0
58	MG	2A	3308	1/1	0.87	0.27	62,62,62,62	0
58	MG	2A	3866	1/1	0.87	0.18	64,64,64,64	0
58	MG	1A	4091	1/1	0.87	0.12	59,59,59,59	0
58	MG	1a	1716	1/1	0.87	0.19	59,59,59,59	0
58	MG	2a	1751	1/1	0.87	0.09	66,66,66,66	0
58	MG	1A	3510	1/1	0.87	0.18	38,38,38,38	0
58	MG	1A	3715	1/1	0.87	0.20	33,33,33,33	0
58	MG	1A	3795	1/1	0.87	0.14	37,37,37,37	0
58	MG	1A	3524	1/1	0.87	0.21	41,41,41,41	0
58	MG	1A	3525	1/1	0.87	0.14	59,59,59,59	0
58	MG	2A	3199	1/1	0.87	0.19	45,45,45,45	0
58	MG	1A	3353	1/1	0.87	0.29	61,61,61,61	0
58	MG	2A	3339	1/1	0.87	0.14	52,52,52,52	0
58	MG	2B	215	1/1	0.87	0.22	56,56,56,56	0
58	MG	1A	3835	1/1	0.87	0.15	43,43,43,43	0
58	MG	2A	3045	1/1	0.87	0.27	51,51,51,51	0
58	MG	1A	3313	1/1	0.87	0.19	36,36,36,36	0
58	MG	2A	3637	1/1	0.87	0.21	49,49,49,49	0
58	MG	1a	1750	1/1	0.87	0.15	69,69,69,69	0
58	MG	2A	3646	1/1	0.87	0.21	43,43,43,43	0
58	MG	2A	3055	1/1	0.87	0.31	57,57,57,57	0
58	MG	2a	1796	1/1	0.87	0.24	64,64,64,64	0
58	MG	1A	3635	1/1	0.87	0.08	41,41,41,41	0
58	MG	1A	3097	1/1	0.87	0.16	34,34,34,34	0
58	MG	1A	3740	1/1	0.87	0.19	61,61,61,61	0
58	MG	28	101	1/1	0.87	0.30	53,53,53,53	0
58	MG	2a	1814	1/1	0.87	0.14	61,61,61,61	0
58	MG	1A	3639	1/1	0.87	0.10	21,21,21,21	0
58	MG	2A	3367	1/1	0.87	0.27	52,52,52,52	0
58	MG	1A	3464	1/1	0.87	0.37	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3225	1/1	0.87	0.28	37,37,37,37	0
58	MG	1a	1648	1/1	0.87	0.18	44,44,44,44	0
58	MG	2A	3693	1/1	0.87	0.11	52,52,52,52	0
58	MG	2A	3240	1/1	0.87	0.13	51,51,51,51	0
58	MG	1A	3150	1/1	0.87	0.21	29,29,29,29	0
58	MG	1a	1654	1/1	0.87	0.18	55,55,55,55	0
58	MG	2n	102	1/1	0.87	0.22	70,70,70,70	0
58	MG	1E	306	1/1	0.87	0.14	42,42,42,42	0
58	MG	1a	1785	1/1	0.87	0.14	40,40,40,40	0
58	MG	2A	3400	1/1	0.87	0.14	60,60,60,60	0
58	MG	1A	3413	1/1	0.87	0.12	52,52,52,52	0
58	MG	1A	3059	1/1	0.87	0.22	31,31,31,31	0
58	MG	2A	3421	1/1	0.87	0.23	65,65,65,65	0
58	MG	2A	3422	1/1	0.87	0.23	32,32,32,32	0
58	MG	2A	3730	1/1	0.87	0.11	35,35,35,35	0
58	MG	2A	3256	1/1	0.87	0.14	39,39,39,39	0
58	MG	2A	3742	1/1	0.87	0.08	53,53,53,53	0
58	MG	2A	3425	1/1	0.87	0.31	51,51,51,51	0
60	ZN	2n	103	1/1	0.87	0.04	82,82,82,82	0
58	MG	1A	3290	1/1	0.88	0.19	34,34,34,34	0
58	MG	2A	3415	1/1	0.88	0.23	47,47,47,47	0
58	MG	2A	3716	1/1	0.88	0.16	29,29,29,29	0
58	MG	2A	3419	1/1	0.88	0.38	44,44,44,44	0
58	MG	1A	3237	1/1	0.88	0.36	33,33,33,33	0
58	MG	1A	3852	1/1	0.88	0.16	41,41,41,41	0
58	MG	1A	4031	1/1	0.88	0.10	41,41,41,41	0
58	MG	2A	3733	1/1	0.88	0.19	51,51,51,51	0
58	MG	2A	3085	1/1	0.88	0.37	41,41,41,41	0
58	MG	1a	1640	1/1	0.88	0.23	53,53,53,53	0
58	MG	2a	1644	1/1	0.88	0.14	57,57,57,57	0
58	MG	2A	3091	1/1	0.88	0.20	58,58,58,58	0
58	MG	1A	3473	1/1	0.88	0.41	54,54,54,54	0
58	MG	1A	3754	1/1	0.88	0.16	49,49,49,49	0
58	MG	2A	3750	1/1	0.88	0.18	33,33,33,33	0
58	MG	2a	1660	1/1	0.88	0.50	55,55,55,55	0
58	MG	1A	3387	1/1	0.88	0.22	46,46,46,46	0
58	MG	1A	3482	1/1	0.88	0.14	35,35,35,35	0
58	MG	1A	3487	1/1	0.88	0.13	33,33,33,33	0
58	MG	2A	3770	1/1	0.88	0.11	44,44,44,44	0
58	MG	2A	3114	1/1	0.88	0.18	61,61,61,61	0
58	MG	1F	305	1/1	0.88	0.16	36,36,36,36	0
58	MG	2a	1676	1/1	0.88	0.20	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3967	1/1	0.88	0.11	25,25,25,25	0
58	MG	1A	3970	1/1	0.88	0.19	39,39,39,39	0
58	MG	1A	3559	1/1	0.88	0.20	37,37,37,37	0
58	MG	2A	3479	1/1	0.88	0.18	63,63,63,63	0
58	MG	2A	3805	1/1	0.88	0.19	48,48,48,48	0
58	MG	1Q	207	1/1	0.88	0.16	39,39,39,39	0
58	MG	1a	1806	1/1	0.88	0.10	47,47,47,47	0
58	MG	1A	3186	1/1	0.88	0.11	55,55,55,55	0
58	MG	2A	3139	1/1	0.88	0.10	50,50,50,50	0
58	MG	1A	3322	1/1	0.88	0.23	51,51,51,51	0
58	MG	2a	1709	1/1	0.88	0.14	56,56,56,56	0
58	MG	2A	3144	1/1	0.88	0.26	40,40,40,40	0
58	MG	2A	3149	1/1	0.88	0.20	49,49,49,49	0
58	MG	2a	1714	1/1	0.88	0.18	47,47,47,47	0
58	MG	2a	1715	1/1	0.88	0.24	54,54,54,54	0
58	MG	2A	3299	1/1	0.88	0.22	60,60,60,60	0
58	MG	1A	3985	1/1	0.88	0.08	33,33,33,33	0
58	MG	1A	3452	1/1	0.88	0.20	41,41,41,41	0
58	MG	2A	3306	1/1	0.88	0.17	49,49,49,49	0
58	MG	1A	3578	1/1	0.88	0.22	36,36,36,36	0
58	MG	1A	3343	1/1	0.88	0.27	49,49,49,49	0
58	MG	1A	3906	1/1	0.88	0.10	38,38,38,38	0
58	MG	2a	1732	1/1	0.88	0.10	62,62,62,62	0
58	MG	1A	3597	1/1	0.88	0.28	46,46,46,46	0
58	MG	2A	3315	1/1	0.88	0.13	62,62,62,62	0
58	MG	1n	101	1/1	0.88	0.21	53,53,53,53	0
58	MG	2A	3860	1/1	0.88	0.27	68,68,68,68	0
58	MG	1A	3456	1/1	0.88	0.22	41,41,41,41	0
58	MG	1A	3005	1/1	0.88	0.23	35,35,35,35	0
58	MG	2A	3573	1/1	0.88	0.12	36,36,36,36	0
58	MG	2a	1753	1/1	0.88	0.17	58,58,58,58	0
58	MG	2A	3185	1/1	0.88	0.09	49,49,49,49	0
58	MG	1x	101	1/1	0.88	0.29	56,56,56,56	0
58	MG	1a	1711	1/1	0.88	0.17	38,38,38,38	0
58	MG	10	108	1/1	0.88	0.21	42,42,42,42	0
58	MG	2A	3612	1/1	0.88	0.17	51,51,51,51	0
58	MG	1A	3511	1/1	0.88	0.27	40,40,40,40	0
58	MG	1A	3412	1/1	0.88	0.27	51,51,51,51	0
58	MG	1A	3462	1/1	0.88	0.26	42,42,42,42	0
58	MG	2A	3346	1/1	0.88	0.32	56,56,56,56	0
58	MG	1a	1725	1/1	0.88	0.14	56,56,56,56	0
58	MG	1a	1729	1/1	0.88	0.19	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	18	106	1/1	0.88	0.12	47,47,47,47	0
58	MG	2A	3633	1/1	0.88	0.24	32,32,32,32	0
58	MG	1A	4013	1/1	0.88	0.08	22,22,22,22	0
58	MG	1A	3528	1/1	0.88	0.21	57,57,57,57	0
58	MG	1a	1601	1/1	0.88	0.13	49,49,49,49	0
58	MG	2A	3655	1/1	0.88	0.20	34,34,34,34	0
58	MG	2F	301	1/1	0.88	0.14	40,40,40,40	0
58	MG	2A	3214	1/1	0.88	0.13	65,65,65,65	0
58	MG	2F	305	1/1	0.88	0.24	46,46,46,46	0
58	MG	2A	3362	1/1	0.88	0.15	48,48,48,48	0
58	MG	2Q	202	1/1	0.88	0.25	52,52,52,52	0
58	MG	2U	202	1/1	0.88	0.19	45,45,45,45	0
58	MG	2W	204	1/1	0.88	0.25	53,53,53,53	0
58	MG	2A	3365	1/1	0.88	0.18	64,64,64,64	0
58	MG	20	102	1/1	0.88	0.13	50,50,50,50	0
58	MG	23	103	1/1	0.88	0.13	41,41,41,41	0
58	MG	1a	1603	1/1	0.88	0.15	51,51,51,51	0
58	MG	2A	3052	1/1	0.88	0.16	39,39,39,39	0
58	MG	1A	3816	1/1	0.88	0.17	49,49,49,49	0
58	MG	2A	3221	1/1	0.88	0.34	42,42,42,42	0
58	MG	2a	1605	1/1	0.88	0.25	59,59,59,59	0
58	MG	1A	3376	1/1	0.88	0.23	27,27,27,27	0
58	MG	2A	3387	1/1	0.88	0.20	55,55,55,55	0
58	MG	2A	3691	1/1	0.88	0.36	51,51,51,51	0
58	MG	2A	3058	1/1	0.88	0.25	55,55,55,55	0
58	MG	2A	3694	1/1	0.88	0.15	40,40,40,40	0
58	MG	1a	1617	1/1	0.88	0.14	37,37,37,37	0
58	MG	1A	3739	1/1	0.88	0.14	12,12,12,12	0
58	MG	1B	222	1/1	0.88	0.21	40,40,40,40	0
58	MG	1a	1761	1/1	0.88	0.09	50,50,50,50	0
58	MG	1A	3354	1/1	0.88	0.22	49,49,49,49	0
58	MG	2A	3705	1/1	0.88	0.18	46,46,46,46	0
58	MG	1A	3703	1/1	0.89	0.15	41,41,41,41	0
58	MG	2A	3096	1/1	0.89	0.21	49,49,49,49	0
58	MG	1a	1784	1/1	0.89	0.13	47,47,47,47	0
58	MG	2A	3718	1/1	0.89	0.22	57,57,57,57	0
58	MG	1O	201	1/1	0.89	0.40	55,55,55,55	0
58	MG	1A	3465	1/1	0.89	0.22	53,53,53,53	0
58	MG	2A	3429	1/1	0.89	0.41	56,56,56,56	0
58	MG	2A	3732	1/1	0.89	0.19	55,55,55,55	0
58	MG	2A	3432	1/1	0.89	0.26	48,48,48,48	0
58	MG	1A	3903	1/1	0.89	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3436	1/1	0.89	0.20	46,46,46,46	0
58	MG	2A	3438	1/1	0.89	0.27	55,55,55,55	0
58	MG	2A	3108	1/1	0.89	0.14	38,38,38,38	0
58	MG	2A	3111	1/1	0.89	0.14	35,35,35,35	0
58	MG	2A	3449	1/1	0.89	0.32	45,45,45,45	0
58	MG	2A	3756	1/1	0.89	0.14	37,37,37,37	0
58	MG	1A	3125	1/1	0.89	0.25	31,31,31,31	0
58	MG	2a	1658	1/1	0.89	0.09	67,67,67,67	0
58	MG	1A	3793	1/1	0.89	0.22	30,30,30,30	0
58	MG	1A	3716	1/1	0.89	0.11	38,38,38,38	0
58	MG	1A	3433	1/1	0.89	0.14	54,54,54,54	0
58	MG	1A	4070	1/1	0.89	0.19	19,19,19,19	0
58	MG	2A	3781	1/1	0.89	0.20	62,62,62,62	0
58	MG	1A	3611	1/1	0.89	0.14	24,24,24,24	0
58	MG	1a	1682	1/1	0.89	0.12	55,55,55,55	0
58	MG	1a	1686	1/1	0.89	0.22	53,53,53,53	0
58	MG	1A	3930	1/1	0.89	0.12	38,38,38,38	0
58	MG	1A	3183	1/1	0.89	0.17	30,30,30,30	0
58	MG	2A	3804	1/1	0.89	0.19	66,66,66,66	0
58	MG	1A	3146	1/1	0.89	0.14	35,35,35,35	0
58	MG	1a	1697	1/1	0.89	0.24	46,46,46,46	0
58	MG	2A	3145	1/1	0.89	0.15	58,58,58,58	0
58	MG	2A	3809	1/1	0.89	0.12	46,46,46,46	0
58	MG	2A	3812	1/1	0.89	0.25	24,24,24,24	0
58	MG	1A	3632	1/1	0.89	0.16	38,38,38,38	0
58	MG	1A	3943	1/1	0.89	0.12	51,51,51,51	0
58	MG	1A	3477	1/1	0.89	0.15	40,40,40,40	0
58	MG	1a	1705	1/1	0.89	0.16	57,57,57,57	0
58	MG	1A	3398	1/1	0.89	0.23	49,49,49,49	0
58	MG	1w	107	1/1	0.89	0.16	40,40,40,40	0
58	MG	12	101	1/1	0.89	0.24	44,44,44,44	0
58	MG	2A	3501	1/1	0.89	0.24	52,52,52,52	0
58	MG	12	103	1/1	0.89	0.27	34,34,34,34	0
58	MG	2A	3314	1/1	0.89	0.13	45,45,45,45	0
58	MG	1A	4098	1/1	0.89	0.15	39,39,39,39	0
58	MG	1x	103	1/1	0.89	0.16	53,53,53,53	0
58	MG	2A	3847	1/1	0.89	0.23	37,37,37,37	0
58	MG	2a	1725	1/1	0.89	0.23	68,68,68,68	0
58	MG	2A	3181	1/1	0.89	0.12	37,37,37,37	0
58	MG	2A	3319	1/1	0.89	0.23	59,59,59,59	0
58	MG	1x	104	1/1	0.89	0.14	59,59,59,59	0
58	MG	2A	3856	1/1	0.89	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
58	MG	2a	1735	1/1	0.89	0.40	56,56,56,56	0
58	MG	1A	3446	1/1	0.89	0.13	52,52,52,52	0
58	MG	1A	3093	1/1	0.89	0.11	37,37,37,37	0
58	MG	1A	3249	1/1	0.89	0.54	51,51,51,51	0
58	MG	2A	3579	1/1	0.89	0.26	54,54,54,54	0
58	MG	1A	3495	1/1	0.89	0.29	32,32,32,32	0
58	MG	1A	3370	1/1	0.89	0.24	41,41,41,41	0
58	MG	2A	3603	1/1	0.89	0.18	55,55,55,55	0
58	MG	2A	3340	1/1	0.89	0.16	49,49,49,49	0
58	MG	1a	1732	1/1	0.89	0.07	43,43,43,43	0
58	MG	2A	3197	1/1	0.89	0.24	52,52,52,52	0
58	MG	1a	1602	1/1	0.89	0.09	59,59,59,59	0
58	MG	2A	3347	1/1	0.89	0.13	57,57,57,57	0
58	MG	1A	3457	1/1	0.89	0.23	59,59,59,59	0
58	MG	1A	3338	1/1	0.89	0.25	45,45,45,45	0
58	MG	1A	3507	1/1	0.89	0.16	39,39,39,39	0
58	MG	1a	1613	1/1	0.89	0.10	56,56,56,56	0
58	MG	1a	1615	1/1	0.89	0.10	47,47,47,47	0
58	MG	2D	304	1/1	0.89	0.20	53,53,53,53	0
58	MG	2D	306	1/1	0.89	0.22	29,29,29,29	0
58	MG	1A	3250	1/1	0.89	0.12	50,50,50,50	0
58	MG	2A	3635	1/1	0.89	0.17	37,37,37,37	0
58	MG	1a	1748	1/1	0.89	0.07	43,43,43,43	0
58	MG	1a	1749	1/1	0.89	0.13	44,44,44,44	0
58	MG	2a	1798	1/1	0.89	0.18	47,47,47,47	0
58	MG	1A	3869	1/1	0.89	0.14	39,39,39,39	0
58	MG	2F	302	1/1	0.89	0.30	53,53,53,53	0
58	MG	1a	1754	1/1	0.89	0.12	42,42,42,42	0
58	MG	1B	233	1/1	0.89	0.14	41,41,41,41	0
58	MG	2A	3372	1/1	0.89	0.15	43,43,43,43	0
58	MG	2A	3663	1/1	0.89	0.11	51,51,51,51	0
58	MG	2U	201	1/1	0.89	0.34	45,45,45,45	0
58	MG	2a	1823	1/1	0.89	0.26	59,59,59,59	0
58	MG	2A	3373	1/1	0.89	0.16	66,66,66,66	0
58	MG	1B	236	1/1	0.89	0.13	34,34,34,34	0
58	MG	1A	3582	1/1	0.89	0.17	26,26,26,26	0
58	MG	2X	102	1/1	0.89	0.12	47,47,47,47	0
58	MG	2A	3380	1/1	0.89	0.15	43,43,43,43	0
58	MG	1A	3968	1/1	0.89	0.10	55,55,55,55	0
58	MG	25	101	1/1	0.89	0.17	57,57,57,57	0
58	MG	1A	3201	1/1	0.89	0.17	39,39,39,39	0
58	MG	2A	3228	1/1	0.89	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3687	1/1	0.89	0.18	53,53,53,53	0
58	MG	2A	3393	1/1	0.89	0.11	59,59,59,59	0
58	MG	2A	3077	1/1	0.89	0.11	36,36,36,36	0
58	MG	1A	3223	1/1	0.89	0.19	30,30,30,30	0
58	MG	2A	3244	1/1	0.89	0.14	41,41,41,41	0
58	MG	1A	3601	1/1	0.89	0.36	57,57,57,57	0
58	MG	2A	3405	1/1	0.89	0.11	63,63,63,63	0
58	MG	1F	314	1/1	0.89	0.15	43,43,43,43	0
58	MG	2A	3249	1/1	0.89	0.11	64,64,64,64	0
58	MG	1G	203	1/1	0.89	0.12	57,57,57,57	0
58	MG	2A	3417	1/1	0.89	0.28	34,34,34,34	0
58	MG	1A	3741	1/1	0.90	0.19	44,44,44,44	0
58	MG	27	102	1/1	0.90	0.28	36,36,36,36	0
58	MG	1a	1653	1/1	0.90	0.10	39,39,39,39	0
58	MG	29	101	1/1	0.90	0.10	60,60,60,60	0
58	MG	1A	3871	1/1	0.90	0.17	47,47,47,47	0
58	MG	2A	3179	1/1	0.90	0.27	50,50,50,50	0
58	MG	1a	1656	1/1	0.90	0.11	44,44,44,44	0
58	MG	1a	1657	1/1	0.90	0.26	49,49,49,49	0
58	MG	1A	3391	1/1	0.90	0.11	15,15,15,15	0
58	MG	1f	201	1/1	0.90	0.28	42,42,42,42	0
58	MG	1A	3878	1/1	0.90	0.23	20,20,20,20	0
58	MG	2A	3686	1/1	0.90	0.19	46,46,46,46	0
58	MG	1a	1663	1/1	0.90	0.10	57,57,57,57	0
58	MG	1m	3001	1/1	0.90	0.08	51,51,51,51	0
58	MG	1A	3880	1/1	0.90	0.14	24,24,24,24	0
58	MG	1A	3259	1/1	0.90	0.19	59,59,59,59	0
58	MG	1A	4007	1/1	0.90	0.24	60,60,60,60	0
58	MG	2A	3385	1/1	0.90	0.23	46,46,46,46	0
58	MG	2A	3701	1/1	0.90	0.11	53,53,53,53	0
58	MG	2A	3201	1/1	0.90	0.32	55,55,55,55	0
58	MG	1A	3885	1/1	0.90	0.17	26,26,26,26	0
58	MG	1a	1675	1/1	0.90	0.16	52,52,52,52	0
58	MG	1E	301	1/1	0.90	0.22	55,55,55,55	0
58	MG	1A	3199	1/1	0.90	0.16	36,36,36,36	0
58	MG	1E	309	1/1	0.90	0.17	19,19,19,19	0
58	MG	1A	3403	1/1	0.90	0.19	24,24,24,24	0
58	MG	1A	3891	1/1	0.90	0.16	22,22,22,22	0
58	MG	1A	3896	1/1	0.90	0.15	37,37,37,37	0
58	MG	1a	1693	1/1	0.90	0.17	46,46,46,46	0
58	MG	2a	1650	1/1	0.90	0.18	60,60,60,60	0
58	MG	1A	3530	1/1	0.90	0.21	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3027	1/1	0.90	0.14	33,33,33,33	0
58	MG	1A	3311	1/1	0.90	0.14	35,35,35,35	0
58	MG	2A	3037	1/1	0.90	0.18	53,53,53,53	0
58	MG	1A	3765	1/1	0.90	0.25	40,40,40,40	0
58	MG	1A	3025	1/1	0.90	0.15	22,22,22,22	0
58	MG	2A	3043	1/1	0.90	0.31	51,51,51,51	0
58	MG	2A	3426	1/1	0.90	0.27	51,51,51,51	0
58	MG	2A	3427	1/1	0.90	0.37	53,53,53,53	0
58	MG	1A	3767	1/1	0.90	0.12	40,40,40,40	0
58	MG	1Q	206	1/1	0.90	0.16	37,37,37,37	0
58	MG	2a	1673	1/1	0.90	0.18	48,48,48,48	0
58	MG	2a	1674	1/1	0.90	0.10	51,51,51,51	0
58	MG	1A	3537	1/1	0.90	0.27	40,40,40,40	0
58	MG	1A	3648	1/1	0.90	0.13	13,13,13,13	0
58	MG	1A	3358	1/1	0.90	0.16	34,34,34,34	0
58	MG	2a	1685	1/1	0.90	0.11	52,52,52,52	0
58	MG	1A	3541	1/1	0.90	0.18	44,44,44,44	0
58	MG	2A	3773	1/1	0.90	0.25	44,44,44,44	0
58	MG	1A	3167	1/1	0.90	0.17	49,49,49,49	0
58	MG	2A	3446	1/1	0.90	0.49	55,55,55,55	0
58	MG	2a	1691	1/1	0.90	0.19	51,51,51,51	0
58	MG	2A	3782	1/1	0.90	0.24	43,43,43,43	0
58	MG	2A	3786	1/1	0.90	0.17	50,50,50,50	0
58	MG	1A	4037	1/1	0.90	0.08	33,33,33,33	0
58	MG	1a	1720	1/1	0.90	0.14	53,53,53,53	0
58	MG	2A	3456	1/1	0.90	0.20	43,43,43,43	0
58	MG	1A	3276	1/1	0.90	0.12	20,20,20,20	0
58	MG	2A	3258	1/1	0.90	0.24	38,38,38,38	0
58	MG	2A	3801	1/1	0.90	0.10	57,57,57,57	0
58	MG	2A	3802	1/1	0.90	0.16	58,58,58,58	0
58	MG	2a	1716	1/1	0.90	0.32	51,51,51,51	0
58	MG	1A	3786	1/1	0.90	0.15	14,14,14,14	0
58	MG	2A	3066	1/1	0.90	0.15	54,54,54,54	0
58	MG	2A	3464	1/1	0.90	0.11	49,49,49,49	0
58	MG	1A	3941	1/1	0.90	0.14	27,27,27,27	0
58	MG	1A	3062	1/1	0.90	0.10	36,36,36,36	0
58	MG	2A	3469	1/1	0.90	0.26	61,61,61,61	0
58	MG	2a	1726	1/1	0.90	0.18	43,43,43,43	0
58	MG	1A	3474	1/1	0.90	0.31	37,37,37,37	0
58	MG	1A	4043	1/1	0.90	0.23	42,42,42,42	0
58	MG	2A	3817	1/1	0.90	0.16	26,26,26,26	0
58	MG	2A	3269	1/1	0.90	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3280	1/1	0.90	0.20	28,28,28,28	0
58	MG	2A	3082	1/1	0.90	0.19	53,53,53,53	0
58	MG	2A	3278	1/1	0.90	0.27	46,46,46,46	0
58	MG	2a	1743	1/1	0.90	0.29	43,43,43,43	0
58	MG	1A	4047	1/1	0.90	0.28	32,32,32,32	0
58	MG	1A	3029	1/1	0.90	0.17	33,33,33,33	0
58	MG	1A	4050	1/1	0.90	0.12	34,34,34,34	0
58	MG	2A	3492	1/1	0.90	0.27	51,51,51,51	0
58	MG	1A	3687	1/1	0.90	0.20	51,51,51,51	0
58	MG	18	105	1/1	0.90	0.27	42,42,42,42	0
58	MG	1A	3688	1/1	0.90	0.11	20,20,20,20	0
58	MG	1A	4058	1/1	0.90	0.14	43,43,43,43	0
58	MG	1A	3091	1/1	0.90	0.21	26,26,26,26	0
58	MG	2A	3853	1/1	0.90	0.14	47,47,47,47	0
58	MG	19	101	1/1	0.90	0.22	55,55,55,55	0
58	MG	1A	3295	1/1	0.90	0.19	27,27,27,27	0
58	MG	2a	1766	1/1	0.90	0.08	46,46,46,46	0
58	MG	1A	3490	1/1	0.90	0.17	39,39,39,39	0
58	MG	2A	3300	1/1	0.90	0.11	59,59,59,59	0
58	MG	2A	3517	1/1	0.90	0.24	51,51,51,51	0
58	MG	1A	3822	1/1	0.90	0.17	64,64,64,64	0
58	MG	2a	1778	1/1	0.90	0.20	39,39,39,39	0
58	MG	2A	3530	1/1	0.90	0.14	25,25,25,25	0
58	MG	2A	3534	1/1	0.90	0.14	29,29,29,29	0
58	MG	2A	3546	1/1	0.90	0.15	45,45,45,45	0
58	MG	2A	3547	1/1	0.90	0.11	42,42,42,42	0
58	MG	2A	3548	1/1	0.90	0.21	38,38,38,38	0
58	MG	1A	3045	1/1	0.90	0.17	26,26,26,26	0
58	MG	2A	3123	1/1	0.90	0.18	68,68,68,68	0
58	MG	1A	3579	1/1	0.90	0.27	40,40,40,40	0
58	MG	1a	1612	1/1	0.90	0.10	51,51,51,51	0
58	MG	2A	3572	1/1	0.90	0.12	30,30,30,30	0
58	MG	2a	1813	1/1	0.90	0.18	42,42,42,42	0
58	MG	1A	3965	1/1	0.90	0.10	30,30,30,30	0
58	MG	1A	3840	1/1	0.90	0.11	34,34,34,34	0
58	MG	1A	3441	1/1	0.90	0.22	37,37,37,37	0
58	MG	2A	3594	1/1	0.90	0.13	53,53,53,53	0
58	MG	2A	3132	1/1	0.90	0.08	61,61,61,61	0
58	MG	1a	1783	1/1	0.90	0.10	54,54,54,54	0
58	MG	1A	3442	1/1	0.90	0.11	37,37,37,37	0
58	MG	1A	3333	1/1	0.90	0.25	43,43,43,43	0
58	MG	2g	201	1/1	0.90	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2k	201	1/1	0.90	0.22	48,48,48,48	0
58	MG	1A	3381	1/1	0.90	0.17	36,36,36,36	0
58	MG	2A	3141	1/1	0.90	0.20	52,52,52,52	0
58	MG	1A	3505	1/1	0.90	0.12	36,36,36,36	0
58	MG	1A	3334	1/1	0.90	0.23	47,47,47,47	0
58	MG	2A	3337	1/1	0.90	0.12	57,57,57,57	0
58	MG	1A	3984	1/1	0.90	0.12	42,42,42,42	0
58	MG	1A	3152	1/1	0.90	0.27	39,39,39,39	0
58	MG	2A	3155	1/1	0.90	0.20	44,44,44,44	0
58	MG	2v	102	1/1	0.90	0.17	57,57,57,57	0
58	MG	2v	103	1/1	0.90	0.35	50,50,50,50	0
58	MG	2A	3156	1/1	0.90	0.21	26,26,26,26	0
58	MG	1A	3986	1/1	0.90	0.20	52,52,52,52	0
58	MG	1a	1801	1/1	0.90	0.15	46,46,46,46	0
58	MG	1a	1643	1/1	0.90	0.14	55,55,55,55	0
58	MG	1A	3298	1/1	0.90	0.12	41,41,41,41	0
58	MG	2A	3651	1/1	0.90	0.16	38,38,38,38	0
58	MG	1A	3612	1/1	0.90	0.26	41,41,41,41	0
58	MG	2x	105	1/1	0.90	0.18	39,39,39,39	0
58	MG	2A	3167	1/1	0.90	0.19	38,38,38,38	0
58	MG	1A	3744	1/1	0.91	0.16	37,37,37,37	0
58	MG	2A	3345	1/1	0.91	0.14	53,53,53,53	0
58	MG	20	101	1/1	0.91	0.32	45,45,45,45	0
58	MG	1N	201	1/1	0.91	0.37	41,41,41,41	0
58	MG	1A	3437	1/1	0.91	0.20	32,32,32,32	0
58	MG	1a	1670	1/1	0.91	0.15	55,55,55,55	0
58	MG	1N	205	1/1	0.91	0.13	41,41,41,41	0
58	MG	2A	3168	1/1	0.91	0.12	43,43,43,43	0
58	MG	27	101	1/1	0.91	0.23	44,44,44,44	0
58	MG	1A	3063	1/1	0.91	0.23	37,37,37,37	0
58	MG	2A	3175	1/1	0.91	0.10	42,42,42,42	0
58	MG	1A	3258	1/1	0.91	0.12	39,39,39,39	0
58	MG	1A	3955	1/1	0.91	0.09	59,59,59,59	0
58	MG	1v	101	1/1	0.91	0.18	64,64,64,64	0
58	MG	1A	3472	1/1	0.91	0.16	49,49,49,49	0
58	MG	1w	102	1/1	0.91	0.15	50,50,50,50	0
58	MG	1A	3100	1/1	0.91	0.17	38,38,38,38	0
58	MG	1A	3371	1/1	0.91	0.17	28,28,28,28	0
58	MG	1A	3678	1/1	0.91	0.12	32,32,32,32	0
58	MG	1S	202	1/1	0.91	0.18	37,37,37,37	0
58	MG	2A	3677	1/1	0.91	0.14	56,56,56,56	0
58	MG	2A	3679	1/1	0.91	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3447	1/1	0.91	0.14	29,29,29,29	0
58	MG	2A	3377	1/1	0.91	0.45	49,49,49,49	0
58	MG	1a	1691	1/1	0.91	0.18	57,57,57,57	0
58	MG	2A	3685	1/1	0.91	0.17	36,36,36,36	0
58	MG	1A	3531	1/1	0.91	0.32	33,33,33,33	0
58	MG	2a	1623	1/1	0.91	0.11	48,48,48,48	0
58	MG	1x	112	1/1	0.91	0.16	53,53,53,53	0
58	MG	2A	3386	1/1	0.91	0.13	51,51,51,51	0
58	MG	1a	1695	1/1	0.91	0.28	56,56,56,56	0
58	MG	2A	3202	1/1	0.91	0.18	34,34,34,34	0
58	MG	2a	1632	1/1	0.91	0.12	52,52,52,52	0
58	MG	2A	3391	1/1	0.91	0.18	48,48,48,48	0
58	MG	1A	3873	1/1	0.91	0.15	40,40,40,40	0
58	MG	2A	3005	1/1	0.91	0.12	56,56,56,56	0
58	MG	2A	3395	1/1	0.91	0.18	44,44,44,44	0
58	MG	2A	3205	1/1	0.91	0.12	52,52,52,52	0
58	MG	2A	3397	1/1	0.91	0.15	57,57,57,57	0
58	MG	1U	202	1/1	0.91	0.32	36,36,36,36	0
58	MG	2a	1652	1/1	0.91	0.28	64,64,64,64	0
58	MG	2A	3708	1/1	0.91	0.14	21,21,21,21	0
58	MG	2a	1656	1/1	0.91	0.22	56,56,56,56	0
58	MG	2A	3007	1/1	0.91	0.13	46,46,46,46	0
58	MG	2A	3008	1/1	0.91	0.21	53,53,53,53	0
58	MG	1A	3260	1/1	0.91	0.10	18,18,18,18	0
58	MG	1V	202	1/1	0.91	0.16	33,33,33,33	0
58	MG	2A	3411	1/1	0.91	0.19	52,52,52,52	0
58	MG	2a	1662	1/1	0.91	0.35	55,55,55,55	0
58	MG	2A	3413	1/1	0.91	0.24	33,33,33,33	0
58	MG	1A	3876	1/1	0.91	0.14	42,42,42,42	0
58	MG	2A	3728	1/1	0.91	0.22	36,36,36,36	0
58	MG	2A	3217	1/1	0.91	0.17	36,36,36,36	0
58	MG	2A	3032	1/1	0.91	0.14	50,50,50,50	0
58	MG	2A	3034	1/1	0.91	0.21	34,34,34,34	0
58	MG	1W	202	1/1	0.91	0.33	44,44,44,44	0
58	MG	1W	207	1/1	0.91	0.17	26,26,26,26	0
58	MG	1X	102	1/1	0.91	0.20	28,28,28,28	0
58	MG	1Y	201	1/1	0.91	0.15	37,37,37,37	0
58	MG	2a	1684	1/1	0.91	0.14	60,60,60,60	0
58	MG	1A	3605	1/1	0.91	0.13	38,38,38,38	0
58	MG	1A	3024	1/1	0.91	0.25	36,36,36,36	0
58	MG	2A	3430	1/1	0.91	0.27	44,44,44,44	0
58	MG	2A	3237	1/1	0.91	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3238	1/1	0.91	0.15	44,44,44,44	0
58	MG	2A	3047	1/1	0.91	0.21	40,40,40,40	0
58	MG	2A	3437	1/1	0.91	0.29	41,41,41,41	0
58	MG	1A	4061	1/1	0.91	0.16	41,41,41,41	0
58	MG	2A	3774	1/1	0.91	0.12	43,43,43,43	0
58	MG	2A	3441	1/1	0.91	0.29	50,50,50,50	0
58	MG	2a	1706	1/1	0.91	0.14	48,48,48,48	0
58	MG	2a	1708	1/1	0.91	0.16	55,55,55,55	0
58	MG	1A	3701	1/1	0.91	0.23	21,21,21,21	0
58	MG	1a	1722	1/1	0.91	0.14	58,58,58,58	0
58	MG	11	102	1/1	0.91	0.12	32,32,32,32	0
58	MG	2A	3448	1/1	0.91	0.28	35,35,35,35	0
58	MG	2A	3056	1/1	0.91	0.20	33,33,33,33	0
58	MG	2A	3790	1/1	0.91	0.10	59,59,59,59	0
58	MG	1A	3702	1/1	0.91	0.17	35,35,35,35	0
58	MG	2a	1719	1/1	0.91	0.12	59,59,59,59	0
58	MG	2A	3795	1/1	0.91	0.19	39,39,39,39	0
58	MG	1A	4067	1/1	0.91	0.11	38,38,38,38	0
58	MG	12	102	1/1	0.91	0.24	46,46,46,46	0
58	MG	2a	1723	1/1	0.91	0.19	59,59,59,59	0
58	MG	2A	3800	1/1	0.91	0.07	68,68,68,68	0
58	MG	1A	3484	1/1	0.91	0.19	27,27,27,27	0
58	MG	1A	3888	1/1	0.91	0.16	24,24,24,24	0
58	MG	2A	3803	1/1	0.91	0.22	73,73,73,73	0
58	MG	1A	3704	1/1	0.91	0.13	19,19,19,19	0
58	MG	1A	3455	1/1	0.91	0.19	36,36,36,36	0
58	MG	2A	3069	1/1	0.91	0.25	25,25,25,25	0
58	MG	2A	3071	1/1	0.91	0.34	44,44,44,44	0
58	MG	1A	3344	1/1	0.91	0.27	38,38,38,38	0
58	MG	1A	3267	1/1	0.91	0.23	44,44,44,44	0
58	MG	1A	3994	1/1	0.91	0.17	24,24,24,24	0
58	MG	2A	3815	1/1	0.91	0.18	28,28,28,28	0
58	MG	1A	3618	1/1	0.91	0.16	48,48,48,48	0
58	MG	1A	3142	1/1	0.91	0.17	27,27,27,27	0
58	MG	2A	3275	1/1	0.91	0.17	47,47,47,47	0
58	MG	2A	3277	1/1	0.91	0.13	43,43,43,43	0
58	MG	1A	3551	1/1	0.91	0.39	55,55,55,55	0
58	MG	1B	204	1/1	0.91	0.31	48,48,48,48	0
58	MG	1a	1604	1/1	0.91	0.17	53,53,53,53	0
58	MG	1a	1757	1/1	0.91	0.11	42,42,42,42	0
58	MG	1a	1758	1/1	0.91	0.14	44,44,44,44	0
58	MG	2a	1762	1/1	0.91	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1B	207	1/1	0.91	0.21	45,45,45,45	0
58	MG	1a	1760	1/1	0.91	0.06	62,62,62,62	0
58	MG	2A	3289	1/1	0.91	0.29	42,42,42,42	0
58	MG	2A	3844	1/1	0.91	0.15	33,33,33,33	0
58	MG	2A	3845	1/1	0.91	0.14	39,39,39,39	0
58	MG	1A	3999	1/1	0.91	0.17	45,45,45,45	0
58	MG	2A	3292	1/1	0.91	0.20	53,53,53,53	0
58	MG	2A	3105	1/1	0.91	0.12	65,65,65,65	0
58	MG	1a	1607	1/1	0.91	0.32	52,52,52,52	0
58	MG	2a	1785	1/1	0.91	0.22	42,42,42,42	0
58	MG	2A	3854	1/1	0.91	0.13	59,59,59,59	0
58	MG	1A	3805	1/1	0.91	0.17	12,12,12,12	0
58	MG	2a	1791	1/1	0.91	0.21	58,58,58,58	0
58	MG	1A	4004	1/1	0.91	0.13	16,16,16,16	0
58	MG	1A	3915	1/1	0.91	0.14	47,47,47,47	0
58	MG	2a	1797	1/1	0.91	0.22	49,49,49,49	0
58	MG	2A	3525	1/1	0.91	0.10	51,51,51,51	0
58	MG	2A	3527	1/1	0.91	0.14	64,64,64,64	0
58	MG	1B	223	1/1	0.91	0.25	41,41,41,41	0
58	MG	2A	3532	1/1	0.91	0.19	27,27,27,27	0
58	MG	2A	3117	1/1	0.91	0.25	40,40,40,40	0
58	MG	2A	3536	1/1	0.91	0.12	55,55,55,55	0
58	MG	1A	4009	1/1	0.91	0.12	59,59,59,59	0
58	MG	1A	3921	1/1	0.91	0.14	22,22,22,22	0
58	MG	1A	3807	1/1	0.91	0.12	35,35,35,35	0
58	MG	2a	1818	1/1	0.91	0.28	54,54,54,54	0
58	MG	1A	3159	1/1	0.91	0.23	32,32,32,32	0
58	MG	1A	3814	1/1	0.91	0.13	18,18,18,18	0
58	MG	1a	1791	1/1	0.91	0.13	54,54,54,54	0
58	MG	2a	1830	1/1	0.91	0.27	49,49,49,49	0
58	MG	1A	3636	1/1	0.91	0.06	23,23,23,23	0
58	MG	2a	1834	1/1	0.91	0.09	52,52,52,52	0
58	MG	2B	213	1/1	0.91	0.25	49,49,49,49	0
58	MG	1A	3461	1/1	0.91	0.17	49,49,49,49	0
58	MG	1a	1638	1/1	0.91	0.12	47,47,47,47	0
58	MG	1A	3824	1/1	0.91	0.15	55,55,55,55	0
58	MG	1A	3331	1/1	0.91	0.18	34,34,34,34	0
58	MG	2A	3587	1/1	0.91	0.20	47,47,47,47	0
58	MG	2D	307	1/1	0.91	0.32	46,46,46,46	0
58	MG	1A	3504	1/1	0.91	0.18	24,24,24,24	0
58	MG	2A	3328	1/1	0.91	0.20	41,41,41,41	0
58	MG	2E	305	1/1	0.91	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3600	1/1	0.91	0.23	49,49,49,49	0
58	MG	1A	4027	1/1	0.91	0.12	25,25,25,25	0
58	MG	1A	3942	1/1	0.91	0.19	30,30,30,30	0
58	MG	2A	3607	1/1	0.91	0.29	46,46,46,46	0
58	MG	2A	3610	1/1	0.91	0.21	53,53,53,53	0
58	MG	1A	3189	1/1	0.91	0.11	37,37,37,37	0
58	MG	1A	3053	1/1	0.91	0.17	31,31,31,31	0
58	MG	1A	3844	1/1	0.91	0.09	45,45,45,45	0
58	MG	2A	3618	1/1	0.91	0.15	27,27,27,27	0
58	MG	1F	312	1/1	0.91	0.22	29,29,29,29	0
58	MG	2W	201	1/1	0.91	0.14	50,50,50,50	0
58	MG	2x	107	1/1	0.91	0.20	32,32,32,32	0
58	MG	1A	3845	1/1	0.91	0.17	51,51,51,51	0
58	MG	1A	3983	1/1	0.92	0.09	56,56,56,56	0
58	MG	2A	3622	1/1	0.92	0.21	28,28,28,28	0
58	MG	1A	3697	1/1	0.92	0.15	26,26,26,26	0
58	MG	1a	1642	1/1	0.92	0.26	53,53,53,53	0
58	MG	2Y	201	1/1	0.92	0.22	47,47,47,47	0
58	MG	2Z	301	1/1	0.92	0.11	64,64,64,64	0
58	MG	2A	3165	1/1	0.92	0.23	62,62,62,62	0
58	MG	1A	3698	1/1	0.92	0.14	22,22,22,22	0
58	MG	1A	3427	1/1	0.92	0.31	54,54,54,54	0
58	MG	1a	1647	1/1	0.92	0.13	41,41,41,41	0
58	MG	2A	3172	1/1	0.92	0.12	47,47,47,47	0
58	MG	2A	3361	1/1	0.92	0.12	44,44,44,44	0
58	MG	1b	301	1/1	0.92	0.14	58,58,58,58	0
58	MG	2A	3647	1/1	0.92	0.20	34,34,34,34	0
58	MG	27	103	1/1	0.92	0.14	40,40,40,40	0
58	MG	2A	3648	1/1	0.92	0.13	47,47,47,47	0
58	MG	2A	3363	1/1	0.92	0.12	48,48,48,48	0
58	MG	1A	3321	1/1	0.92	0.15	22,22,22,22	0
58	MG	1A	3481	1/1	0.92	0.27	41,41,41,41	0
58	MG	2A	3369	1/1	0.92	0.44	69,69,69,69	0
58	MG	1A	3434	1/1	0.92	0.15	36,36,36,36	0
58	MG	2A	3666	1/1	0.92	0.08	45,45,45,45	0
58	MG	1A	3990	1/1	0.92	0.19	20,20,20,20	0
58	MG	2A	3669	1/1	0.92	0.12	27,27,27,27	0
58	MG	2A	3180	1/1	0.92	0.14	45,45,45,45	0
58	MG	2A	3672	1/1	0.92	0.24	43,43,43,43	0
58	MG	2a	1614	1/1	0.92	0.21	61,61,61,61	0
58	MG	1A	3857	1/1	0.92	0.10	44,44,44,44	0
58	MG	1A	3283	1/1	0.92	0.31	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3172	1/1	0.92	0.18	37,37,37,37	0
58	MG	2A	3378	1/1	0.92	0.32	41,41,41,41	0
58	MG	2a	1620	1/1	0.92	0.21	47,47,47,47	0
58	MG	2A	3680	1/1	0.92	0.14	51,51,51,51	0
58	MG	1A	3570	1/1	0.92	0.22	33,33,33,33	0
58	MG	2A	3381	1/1	0.92	0.13	54,54,54,54	0
58	MG	2A	3382	1/1	0.92	0.21	58,58,58,58	0
58	MG	1A	3997	1/1	0.92	0.14	42,42,42,42	0
58	MG	1w	103	1/1	0.92	0.19	65,65,65,65	0
58	MG	1a	1664	1/1	0.92	0.19	45,45,45,45	0
58	MG	1A	3575	1/1	0.92	0.15	41,41,41,41	0
58	MG	1A	3577	1/1	0.92	0.24	41,41,41,41	0
58	MG	2A	3390	1/1	0.92	0.34	57,57,57,57	0
58	MG	1A	3292	1/1	0.92	0.22	49,49,49,49	0
58	MG	2A	3200	1/1	0.92	0.21	42,42,42,42	0
58	MG	1F	306	1/1	0.92	0.16	25,25,25,25	0
58	MG	1A	3491	1/1	0.92	0.15	35,35,35,35	0
58	MG	1A	3440	1/1	0.92	0.17	42,42,42,42	0
58	MG	1a	1677	1/1	0.92	0.19	43,43,43,43	0
58	MG	1A	3589	1/1	0.92	0.19	37,37,37,37	0
58	MG	2A	3207	1/1	0.92	0.22	36,36,36,36	0
58	MG	2A	3002	1/1	0.92	0.30	45,45,45,45	0
58	MG	1A	3877	1/1	0.92	0.23	24,24,24,24	0
58	MG	1A	3733	1/1	0.92	0.12	49,49,49,49	0
58	MG	1a	1684	1/1	0.92	0.30	51,51,51,51	0
58	MG	1A	3591	1/1	0.92	0.27	40,40,40,40	0
58	MG	1a	1687	1/1	0.92	0.12	49,49,49,49	0
58	MG	2A	3720	1/1	0.92	0.20	58,58,58,58	0
58	MG	1A	4015	1/1	0.92	0.17	23,23,23,23	0
58	MG	2A	3724	1/1	0.92	0.16	35,35,35,35	0
58	MG	2A	3018	1/1	0.92	0.23	37,37,37,37	0
58	MG	1A	3738	1/1	0.92	0.13	23,23,23,23	0
58	MG	2A	3731	1/1	0.92	0.17	48,48,48,48	0
58	MG	1A	3493	1/1	0.92	0.11	37,37,37,37	0
58	MG	1a	1692	1/1	0.92	0.33	50,50,50,50	0
58	MG	1Q	202	1/1	0.92	0.15	21,21,21,21	0
58	MG	1A	3330	1/1	0.92	0.15	32,32,32,32	0
58	MG	1A	3496	1/1	0.92	0.20	30,30,30,30	0
58	MG	1A	3497	1/1	0.92	0.18	36,36,36,36	0
58	MG	2a	1686	1/1	0.92	0.15	52,52,52,52	0
58	MG	2A	3229	1/1	0.92	0.16	41,41,41,41	0
58	MG	2A	3230	1/1	0.92	0.36	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3754	1/1	0.92	0.21	43,43,43,43	0
58	MG	1A	3890	1/1	0.92	0.14	24,24,24,24	0
58	MG	1a	1700	1/1	0.92	0.27	56,56,56,56	0
58	MG	1A	3050	1/1	0.92	0.20	28,28,28,28	0
58	MG	2A	3762	1/1	0.92	0.14	41,41,41,41	0
58	MG	2A	3764	1/1	0.92	0.14	51,51,51,51	0
58	MG	1A	3210	1/1	0.92	0.12	46,46,46,46	0
58	MG	1A	3897	1/1	0.92	0.08	28,28,28,28	0
58	MG	1A	3380	1/1	0.92	0.17	31,31,31,31	0
58	MG	1A	3503	1/1	0.92	0.14	26,26,26,26	0
58	MG	2a	1711	1/1	0.92	0.11	53,53,53,53	0
58	MG	1A	3121	1/1	0.92	0.21	27,27,27,27	0
58	MG	1A	3084	1/1	0.92	0.19	21,21,21,21	0
58	MG	1A	3614	1/1	0.92	0.17	31,31,31,31	0
58	MG	2A	3784	1/1	0.92	0.19	43,43,43,43	0
58	MG	2A	3785	1/1	0.92	0.09	31,31,31,31	0
58	MG	2A	3253	1/1	0.92	0.09	67,67,67,67	0
58	MG	2A	3452	1/1	0.92	0.25	42,42,42,42	0
58	MG	1A	3184	1/1	0.92	0.20	47,47,47,47	0
58	MG	2A	3255	1/1	0.92	0.19	51,51,51,51	0
58	MG	2A	3458	1/1	0.92	0.19	55,55,55,55	0
58	MG	1A	3917	1/1	0.92	0.20	29,29,29,29	0
58	MG	1A	3221	1/1	0.92	0.24	28,28,28,28	0
58	MG	2A	3797	1/1	0.92	0.18	50,50,50,50	0
58	MG	1A	3922	1/1	0.92	0.21	20,20,20,20	0
58	MG	1a	1724	1/1	0.92	0.18	50,50,50,50	0
58	MG	1Y	202	1/1	0.92	0.14	32,32,32,32	0
58	MG	2A	3068	1/1	0.92	0.30	37,37,37,37	0
58	MG	1A	3771	1/1	0.92	0.15	20,20,20,20	0
58	MG	1Z	301	1/1	0.92	0.11	59,59,59,59	0
58	MG	2a	1736	1/1	0.92	0.28	45,45,45,45	0
58	MG	10	102	1/1	0.92	0.19	40,40,40,40	0
58	MG	1A	3627	1/1	0.92	0.07	59,59,59,59	0
58	MG	1A	3302	1/1	0.92	0.20	49,49,49,49	0
58	MG	2A	3808	1/1	0.92	0.14	45,45,45,45	0
58	MG	1a	1739	1/1	0.92	0.24	38,38,38,38	0
58	MG	1A	3394	1/1	0.92	0.22	33,33,33,33	0
58	MG	1a	1741	1/1	0.92	0.25	46,46,46,46	0
58	MG	2A	3279	1/1	0.92	0.11	45,45,45,45	0
58	MG	2a	1755	1/1	0.92	0.19	46,46,46,46	0
58	MG	2A	3489	1/1	0.92	0.19	58,58,58,58	0
58	MG	1A	3778	1/1	0.92	0.11	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3520	1/1	0.92	0.22	37,37,37,37	0
58	MG	2A	3493	1/1	0.92	0.13	55,55,55,55	0
58	MG	1A	3780	1/1	0.92	0.17	18,18,18,18	0
58	MG	2A	3825	1/1	0.92	0.18	46,46,46,46	0
58	MG	1A	3458	1/1	0.92	0.20	43,43,43,43	0
58	MG	2A	3098	1/1	0.92	0.23	38,38,38,38	0
58	MG	1A	3016	1/1	0.92	0.21	41,41,41,41	0
58	MG	13	102	1/1	0.92	0.17	49,49,49,49	0
58	MG	1A	3057	1/1	0.92	0.24	36,36,36,36	0
58	MG	1A	3345	1/1	0.92	0.20	50,50,50,50	0
58	MG	1A	3233	1/1	0.92	0.14	35,35,35,35	0
58	MG	1A	3235	1/1	0.92	0.16	46,46,46,46	0
58	MG	2a	1780	1/1	0.92	0.16	49,49,49,49	0
58	MG	1A	3656	1/1	0.92	0.15	27,27,27,27	0
58	MG	1A	3409	1/1	0.92	0.23	35,35,35,35	0
58	MG	2A	3520	1/1	0.92	0.26	33,33,33,33	0
58	MG	2A	3522	1/1	0.92	0.09	52,52,52,52	0
58	MG	2A	3113	1/1	0.92	0.29	54,54,54,54	0
58	MG	1A	3662	1/1	0.92	0.21	28,28,28,28	0
58	MG	1A	3355	1/1	0.92	0.10	54,54,54,54	0
58	MG	2A	3122	1/1	0.92	0.20	43,43,43,43	0
58	MG	2A	3533	1/1	0.92	0.11	40,40,40,40	0
58	MG	1A	3356	1/1	0.92	0.23	53,53,53,53	0
58	MG	1A	4087	1/1	0.92	0.22	36,36,36,36	0
58	MG	2A	3540	1/1	0.92	0.18	47,47,47,47	0
58	MG	2a	1808	1/1	0.92	0.15	53,53,53,53	0
58	MG	1A	3668	1/1	0.92	0.15	18,18,18,18	0
58	MG	2A	3311	1/1	0.92	0.11	26,26,26,26	0
58	MG	1A	3540	1/1	0.92	0.22	43,43,43,43	0
58	MG	2B	201	1/1	0.92	0.12	59,59,59,59	0
58	MG	2A	3554	1/1	0.92	0.15	32,32,32,32	0
58	MG	2A	3556	1/1	0.92	0.19	25,25,25,25	0
58	MG	2a	1819	1/1	0.92	0.12	68,68,68,68	0
58	MG	2a	1820	1/1	0.92	0.28	55,55,55,55	0
58	MG	2a	1821	1/1	0.92	0.12	59,59,59,59	0
58	MG	2A	3129	1/1	0.92	0.12	50,50,50,50	0
58	MG	1A	3468	1/1	0.92	0.16	26,26,26,26	0
58	MG	2A	3564	1/1	0.92	0.20	17,17,17,17	0
58	MG	2A	3565	1/1	0.92	0.21	34,34,34,34	0
58	MG	1A	4094	1/1	0.92	0.13	38,38,38,38	0
58	MG	1A	3542	1/1	0.92	0.30	63,63,63,63	0
58	MG	2A	3134	1/1	0.92	0.15	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2d	302	1/1	0.92	0.11	52,52,52,52	0
58	MG	1A	3821	1/1	0.92	0.12	60,60,60,60	0
58	MG	2A	3321	1/1	0.92	0.19	58,58,58,58	0
58	MG	2D	302	1/1	0.92	0.42	52,52,52,52	0
58	MG	1A	3133	1/1	0.92	0.17	55,55,55,55	0
58	MG	1A	3546	1/1	0.92	0.32	34,34,34,34	0
58	MG	2A	3589	1/1	0.92	0.31	42,42,42,42	0
58	MG	2D	308	1/1	0.92	0.10	48,48,48,48	0
58	MG	2A	3330	1/1	0.92	0.23	44,44,44,44	0
58	MG	2E	302	1/1	0.92	0.13	55,55,55,55	0
58	MG	1A	3686	1/1	0.92	0.13	42,42,42,42	0
58	MG	1A	3317	1/1	0.92	0.14	21,21,21,21	0
58	MG	1B	211	1/1	0.92	0.11	32,32,32,32	0
58	MG	1A	3134	1/1	0.92	0.19	33,33,33,33	0
58	MG	2A	3606	1/1	0.92	0.25	64,64,64,64	0
58	MG	1A	3102	1/1	0.92	0.16	41,41,41,41	0
58	MG	2A	3150	1/1	0.92	0.18	41,41,41,41	0
58	MG	1B	220	1/1	0.92	0.20	26,26,26,26	0
58	MG	1a	1635	1/1	0.92	0.11	49,49,49,49	0
58	MG	2P	202	1/1	0.92	0.13	44,44,44,44	0
58	MG	2A	3344	1/1	0.92	0.10	65,65,65,65	0
58	MG	1A	3842	1/1	0.92	0.16	24,24,24,24	0
58	MG	1a	1637	1/1	0.92	0.11	38,38,38,38	0
58	MG	2A	3623	1/1	0.93	0.17	39,39,39,39	0
58	MG	1a	1685	1/1	0.93	0.07	57,57,57,57	0
58	MG	2W	202	1/1	0.93	0.16	31,31,31,31	0
58	MG	2W	203	1/1	0.93	0.22	39,39,39,39	0
58	MG	2A	3626	1/1	0.93	0.08	57,57,57,57	0
58	MG	1U	201	1/1	0.93	0.17	27,27,27,27	0
58	MG	2A	3366	1/1	0.93	0.52	43,43,43,43	0
58	MG	1A	3866	1/1	0.93	0.19	37,37,37,37	0
58	MG	2A	3368	1/1	0.93	0.33	59,59,59,59	0
58	MG	2A	3634	1/1	0.93	0.13	48,48,48,48	0
58	MG	1A	3222	1/1	0.93	0.28	36,36,36,36	0
58	MG	23	101	1/1	0.93	0.15	63,63,63,63	0
58	MG	2A	3636	1/1	0.93	0.18	48,48,48,48	0
58	MG	2A	3370	1/1	0.93	0.23	41,41,41,41	0
58	MG	2A	3638	1/1	0.93	0.17	36,36,36,36	0
58	MG	25	103	1/1	0.93	0.22	39,39,39,39	0
58	MG	25	105	1/1	0.93	0.16	61,61,61,61	0
58	MG	1x	106	1/1	0.93	0.24	50,50,50,50	0
58	MG	2A	3645	1/1	0.93	0.14	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1x	109	1/1	0.93	0.17	63,63,63,63	0
58	MG	1x	110	1/1	0.93	0.19	58,58,58,58	0
58	MG	1A	3439	1/1	0.93	0.14	39,39,39,39	0
58	MG	2A	3650	1/1	0.93	0.18	51,51,51,51	0
58	MG	1A	4060	1/1	0.93	0.15	41,41,41,41	0
58	MG	2a	1602	1/1	0.93	0.24	60,60,60,60	0
58	MG	2a	1604	1/1	0.93	0.09	62,62,62,62	0
58	MG	2A	3198	1/1	0.93	0.33	52,52,52,52	0
58	MG	1V	206	1/1	0.93	0.14	45,45,45,45	0
58	MG	1W	201	1/1	0.93	0.20	37,37,37,37	0
58	MG	1A	3870	1/1	0.93	0.20	43,43,43,43	0
58	MG	1W	205	1/1	0.93	0.14	36,36,36,36	0
58	MG	1A	3969	1/1	0.93	0.10	38,38,38,38	0
58	MG	1a	1698	1/1	0.93	0.24	45,45,45,45	0
58	MG	1A	3475	1/1	0.93	0.19	52,52,52,52	0
58	MG	1A	3974	1/1	0.93	0.34	51,51,51,51	0
58	MG	2A	3208	1/1	0.93	0.21	48,48,48,48	0
58	MG	2A	3675	1/1	0.93	0.12	43,43,43,43	0
58	MG	2A	3389	1/1	0.93	0.09	53,53,53,53	0
58	MG	2A	3020	1/1	0.93	0.13	55,55,55,55	0
58	MG	1a	1701	1/1	0.93	0.07	53,53,53,53	0
58	MG	1A	3872	1/1	0.93	0.22	40,40,40,40	0
58	MG	1A	3979	1/1	0.93	0.19	52,52,52,52	0
58	MG	1A	4079	1/1	0.93	0.18	30,30,30,30	0
58	MG	2A	3036	1/1	0.93	0.15	26,26,26,26	0
58	MG	1A	3527	1/1	0.93	0.24	62,62,62,62	0
58	MG	2A	3398	1/1	0.93	0.11	48,48,48,48	0
58	MG	2A	3218	1/1	0.93	0.36	45,45,45,45	0
58	MG	2A	3219	1/1	0.93	0.25	43,43,43,43	0
58	MG	2a	1633	1/1	0.93	0.38	56,56,56,56	0
58	MG	2a	1636	1/1	0.93	0.36	70,70,70,70	0
58	MG	2A	3404	1/1	0.93	0.10	51,51,51,51	0
58	MG	1a	1708	1/1	0.93	0.12	39,39,39,39	0
58	MG	2A	3406	1/1	0.93	0.13	32,32,32,32	0
58	MG	1A	3095	1/1	0.93	0.13	34,34,34,34	0
58	MG	1A	4086	1/1	0.93	0.29	52,52,52,52	0
58	MG	1A	3388	1/1	0.93	0.23	57,57,57,57	0
58	MG	2a	1647	1/1	0.93	0.14	40,40,40,40	0
58	MG	2a	1649	1/1	0.93	0.15	55,55,55,55	0
58	MG	1A	4088	1/1	0.93	0.29	49,49,49,49	0
58	MG	2a	1651	1/1	0.93	0.18	46,46,46,46	0
58	MG	1A	3603	1/1	0.93	0.26	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1654	1/1	0.93	0.11	45,45,45,45	0
58	MG	2A	3226	1/1	0.93	0.30	55,55,55,55	0
58	MG	2A	3049	1/1	0.93	0.16	40,40,40,40	0
58	MG	1A	3026	1/1	0.93	0.13	57,57,57,57	0
58	MG	1A	3782	1/1	0.93	0.10	31,31,31,31	0
58	MG	1A	3316	1/1	0.93	0.31	45,45,45,45	0
58	MG	1A	4095	1/1	0.93	0.24	49,49,49,49	0
58	MG	1A	3232	1/1	0.93	0.25	20,20,20,20	0
58	MG	15	106	1/1	0.93	0.19	39,39,39,39	0
58	MG	2A	3428	1/1	0.93	0.41	48,48,48,48	0
58	MG	2A	3059	1/1	0.93	0.16	56,56,56,56	0
58	MG	2A	3722	1/1	0.93	0.15	51,51,51,51	0
58	MG	2A	3723	1/1	0.93	0.06	58,58,58,58	0
58	MG	1A	3886	1/1	0.93	0.13	25,25,25,25	0
58	MG	2A	3726	1/1	0.93	0.21	53,53,53,53	0
58	MG	1A	3609	1/1	0.93	0.15	34,34,34,34	0
58	MG	2A	3433	1/1	0.93	0.16	51,51,51,51	0
58	MG	1A	3787	1/1	0.93	0.16	21,21,21,21	0
58	MG	2A	3248	1/1	0.93	0.12	68,68,68,68	0
58	MG	2a	1682	1/1	0.93	0.18	42,42,42,42	0
58	MG	1A	3485	1/1	0.93	0.14	40,40,40,40	0
58	MG	1A	3011	1/1	0.93	0.19	28,28,28,28	0
58	MG	1A	3489	1/1	0.93	0.24	38,38,38,38	0
58	MG	2A	3252	1/1	0.93	0.19	57,57,57,57	0
58	MG	1A	3195	1/1	0.93	0.21	27,27,27,27	0
58	MG	1B	213	1/1	0.93	0.23	63,63,63,63	0
58	MG	1A	3714	1/1	0.93	0.22	26,26,26,26	0
58	MG	1B	216	1/1	0.93	0.07	52,52,52,52	0
58	MG	1a	1746	1/1	0.93	0.12	53,53,53,53	0
58	MG	2A	3451	1/1	0.93	0.26	42,42,42,42	0
58	MG	2a	1702	1/1	0.93	0.18	50,50,50,50	0
58	MG	2A	3075	1/1	0.93	0.20	38,38,38,38	0
58	MG	2A	3761	1/1	0.93	0.13	62,62,62,62	0
58	MG	1a	1747	1/1	0.93	0.07	49,49,49,49	0
58	MG	2a	1707	1/1	0.93	0.26	58,58,58,58	0
58	MG	2A	3763	1/1	0.93	0.12	41,41,41,41	0
58	MG	2A	3261	1/1	0.93	0.14	52,52,52,52	0
58	MG	2A	3078	1/1	0.93	0.21	19,19,19,19	0
58	MG	2A	3769	1/1	0.93	0.23	46,46,46,46	0
58	MG	2A	3079	1/1	0.93	0.13	43,43,43,43	0
58	MG	1A	3616	1/1	0.93	0.19	44,44,44,44	0
58	MG	1A	3158	1/1	0.93	0.28	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4003	1/1	0.93	0.20	7,7,7,7	0
58	MG	1A	3902	1/1	0.93	0.15	13,13,13,13	0
58	MG	1B	225	1/1	0.93	0.20	41,41,41,41	0
58	MG	2A	3274	1/1	0.93	0.29	49,49,49,49	0
58	MG	2A	3472	1/1	0.93	0.15	52,52,52,52	0
58	MG	1A	3800	1/1	0.93	0.20	37,37,37,37	0
58	MG	2A	3095	1/1	0.93	0.21	36,36,36,36	0
58	MG	1A	3054	1/1	0.93	0.11	41,41,41,41	0
58	MG	1A	3806	1/1	0.93	0.22	30,30,30,30	0
58	MG	2A	3482	1/1	0.93	0.28	34,34,34,34	0
58	MG	1A	3545	1/1	0.93	0.26	19,19,19,19	0
58	MG	1A	3239	1/1	0.93	0.32	27,27,27,27	0
58	MG	2a	1730	1/1	0.93	0.20	41,41,41,41	0
58	MG	1A	4014	1/1	0.93	0.19	33,33,33,33	0
58	MG	1A	3813	1/1	0.93	0.08	39,39,39,39	0
58	MG	1a	1769	1/1	0.93	0.07	45,45,45,45	0
58	MG	2A	3107	1/1	0.93	0.20	43,43,43,43	0
58	MG	2a	1737	1/1	0.93	0.10	42,42,42,42	0
58	MG	1A	3002	1/1	0.93	0.15	48,48,48,48	0
58	MG	2a	1739	1/1	0.93	0.19	50,50,50,50	0
58	MG	1a	1772	1/1	0.93	0.16	58,58,58,58	0
58	MG	2A	3291	1/1	0.93	0.29	54,54,54,54	0
58	MG	1a	1632	1/1	0.93	0.23	43,43,43,43	0
58	MG	1A	4018	1/1	0.93	0.14	37,37,37,37	0
58	MG	1A	3104	1/1	0.93	0.12	23,23,23,23	0
58	MG	2A	3499	1/1	0.93	0.18	47,47,47,47	0
58	MG	2A	3115	1/1	0.93	0.25	46,46,46,46	0
58	MG	2A	3811	1/1	0.93	0.16	42,42,42,42	0
58	MG	2A	3116	1/1	0.93	0.23	41,41,41,41	0
58	MG	1a	1776	1/1	0.93	0.09	52,52,52,52	0
58	MG	1A	3113	1/1	0.93	0.15	32,32,32,32	0
58	MG	2A	3302	1/1	0.93	0.12	48,48,48,48	0
58	MG	1A	3553	1/1	0.93	0.22	44,44,44,44	0
58	MG	1a	1639	1/1	0.93	0.16	50,50,50,50	0
58	MG	2a	1763	1/1	0.93	0.18	48,48,48,48	0
58	MG	1A	3735	1/1	0.93	0.19	63,63,63,63	0
58	MG	1a	1789	1/1	0.93	0.07	34,34,34,34	0
58	MG	2A	3524	1/1	0.93	0.15	41,41,41,41	0
58	MG	1a	1790	1/1	0.93	0.06	43,43,43,43	0
58	MG	1A	3115	1/1	0.93	0.19	25,25,25,25	0
58	MG	2A	3312	1/1	0.93	0.24	36,36,36,36	0
58	MG	1A	3415	1/1	0.93	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
58	MG	1F	311	1/1	0.93	0.23	46,46,46,46	0
58	MG	1A	3839	1/1	0.93	0.17	42,42,42,42	0
58	MG	1A	3372	1/1	0.93	0.30	31,31,31,31	0
58	MG	2A	3539	1/1	0.93	0.13	46,46,46,46	0
58	MG	1A	3418	1/1	0.93	0.23	27,27,27,27	0
58	MG	2A	3542	1/1	0.93	0.20	44,44,44,44	0
58	MG	2A	3544	1/1	0.93	0.16	39,39,39,39	0
58	MG	2a	1792	1/1	0.93	0.13	53,53,53,53	0
58	MG	1I	201	1/1	0.93	0.14	42,42,42,42	0
58	MG	1A	3216	1/1	0.93	0.18	38,38,38,38	0
58	MG	1a	1655	1/1	0.93	0.13	38,38,38,38	0
58	MG	2A	3549	1/1	0.93	0.22	36,36,36,36	0
58	MG	2a	1799	1/1	0.93	0.15	46,46,46,46	0
58	MG	2A	3552	1/1	0.93	0.14	36,36,36,36	0
58	MG	2A	3142	1/1	0.93	0.20	42,42,42,42	0
58	MG	1A	3945	1/1	0.93	0.14	45,45,45,45	0
58	MG	2A	3558	1/1	0.93	0.28	44,44,44,44	0
58	MG	2A	3559	1/1	0.93	0.08	53,53,53,53	0
58	MG	2a	1812	1/1	0.93	0.14	50,50,50,50	0
58	MG	1N	204	1/1	0.93	0.20	43,43,43,43	0
58	MG	1A	3180	1/1	0.93	0.13	20,20,20,20	0
58	MG	2A	3563	1/1	0.93	0.12	45,45,45,45	0
58	MG	1a	1659	1/1	0.93	0.10	44,44,44,44	0
58	MG	2A	3336	1/1	0.93	0.19	44,44,44,44	0
58	MG	1a	1660	1/1	0.93	0.16	48,48,48,48	0
58	MG	2A	3570	1/1	0.93	0.16	25,25,25,25	0
58	MG	1A	3506	1/1	0.93	0.15	28,28,28,28	0
58	MG	1A	3948	1/1	0.93	0.12	25,25,25,25	0
58	MG	2a	1825	1/1	0.93	0.17	51,51,51,51	0
58	MG	1P	202	1/1	0.93	0.14	20,20,20,20	0
58	MG	2a	1828	1/1	0.93	0.18	54,54,54,54	0
58	MG	2A	3341	1/1	0.93	0.22	62,62,62,62	0
58	MG	1a	1668	1/1	0.93	0.17	61,61,61,61	0
58	MG	1A	3219	1/1	0.93	0.29	25,25,25,25	0
58	MG	2a	1833	1/1	0.93	0.09	65,65,65,65	0
58	MG	1A	3850	1/1	0.93	0.20	31,31,31,31	0
58	MG	2B	216	1/1	0.93	0.16	42,42,42,42	0
58	MG	2B	218	1/1	0.93	0.10	65,65,65,65	0
58	MG	2A	3592	1/1	0.93	0.16	32,32,32,32	0
58	MG	2i	201	1/1	0.93	0.10	57,57,57,57	0
58	MG	2A	3593	1/1	0.93	0.07	65,65,65,65	0
58	MG	1Q	204	1/1	0.93	0.18	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3749	1/1	0.93	0.22	15,15,15,15	0
58	MG	2A	3596	1/1	0.93	0.14	46,46,46,46	0
58	MG	1A	3148	1/1	0.93	0.11	24,24,24,24	0
58	MG	2A	3602	1/1	0.93	0.14	44,44,44,44	0
58	MG	2A	3348	1/1	0.93	0.31	46,46,46,46	0
58	MG	1A	3854	1/1	0.93	0.13	36,36,36,36	0
58	MG	1A	3307	1/1	0.93	0.20	27,27,27,27	0
58	MG	2A	3352	1/1	0.93	0.28	49,49,49,49	0
58	MG	2A	3608	1/1	0.93	0.19	48,48,48,48	0
58	MG	1A	3670	1/1	0.93	0.12	48,48,48,48	0
58	MG	2A	3174	1/1	0.93	0.26	53,53,53,53	0
58	MG	1a	1679	1/1	0.93	0.08	57,57,57,57	0
58	MG	2F	304	1/1	0.93	0.17	41,41,41,41	0
58	MG	1w	106	1/1	0.93	0.14	56,56,56,56	0
58	MG	2x	102	1/1	0.93	0.18	46,46,46,46	0
58	MG	2F	308	1/1	0.93	0.18	43,43,43,43	0
58	MG	2A	3358	1/1	0.93	0.12	48,48,48,48	0
58	MG	1A	3762	1/1	0.93	0.17	16,16,16,16	0
58	MG	1A	3094	1/1	0.93	0.22	20,20,20,20	0
58	MG	1A	3515	1/1	0.93	0.13	37,37,37,37	0
58	MG	1R	201	1/1	0.94	0.14	35,35,35,35	0
58	MG	1A	3689	1/1	0.94	0.15	53,53,53,53	0
58	MG	1A	3690	1/1	0.94	0.21	18,18,18,18	0
58	MG	1A	3386	1/1	0.94	0.13	28,28,28,28	0
58	MG	2A	3577	1/1	0.94	0.15	25,25,25,25	0
58	MG	1a	1726	1/1	0.94	0.20	46,46,46,46	0
58	MG	2E	308	1/1	0.94	0.12	33,33,33,33	0
58	MG	2E	310	1/1	0.94	0.14	52,52,52,52	0
58	MG	2A	3580	1/1	0.94	0.25	32,32,32,32	0
58	MG	1a	1727	1/1	0.94	0.21	48,48,48,48	0
58	MG	2A	3584	1/1	0.94	0.13	49,49,49,49	0
58	MG	1A	3692	1/1	0.94	0.15	21,21,21,21	0
58	MG	2A	3588	1/1	0.94	0.31	45,45,45,45	0
58	MG	2A	3322	1/1	0.94	0.19	53,53,53,53	0
58	MG	2O	201	1/1	0.94	0.17	45,45,45,45	0
58	MG	2A	3591	1/1	0.94	0.18	32,32,32,32	0
58	MG	2A	3110	1/1	0.94	0.15	44,44,44,44	0
58	MG	1a	1730	1/1	0.94	0.14	40,40,40,40	0
58	MG	2R	201	1/1	0.94	0.22	43,43,43,43	0
58	MG	2A	3329	1/1	0.94	0.16	42,42,42,42	0
58	MG	1A	3696	1/1	0.94	0.16	28,28,28,28	0
58	MG	2A	3331	1/1	0.94	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3257	1/1	0.94	0.19	39,39,39,39	0
58	MG	1A	3088	1/1	0.94	0.20	25,25,25,25	0
58	MG	1A	3105	1/1	0.94	0.14	21,21,21,21	0
58	MG	1U	203	1/1	0.94	0.15	30,30,30,30	0
58	MG	1A	4019	1/1	0.94	0.13	40,40,40,40	0
58	MG	2A	3118	1/1	0.94	0.28	42,42,42,42	0
58	MG	2A	3119	1/1	0.94	0.23	26,26,26,26	0
58	MG	2A	3609	1/1	0.94	0.13	41,41,41,41	0
58	MG	1A	3326	1/1	0.94	0.32	43,43,43,43	0
58	MG	1A	3395	1/1	0.94	0.38	26,26,26,26	0
58	MG	1A	3470	1/1	0.94	0.14	29,29,29,29	0
58	MG	2A	3614	1/1	0.94	0.21	49,49,49,49	0
58	MG	2A	3125	1/1	0.94	0.09	41,41,41,41	0
58	MG	1A	3396	1/1	0.94	0.19	48,48,48,48	0
58	MG	25	104	1/1	0.94	0.12	49,49,49,49	0
58	MG	1A	3708	1/1	0.94	0.17	22,22,22,22	0
58	MG	1A	3106	1/1	0.94	0.16	39,39,39,39	0
58	MG	1A	3328	1/1	0.94	0.16	45,45,45,45	0
58	MG	1A	3566	1/1	0.94	0.27	46,46,46,46	0
58	MG	2A	3350	1/1	0.94	0.22	57,57,57,57	0
58	MG	1A	3262	1/1	0.94	0.16	27,27,27,27	0
58	MG	28	102	1/1	0.94	0.15	54,54,54,54	0
58	MG	2A	3133	1/1	0.94	0.24	32,32,32,32	0
58	MG	2A	3629	1/1	0.94	0.18	56,56,56,56	0
58	MG	1a	1753	1/1	0.94	0.17	53,53,53,53	0
58	MG	1A	3265	1/1	0.94	0.11	55,55,55,55	0
58	MG	1A	3108	1/1	0.94	0.20	19,19,19,19	0
58	MG	2A	3137	1/1	0.94	0.16	33,33,33,33	0
58	MG	1Y	205	1/1	0.94	0.10	49,49,49,49	0
58	MG	1A	4034	1/1	0.94	0.15	13,13,13,13	0
58	MG	10	101	1/1	0.94	0.11	31,31,31,31	0
58	MG	1A	3573	1/1	0.94	0.11	53,53,53,53	0
58	MG	2A	3143	1/1	0.94	0.27	31,31,31,31	0
58	MG	2A	3642	1/1	0.94	0.14	35,35,35,35	0
58	MG	2A	3364	1/1	0.94	0.21	54,54,54,54	0
58	MG	2a	1615	1/1	0.94	0.22	49,49,49,49	0
58	MG	1A	3574	1/1	0.94	0.21	24,24,24,24	0
58	MG	1A	3406	1/1	0.94	0.18	45,45,45,45	0
58	MG	2A	3146	1/1	0.94	0.20	41,41,41,41	0
58	MG	2A	3649	1/1	0.94	0.17	35,35,35,35	0
58	MG	2A	3148	1/1	0.94	0.20	25,25,25,25	0
58	MG	1A	3576	1/1	0.94	0.23	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3110	1/1	0.94	0.16	22,22,22,22	0
58	MG	1A	3153	1/1	0.94	0.20	27,27,27,27	0
58	MG	2A	3659	1/1	0.94	0.15	47,47,47,47	0
58	MG	11	105	1/1	0.94	0.08	53,53,53,53	0
58	MG	1A	3089	1/1	0.94	0.18	37,37,37,37	0
58	MG	2A	3664	1/1	0.94	0.22	37,37,37,37	0
58	MG	2a	1629	1/1	0.94	0.20	58,58,58,58	0
58	MG	1A	3486	1/1	0.94	0.22	35,35,35,35	0
58	MG	1A	3587	1/1	0.94	0.17	48,48,48,48	0
58	MG	1A	3901	1/1	0.94	0.11	28,28,28,28	0
58	MG	1a	1781	1/1	0.94	0.19	39,39,39,39	0
58	MG	2A	3379	1/1	0.94	0.32	57,57,57,57	0
58	MG	2A	3164	1/1	0.94	0.24	24,24,24,24	0
58	MG	1A	3009	1/1	0.94	0.15	15,15,15,15	0
58	MG	1A	4049	1/1	0.94	0.12	27,27,27,27	0
58	MG	15	107	1/1	0.94	0.17	46,46,46,46	0
58	MG	1A	3590	1/1	0.94	0.16	43,43,43,43	0
58	MG	2A	3170	1/1	0.94	0.09	53,53,53,53	0
58	MG	18	103	1/1	0.94	0.24	33,33,33,33	0
58	MG	1A	4052	1/1	0.94	0.17	42,42,42,42	0
58	MG	1A	3905	1/1	0.94	0.20	24,24,24,24	0
58	MG	2a	1653	1/1	0.94	0.16	47,47,47,47	0
58	MG	1A	3488	1/1	0.94	0.15	39,39,39,39	0
58	MG	1A	4057	1/1	0.94	0.22	46,46,46,46	0
58	MG	2A	3392	1/1	0.94	0.20	59,59,59,59	0
58	MG	1A	3909	1/1	0.94	0.17	40,40,40,40	0
58	MG	1A	3594	1/1	0.94	0.27	34,34,34,34	0
58	MG	1A	3912	1/1	0.94	0.22	27,27,27,27	0
58	MG	1A	3118	1/1	0.94	0.28	37,37,37,37	0
58	MG	2A	3183	1/1	0.94	0.27	40,40,40,40	0
58	MG	2A	3700	1/1	0.94	0.22	34,34,34,34	0
58	MG	1A	3340	1/1	0.94	0.15	32,32,32,32	0
58	MG	1A	3919	1/1	0.94	0.17	22,22,22,22	0
58	MG	1a	1804	1/1	0.94	0.07	58,58,58,58	0
58	MG	2A	3402	1/1	0.94	0.26	46,46,46,46	0
58	MG	2a	1668	1/1	0.94	0.10	59,59,59,59	0
58	MG	1A	3753	1/1	0.94	0.32	47,47,47,47	0
58	MG	1A	3066	1/1	0.94	0.32	39,39,39,39	0
58	MG	1A	4071	1/1	0.94	0.17	47,47,47,47	0
58	MG	1A	3040	1/1	0.94	0.31	43,43,43,43	0
58	MG	2a	1677	1/1	0.94	0.20	35,35,35,35	0
58	MG	2A	3196	1/1	0.94	0.38	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4078	1/1	0.94	0.15	45,45,45,45	0
58	MG	2A	3412	1/1	0.94	0.21	44,44,44,44	0
58	MG	1A	3123	1/1	0.94	0.18	33,33,33,33	0
58	MG	1A	3928	1/1	0.94	0.12	23,23,23,23	0
58	MG	1A	3494	1/1	0.94	0.20	46,46,46,46	0
58	MG	1d	301	1/1	0.94	0.38	51,51,51,51	0
58	MG	1A	4082	1/1	0.94	0.23	18,18,18,18	0
58	MG	1A	3423	1/1	0.94	0.16	36,36,36,36	0
58	MG	1A	3606	1/1	0.94	0.12	29,29,29,29	0
58	MG	1A	3934	1/1	0.94	0.17	37,37,37,37	0
58	MG	2A	3206	1/1	0.94	0.30	47,47,47,47	0
58	MG	1A	3352	1/1	0.94	0.33	50,50,50,50	0
58	MG	1a	1634	1/1	0.94	0.25	21,21,21,21	0
58	MG	2a	1703	1/1	0.94	0.08	55,55,55,55	0
58	MG	1A	4090	1/1	0.94	0.07	81,81,81,81	0
58	MG	1A	3430	1/1	0.94	0.14	39,39,39,39	0
58	MG	2A	3740	1/1	0.94	0.18	45,45,45,45	0
58	MG	2A	3741	1/1	0.94	0.24	40,40,40,40	0
58	MG	1A	3940	1/1	0.94	0.12	23,23,23,23	0
58	MG	1A	3610	1/1	0.94	0.15	19,19,19,19	0
58	MG	1A	3774	1/1	0.94	0.20	17,17,17,17	0
58	MG	1A	3431	1/1	0.94	0.14	35,35,35,35	0
58	MG	1A	3944	1/1	0.94	0.12	33,33,33,33	0
58	MG	1A	3225	1/1	0.94	0.13	27,27,27,27	0
58	MG	2A	3439	1/1	0.94	0.18	41,41,41,41	0
58	MG	2A	3757	1/1	0.94	0.19	46,46,46,46	0
58	MG	1a	1644	1/1	0.94	0.12	52,52,52,52	0
58	MG	1A	4099	1/1	0.94	0.24	47,47,47,47	0
58	MG	2A	3760	1/1	0.94	0.16	48,48,48,48	0
58	MG	1A	3500	1/1	0.94	0.23	46,46,46,46	0
58	MG	2A	3445	1/1	0.94	0.28	49,49,49,49	0
58	MG	1B	206	1/1	0.94	0.18	40,40,40,40	0
58	MG	2A	3447	1/1	0.94	0.31	42,42,42,42	0
58	MG	1A	3226	1/1	0.94	0.27	38,38,38,38	0
58	MG	1A	3615	1/1	0.94	0.20	19,19,19,19	0
58	MG	1B	210	1/1	0.94	0.27	50,50,50,50	0
58	MG	2A	3772	1/1	0.94	0.12	49,49,49,49	0
58	MG	1A	3055	1/1	0.94	0.13	32,32,32,32	0
58	MG	1A	3128	1/1	0.94	0.26	25,25,25,25	0
58	MG	2A	3778	1/1	0.94	0.20	52,52,52,52	0
58	MG	2A	3454	1/1	0.94	0.27	46,46,46,46	0
58	MG	2A	3455	1/1	0.94	0.36	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3001	1/1	0.94	0.15	37,37,37,37	0
58	MG	2A	3003	1/1	0.94	0.35	52,52,52,52	0
58	MG	1B	214	1/1	0.94	0.11	45,45,45,45	0
58	MG	2A	3236	1/1	0.94	0.20	45,45,45,45	0
58	MG	1A	3621	1/1	0.94	0.14	36,36,36,36	0
58	MG	1A	3234	1/1	0.94	0.12	37,37,37,37	0
58	MG	2A	3239	1/1	0.94	0.14	41,41,41,41	0
58	MG	1A	3629	1/1	0.94	0.15	27,27,27,27	0
58	MG	1A	3082	1/1	0.94	0.20	37,37,37,37	0
58	MG	1A	3185	1/1	0.94	0.27	39,39,39,39	0
58	MG	2A	3014	1/1	0.94	0.14	29,29,29,29	0
58	MG	1a	1665	1/1	0.94	0.15	48,48,48,48	0
58	MG	1a	1666	1/1	0.94	0.18	44,44,44,44	0
58	MG	1A	3304	1/1	0.94	0.13	16,16,16,16	0
58	MG	2A	3030	1/1	0.94	0.12	33,33,33,33	0
58	MG	1A	3047	1/1	0.94	0.21	25,25,25,25	0
58	MG	2A	3483	1/1	0.94	0.26	41,41,41,41	0
58	MG	1A	3135	1/1	0.94	0.18	28,28,28,28	0
58	MG	1A	3638	1/1	0.94	0.08	19,19,19,19	0
58	MG	1B	228	1/1	0.94	0.24	33,33,33,33	0
58	MG	1a	1673	1/1	0.94	0.20	39,39,39,39	0
58	MG	1A	3517	1/1	0.94	0.21	48,48,48,48	0
58	MG	2a	1770	1/1	0.94	0.14	61,61,61,61	0
58	MG	1A	3801	1/1	0.94	0.19	40,40,40,40	0
58	MG	1A	3641	1/1	0.94	0.15	45,45,45,45	0
58	MG	1A	3644	1/1	0.94	0.12	32,32,32,32	0
58	MG	2A	3814	1/1	0.94	0.19	44,44,44,44	0
58	MG	1B	234	1/1	0.94	0.16	46,46,46,46	0
58	MG	1a	1680	1/1	0.94	0.11	44,44,44,44	0
58	MG	2a	1783	1/1	0.94	0.19	46,46,46,46	0
58	MG	1B	235	1/1	0.94	0.20	57,57,57,57	0
58	MG	2a	1786	1/1	0.94	0.18	56,56,56,56	0
58	MG	1A	3518	1/1	0.94	0.23	47,47,47,47	0
58	MG	1A	3977	1/1	0.94	0.15	48,48,48,48	0
58	MG	1D	311	1/1	0.94	0.18	35,35,35,35	0
58	MG	1A	3647	1/1	0.94	0.22	41,41,41,41	0
58	MG	2A	3506	1/1	0.94	0.24	53,53,53,53	0
58	MG	2a	1795	1/1	0.94	0.21	54,54,54,54	0
58	MG	1A	3243	1/1	0.94	0.25	36,36,36,36	0
58	MG	2A	3831	1/1	0.94	0.13	32,32,32,32	0
58	MG	2A	3508	1/1	0.94	0.18	51,51,51,51	0
58	MG	2A	3833	1/1	0.94	0.19	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3834	1/1	0.94	0.20	25,25,25,25	0
58	MG	2A	3509	1/1	0.94	0.09	47,47,47,47	0
58	MG	2a	1804	1/1	0.94	0.19	51,51,51,51	0
58	MG	1A	3521	1/1	0.94	0.16	19,19,19,19	0
58	MG	2A	3839	1/1	0.94	0.07	52,52,52,52	0
58	MG	2a	1810	1/1	0.94	0.22	41,41,41,41	0
58	MG	1A	3655	1/1	0.94	0.19	26,26,26,26	0
58	MG	2A	3276	1/1	0.94	0.16	54,54,54,54	0
58	MG	1A	3448	1/1	0.94	0.10	21,21,21,21	0
58	MG	2A	3061	1/1	0.94	0.12	34,34,34,34	0
58	MG	2a	1815	1/1	0.94	0.15	59,59,59,59	0
58	MG	1A	3660	1/1	0.94	0.18	33,33,33,33	0
58	MG	1A	3823	1/1	0.94	0.22	15,15,15,15	0
58	MG	1A	3450	1/1	0.94	0.45	32,32,32,32	0
58	MG	2A	3852	1/1	0.94	0.23	52,52,52,52	0
58	MG	1A	3451	1/1	0.94	0.17	27,27,27,27	0
58	MG	1A	3061	1/1	0.94	0.12	25,25,25,25	0
58	MG	2A	3531	1/1	0.94	0.25	54,54,54,54	0
58	MG	1A	3453	1/1	0.94	0.18	25,25,25,25	0
58	MG	2A	3857	1/1	0.94	0.15	51,51,51,51	0
58	MG	2A	3858	1/1	0.94	0.17	51,51,51,51	0
58	MG	1A	3193	1/1	0.94	0.22	30,30,30,30	0
58	MG	2A	3070	1/1	0.94	0.20	45,45,45,45	0
58	MG	1A	3375	1/1	0.94	0.21	40,40,40,40	0
58	MG	2A	3538	1/1	0.94	0.12	38,38,38,38	0
58	MG	1A	3014	1/1	0.94	0.20	19,19,19,19	0
58	MG	1A	3251	1/1	0.94	0.17	25,25,25,25	0
58	MG	2A	3870	1/1	0.94	0.13	50,50,50,50	0
58	MG	2e	201	1/1	0.94	0.06	60,60,60,60	0
58	MG	2f	202	1/1	0.94	0.21	51,51,51,51	0
58	MG	1A	3379	1/1	0.94	0.39	27,27,27,27	0
58	MG	2A	3543	1/1	0.94	0.32	47,47,47,47	0
58	MG	1A	3252	1/1	0.94	0.18	51,51,51,51	0
58	MG	2A	3296	1/1	0.94	0.13	43,43,43,43	0
58	MG	1A	3849	1/1	0.94	0.21	58,58,58,58	0
58	MG	1A	3196	1/1	0.94	0.21	25,25,25,25	0
58	MG	1A	4000	1/1	0.94	0.10	39,39,39,39	0
58	MG	2B	208	1/1	0.94	0.13	43,43,43,43	0
58	MG	2q	202	1/1	0.94	0.18	55,55,55,55	0
58	MG	2B	209	1/1	0.94	0.11	49,49,49,49	0
58	MG	1a	1710	1/1	0.94	0.16	50,50,50,50	0
58	MG	2A	3553	1/1	0.94	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2B	212	1/1	0.94	0.24	59,59,59,59	0
58	MG	2A	3083	1/1	0.94	0.12	36,36,36,36	0
58	MG	2w	101	1/1	0.94	0.22	46,46,46,46	0
58	MG	2A	3555	1/1	0.94	0.20	34,34,34,34	0
58	MG	1A	3684	1/1	0.94	0.16	14,14,14,14	0
58	MG	1A	3144	1/1	0.94	0.11	24,24,24,24	0
58	MG	2A	3088	1/1	0.94	0.24	47,47,47,47	0
58	MG	1Q	205	1/1	0.94	0.12	58,58,58,58	0
58	MG	2A	3309	1/1	0.94	0.10	56,56,56,56	0
58	MG	2D	303	1/1	0.94	0.12	34,34,34,34	0
58	MG	1a	1715	1/1	0.94	0.28	46,46,46,46	0
58	MG	1A	3320	1/1	0.94	0.21	25,25,25,25	0
58	MG	2x	106	1/1	0.94	0.24	40,40,40,40	0
58	MG	1a	1717	1/1	0.94	0.20	46,46,46,46	0
58	MG	2y	101	1/1	0.94	0.22	58,58,58,58	0
58	MG	1A	3544	1/1	0.94	0.25	40,40,40,40	0
58	MG	1A	3244	1/1	0.95	0.22	21,21,21,21	0
58	MG	2A	3671	1/1	0.95	0.19	41,41,41,41	0
58	MG	1A	3246	1/1	0.95	0.17	39,39,39,39	0
58	MG	1F	310	1/1	0.95	0.18	33,33,33,33	0
58	MG	1A	4012	1/1	0.95	0.16	14,14,14,14	0
58	MG	1A	3757	1/1	0.95	0.17	32,32,32,32	0
58	MG	1F	313	1/1	0.95	0.21	32,32,32,32	0
58	MG	2A	3009	1/1	0.95	0.20	32,32,32,32	0
58	MG	1A	3645	1/1	0.95	0.13	37,37,37,37	0
58	MG	1G	202	1/1	0.95	0.24	44,44,44,44	0
58	MG	2A	3015	1/1	0.95	0.12	36,36,36,36	0
58	MG	2A	3683	1/1	0.95	0.11	56,56,56,56	0
58	MG	2a	1603	1/1	0.95	0.15	57,57,57,57	0
58	MG	1A	3247	1/1	0.95	0.12	32,32,32,32	0
58	MG	1A	4016	1/1	0.95	0.09	36,36,36,36	0
58	MG	2A	3024	1/1	0.95	0.10	42,42,42,42	0
58	MG	2A	3025	1/1	0.95	0.26	39,39,39,39	0
58	MG	2A	3688	1/1	0.95	0.28	49,49,49,49	0
58	MG	2A	3690	1/1	0.95	0.16	53,53,53,53	0
58	MG	1A	3136	1/1	0.95	0.18	21,21,21,21	0
58	MG	2A	3232	1/1	0.95	0.21	39,39,39,39	0
58	MG	2A	3233	1/1	0.95	0.19	34,34,34,34	0
58	MG	2A	3234	1/1	0.95	0.12	33,33,33,33	0
58	MG	2A	3235	1/1	0.95	0.21	41,41,41,41	0
58	MG	1A	3555	1/1	0.95	0.15	38,38,38,38	0
58	MG	2A	3440	1/1	0.95	0.32	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3161	1/1	0.95	0.27	28,28,28,28	0
58	MG	1A	3769	1/1	0.95	0.18	15,15,15,15	0
58	MG	1A	3557	1/1	0.95	0.16	28,28,28,28	0
58	MG	1A	3305	1/1	0.95	0.29	39,39,39,39	0
58	MG	1O	205	1/1	0.95	0.31	47,47,47,47	0
58	MG	1a	1688	1/1	0.95	0.22	31,31,31,31	0
58	MG	2A	3041	1/1	0.95	0.24	48,48,48,48	0
58	MG	2A	3713	1/1	0.95	0.39	52,52,52,52	0
58	MG	1A	3773	1/1	0.95	0.13	23,23,23,23	0
58	MG	1A	3657	1/1	0.95	0.10	51,51,51,51	0
58	MG	1A	3904	1/1	0.95	0.16	26,26,26,26	0
58	MG	1A	3560	1/1	0.95	0.15	23,23,23,23	0
58	MG	1A	3563	1/1	0.95	0.18	23,23,23,23	0
58	MG	1A	3907	1/1	0.95	0.22	25,25,25,25	0
58	MG	1A	3908	1/1	0.95	0.09	28,28,28,28	0
58	MG	2a	1638	1/1	0.95	0.17	38,38,38,38	0
58	MG	1Q	208	1/1	0.95	0.18	34,34,34,34	0
58	MG	1A	3162	1/1	0.95	0.09	39,39,39,39	0
58	MG	1A	3137	1/1	0.95	0.20	32,32,32,32	0
58	MG	2a	1643	1/1	0.95	0.14	60,60,60,60	0
58	MG	1A	3911	1/1	0.95	0.13	29,29,29,29	0
58	MG	1A	4036	1/1	0.95	0.12	41,41,41,41	0
58	MG	1a	1702	1/1	0.95	0.25	41,41,41,41	0
58	MG	1A	3367	1/1	0.95	0.11	35,35,35,35	0
58	MG	1A	3310	1/1	0.95	0.39	48,48,48,48	0
58	MG	2A	3263	1/1	0.95	0.39	58,58,58,58	0
58	MG	2A	3738	1/1	0.95	0.12	33,33,33,33	0
58	MG	1T	203	1/1	0.95	0.20	35,35,35,35	0
58	MG	1A	3916	1/1	0.95	0.10	30,30,30,30	0
58	MG	1A	3212	1/1	0.95	0.10	26,26,26,26	0
58	MG	1A	3918	1/1	0.95	0.18	23,23,23,23	0
58	MG	2A	3480	1/1	0.95	0.34	40,40,40,40	0
58	MG	1A	3671	1/1	0.95	0.12	38,38,38,38	0
58	MG	2A	3748	1/1	0.95	0.22	53,53,53,53	0
58	MG	1U	207	1/1	0.95	0.18	27,27,27,27	0
58	MG	2A	3751	1/1	0.95	0.14	47,47,47,47	0
58	MG	2A	3273	1/1	0.95	0.11	51,51,51,51	0
58	MG	2a	1663	1/1	0.95	0.17	61,61,61,61	0
58	MG	1A	3672	1/1	0.95	0.14	35,35,35,35	0
58	MG	2A	3485	1/1	0.95	0.23	28,28,28,28	0
58	MG	1A	3215	1/1	0.95	0.13	28,28,28,28	0
58	MG	1A	4045	1/1	0.95	0.14	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3077	1/1	0.95	0.21	32,32,32,32	0
58	MG	1A	3926	1/1	0.95	0.11	26,26,26,26	0
58	MG	1a	1719	1/1	0.95	0.19	28,28,28,28	0
58	MG	1A	3096	1/1	0.95	0.26	45,45,45,45	0
58	MG	2a	1675	1/1	0.95	0.12	42,42,42,42	0
58	MG	1A	3677	1/1	0.95	0.14	28,28,28,28	0
58	MG	2A	3767	1/1	0.95	0.20	33,33,33,33	0
58	MG	1A	4051	1/1	0.95	0.17	36,36,36,36	0
58	MG	1A	3143	1/1	0.95	0.12	36,36,36,36	0
58	MG	2a	1681	1/1	0.95	0.09	51,51,51,51	0
58	MG	2A	3496	1/1	0.95	0.22	32,32,32,32	0
58	MG	2A	3771	1/1	0.95	0.16	50,50,50,50	0
58	MG	1A	3176	1/1	0.95	0.17	30,30,30,30	0
58	MG	2A	3287	1/1	0.95	0.13	57,57,57,57	0
58	MG	1A	3683	1/1	0.95	0.19	20,20,20,20	0
58	MG	2A	3500	1/1	0.95	0.13	46,46,46,46	0
58	MG	1A	3502	1/1	0.95	0.36	44,44,44,44	0
58	MG	1A	3935	1/1	0.95	0.16	25,25,25,25	0
58	MG	1A	3936	1/1	0.95	0.14	32,32,32,32	0
58	MG	2A	3783	1/1	0.95	0.07	54,54,54,54	0
58	MG	2a	1694	1/1	0.95	0.27	48,48,48,48	0
58	MG	2a	1695	1/1	0.95	0.14	57,57,57,57	0
58	MG	1a	1731	1/1	0.95	0.10	54,54,54,54	0
58	MG	1Z	302	1/1	0.95	0.21	37,37,37,37	0
58	MG	2A	3294	1/1	0.95	0.32	54,54,54,54	0
58	MG	2A	3787	1/1	0.95	0.14	44,44,44,44	0
58	MG	2A	3093	1/1	0.95	0.17	37,37,37,37	0
58	MG	1A	3035	1/1	0.95	0.13	35,35,35,35	0
58	MG	2A	3513	1/1	0.95	0.11	44,44,44,44	0
58	MG	2A	3791	1/1	0.95	0.12	63,63,63,63	0
58	MG	2A	3792	1/1	0.95	0.16	45,45,45,45	0
58	MG	2A	3514	1/1	0.95	0.26	34,34,34,34	0
58	MG	2A	3794	1/1	0.95	0.19	30,30,30,30	0
58	MG	1a	1735	1/1	0.95	0.09	37,37,37,37	0
58	MG	1A	3581	1/1	0.95	0.17	30,30,30,30	0
58	MG	1A	3802	1/1	0.95	0.19	14,14,14,14	0
58	MG	2A	3798	1/1	0.95	0.21	54,54,54,54	0
58	MG	1a	1738	1/1	0.95	0.23	46,46,46,46	0
58	MG	2A	3102	1/1	0.95	0.12	45,45,45,45	0
58	MG	10	106	1/1	0.95	0.14	31,31,31,31	0
58	MG	2A	3526	1/1	0.95	0.15	26,26,26,26	0
58	MG	1A	3803	1/1	0.95	0.21	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3124	1/1	0.95	0.18	30,30,30,30	0
58	MG	11	101	1/1	0.95	0.24	29,29,29,29	0
58	MG	1A	3264	1/1	0.95	0.12	41,41,41,41	0
58	MG	11	103	1/1	0.95	0.18	26,26,26,26	0
58	MG	2a	1727	1/1	0.95	0.23	57,57,57,57	0
58	MG	1A	3051	1/1	0.95	0.20	17,17,17,17	0
58	MG	1A	3013	1/1	0.95	0.12	18,18,18,18	0
58	MG	2A	3810	1/1	0.95	0.14	49,49,49,49	0
58	MG	11	106	1/1	0.95	0.19	36,36,36,36	0
58	MG	1A	4075	1/1	0.95	0.20	24,24,24,24	0
58	MG	1A	3129	1/1	0.95	0.12	23,23,23,23	0
58	MG	1A	3325	1/1	0.95	0.18	46,46,46,46	0
58	MG	1A	3268	1/1	0.95	0.14	37,37,37,37	0
58	MG	1A	3512	1/1	0.95	0.19	35,35,35,35	0
58	MG	15	103	1/1	0.95	0.12	28,28,28,28	0
58	MG	1A	3699	1/1	0.95	0.12	17,17,17,17	0
58	MG	2A	3822	1/1	0.95	0.17	30,30,30,30	0
58	MG	2a	1747	1/1	0.95	0.14	52,52,52,52	0
58	MG	1A	3270	1/1	0.95	0.20	27,27,27,27	0
58	MG	2A	3325	1/1	0.95	0.39	52,52,52,52	0
58	MG	1A	3271	1/1	0.95	0.28	51,51,51,51	0
58	MG	2A	3827	1/1	0.95	0.08	53,53,53,53	0
58	MG	1A	3828	1/1	0.95	0.14	14,14,14,14	0
58	MG	2A	3126	1/1	0.95	0.14	39,39,39,39	0
58	MG	1a	1763	1/1	0.95	0.09	58,58,58,58	0
58	MG	1A	3832	1/1	0.95	0.19	29,29,29,29	0
58	MG	2A	3333	1/1	0.95	0.28	58,58,58,58	0
58	MG	1a	1765	1/1	0.95	0.08	44,44,44,44	0
58	MG	1A	3329	1/1	0.95	0.27	47,47,47,47	0
58	MG	1a	1767	1/1	0.95	0.17	47,47,47,47	0
58	MG	1A	3060	1/1	0.95	0.25	38,38,38,38	0
58	MG	1A	3837	1/1	0.95	0.30	42,42,42,42	0
58	MG	1A	3838	1/1	0.95	0.20	53,53,53,53	0
58	MG	2A	3566	1/1	0.95	0.24	54,54,54,54	0
58	MG	1A	3962	1/1	0.95	0.15	38,38,38,38	0
58	MG	2a	1768	1/1	0.95	0.10	44,44,44,44	0
58	MG	1A	3273	1/1	0.95	0.13	54,54,54,54	0
58	MG	1A	3705	1/1	0.95	0.20	18,18,18,18	0
58	MG	2A	3138	1/1	0.95	0.19	29,29,29,29	0
58	MG	1A	3522	1/1	0.95	0.13	25,25,25,25	0
58	MG	2a	1777	1/1	0.95	0.17	56,56,56,56	0
58	MG	1a	1777	1/1	0.95	0.18	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1779	1/1	0.95	0.08	46,46,46,46	0
58	MG	1A	3709	1/1	0.95	0.13	21,21,21,21	0
58	MG	1B	201	1/1	0.95	0.21	30,30,30,30	0
58	MG	2a	1784	1/1	0.95	0.16	57,57,57,57	0
58	MG	1B	203	1/1	0.95	0.20	31,31,31,31	0
58	MG	1a	1609	1/1	0.95	0.25	40,40,40,40	0
58	MG	1a	1610	1/1	0.95	0.12	49,49,49,49	0
58	MG	1a	1786	1/1	0.95	0.10	46,46,46,46	0
58	MG	1A	3274	1/1	0.95	0.17	29,29,29,29	0
58	MG	1A	3230	1/1	0.95	0.17	25,25,25,25	0
58	MG	1a	1614	1/1	0.95	0.16	47,47,47,47	0
58	MG	1A	3971	1/1	0.95	0.21	16,16,16,16	0
58	MG	2A	3869	1/1	0.95	0.11	53,53,53,53	0
58	MG	1a	1616	1/1	0.95	0.14	61,61,61,61	0
58	MG	1A	3526	1/1	0.95	0.18	40,40,40,40	0
58	MG	2A	3597	1/1	0.95	0.26	43,43,43,43	0
58	MG	2A	3599	1/1	0.95	0.15	36,36,36,36	0
58	MG	2a	1802	1/1	0.95	0.12	52,52,52,52	0
58	MG	1A	3847	1/1	0.95	0.12	35,35,35,35	0
58	MG	1a	1621	1/1	0.95	0.19	40,40,40,40	0
58	MG	1A	3188	1/1	0.95	0.19	24,24,24,24	0
58	MG	2A	3604	1/1	0.95	0.17	47,47,47,47	0
58	MG	1A	3116	1/1	0.95	0.17	26,26,26,26	0
58	MG	1A	3529	1/1	0.95	0.09	54,54,54,54	0
58	MG	1a	1626	1/1	0.95	0.10	53,53,53,53	0
58	MG	1A	3721	1/1	0.95	0.33	50,50,50,50	0
58	MG	1A	3982	1/1	0.95	0.16	31,31,31,31	0
58	MG	2A	3169	1/1	0.95	0.10	44,44,44,44	0
58	MG	1A	3853	1/1	0.95	0.19	43,43,43,43	0
58	MG	1a	1633	1/1	0.95	0.27	46,46,46,46	0
58	MG	2A	3613	1/1	0.95	0.16	44,44,44,44	0
58	MG	1B	217	1/1	0.95	0.15	37,37,37,37	0
58	MG	1B	218	1/1	0.95	0.14	27,27,27,27	0
58	MG	1B	219	1/1	0.95	0.27	34,34,34,34	0
58	MG	1a	1814	1/1	0.95	0.08	41,41,41,41	0
58	MG	2A	3177	1/1	0.95	0.26	28,28,28,28	0
58	MG	1A	3279	1/1	0.95	0.11	40,40,40,40	0
58	MG	2a	1827	1/1	0.95	0.14	65,65,65,65	0
58	MG	1A	3408	1/1	0.95	0.15	36,36,36,36	0
58	MG	1A	3154	1/1	0.95	0.19	34,34,34,34	0
58	MG	2A	3625	1/1	0.95	0.12	39,39,39,39	0
58	MG	1A	3471	1/1	0.95	0.11	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3339	1/1	0.95	0.30	45,45,45,45	0
58	MG	1A	3155	1/1	0.95	0.17	24,24,24,24	0
58	MG	1l	202	1/1	0.95	0.13	49,49,49,49	0
58	MG	1A	3736	1/1	0.95	0.20	29,29,29,29	0
58	MG	1a	1645	1/1	0.95	0.29	51,51,51,51	0
58	MG	1A	3117	1/1	0.95	0.20	27,27,27,27	0
58	MG	1A	3992	1/1	0.95	0.24	35,35,35,35	0
58	MG	1A	3993	1/1	0.95	0.14	18,18,18,18	0
58	MG	1A	3291	1/1	0.95	0.11	41,41,41,41	0
58	MG	1w	104	1/1	0.95	0.23	47,47,47,47	0
58	MG	2l	202	1/1	0.95	0.10	53,53,53,53	0
58	MG	2l	203	1/1	0.95	0.11	54,54,54,54	0
58	MG	1A	3157	1/1	0.95	0.17	39,39,39,39	0
58	MG	1A	3416	1/1	0.95	0.15	29,29,29,29	0
58	MG	1A	3634	1/1	0.95	0.16	19,19,19,19	0
58	MG	1A	3743	1/1	0.95	0.11	45,45,45,45	0
58	MG	1A	3349	1/1	0.95	0.19	30,30,30,30	0
58	MG	1D	307	1/1	0.95	0.15	26,26,26,26	0
58	MG	2r	101	1/1	0.95	0.18	44,44,44,44	0
58	MG	1A	3049	1/1	0.95	0.18	11,11,11,11	0
58	MG	1A	3241	1/1	0.95	0.12	31,31,31,31	0
58	MG	2A	3401	1/1	0.95	0.13	43,43,43,43	0
58	MG	2V	202	1/1	0.95	0.20	60,60,60,60	0
58	MG	2A	3653	1/1	0.95	0.12	55,55,55,55	0
58	MG	1A	3747	1/1	0.95	0.08	36,36,36,36	0
58	MG	1x	107	1/1	0.95	0.23	40,40,40,40	0
58	MG	2A	3657	1/1	0.95	0.19	53,53,53,53	0
58	MG	2A	3658	1/1	0.95	0.34	44,44,44,44	0
58	MG	1E	302	1/1	0.95	0.14	32,32,32,32	0
58	MG	1E	304	1/1	0.95	0.11	20,20,20,20	0
58	MG	2A	3662	1/1	0.95	0.20	53,53,53,53	0
58	MG	2A	3407	1/1	0.95	0.11	58,58,58,58	0
58	MG	1x	111	1/1	0.95	0.12	46,46,46,46	0
58	MG	1A	3203	1/1	0.95	0.21	34,34,34,34	0
58	MG	1A	3751	1/1	0.95	0.17	15,15,15,15	0
58	MG	2A	3668	1/1	0.95	0.33	43,43,43,43	0
59	K	2A	3465	1/1	0.95	0.16	50,50,50,50	0
60	ZN	15	108	1/1	0.95	0.07	60,60,60,60	0
60	ZN	2Y	202	1/1	0.95	0.10	81,81,81,81	0
60	ZN	24	501	1/1	0.95	0.06	89,89,89,89	0
58	MG	1A	3550	1/1	0.95	0.18	39,39,39,39	0
58	MG	2A	3182	1/1	0.96	0.26	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3694	1/1	0.96	0.13	20,20,20,20	0
58	MG	1A	3377	1/1	0.96	0.20	34,34,34,34	0
58	MG	1a	1641	1/1	0.96	0.18	47,47,47,47	0
58	MG	23	102	1/1	0.96	0.16	33,33,33,33	0
58	MG	1A	3197	1/1	0.96	0.13	26,26,26,26	0
58	MG	1A	3324	1/1	0.96	0.18	28,28,28,28	0
58	MG	2A	3661	1/1	0.96	0.12	37,37,37,37	0
58	MG	1A	3592	1/1	0.96	0.14	37,37,37,37	0
58	MG	1A	3449	1/1	0.96	0.15	27,27,27,27	0
58	MG	2A	3193	1/1	0.96	0.29	58,58,58,58	0
58	MG	2A	3403	1/1	0.96	0.11	58,58,58,58	0
58	MG	1n	102	1/1	0.96	0.12	44,44,44,44	0
58	MG	1t	201	1/1	0.96	0.10	42,42,42,42	0
58	MG	1A	3101	1/1	0.96	0.23	51,51,51,51	0
58	MG	1A	3843	1/1	0.96	0.11	29,29,29,29	0
58	MG	1A	3078	1/1	0.96	0.09	23,23,23,23	0
58	MG	1A	3599	1/1	0.96	0.20	45,45,45,45	0
58	MG	1a	1652	1/1	0.96	0.16	33,33,33,33	0
58	MG	1A	3600	1/1	0.96	0.12	25,25,25,25	0
58	MG	1D	302	1/1	0.96	0.17	33,33,33,33	0
58	MG	2A	3414	1/1	0.96	0.27	49,49,49,49	0
58	MG	1D	303	1/1	0.96	0.15	32,32,32,32	0
58	MG	1A	3516	1/1	0.96	0.10	44,44,44,44	0
58	MG	2a	1607	1/1	0.96	0.08	56,56,56,56	0
58	MG	1D	308	1/1	0.96	0.19	34,34,34,34	0
58	MG	2A	3420	1/1	0.96	0.35	43,43,43,43	0
58	MG	1A	3382	1/1	0.96	0.16	41,41,41,41	0
58	MG	1A	3383	1/1	0.96	0.26	19,19,19,19	0
58	MG	1A	3710	1/1	0.96	0.13	9,9,9,9	0
58	MG	1a	1661	1/1	0.96	0.17	55,55,55,55	0
58	MG	1A	3711	1/1	0.96	0.12	34,34,34,34	0
58	MG	1x	108	1/1	0.96	0.12	16,16,16,16	0
58	MG	2A	3689	1/1	0.96	0.10	45,45,45,45	0
58	MG	1A	3712	1/1	0.96	0.20	22,22,22,22	0
58	MG	1A	3277	1/1	0.96	0.14	33,33,33,33	0
58	MG	1A	3132	1/1	0.96	0.23	29,29,29,29	0
58	MG	2A	3431	1/1	0.96	0.11	55,55,55,55	0
58	MG	2A	3695	1/1	0.96	0.13	49,49,49,49	0
58	MG	1A	3048	1/1	0.96	0.20	19,19,19,19	0
58	MG	1E	312	1/1	0.96	0.11	28,28,28,28	0
58	MG	1E	313	1/1	0.96	0.19	40,40,40,40	0
58	MG	2A	3435	1/1	0.96	0.43	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4001	1/1	0.96	0.14	33,33,33,33	0
58	MG	1A	3859	1/1	0.96	0.20	14,14,14,14	0
58	MG	1F	307	1/1	0.96	0.16	33,33,33,33	0
58	MG	2a	1630	1/1	0.96	0.23	56,56,56,56	0
58	MG	1A	3607	1/1	0.96	0.35	40,40,40,40	0
58	MG	1A	3718	1/1	0.96	0.17	38,38,38,38	0
58	MG	2a	1634	1/1	0.96	0.28	68,68,68,68	0
58	MG	1A	4005	1/1	0.96	0.14	14,14,14,14	0
58	MG	1a	1676	1/1	0.96	0.33	49,49,49,49	0
58	MG	2A	3711	1/1	0.96	0.23	63,63,63,63	0
58	MG	2a	1639	1/1	0.96	0.31	49,49,49,49	0
58	MG	2A	3712	1/1	0.96	0.15	52,52,52,52	0
58	MG	2A	3010	1/1	0.96	0.27	38,38,38,38	0
58	MG	2A	3714	1/1	0.96	0.19	20,20,20,20	0
58	MG	2A	3715	1/1	0.96	0.24	30,30,30,30	0
58	MG	1A	3523	1/1	0.96	0.14	23,23,23,23	0
58	MG	2a	1645	1/1	0.96	0.16	54,54,54,54	0
58	MG	1A	4008	1/1	0.96	0.08	46,46,46,46	0
58	MG	1A	3865	1/1	0.96	0.16	31,31,31,31	0
58	MG	2A	3017	1/1	0.96	0.34	40,40,40,40	0
58	MG	1A	3081	1/1	0.96	0.22	31,31,31,31	0
58	MG	2A	3019	1/1	0.96	0.28	28,28,28,28	0
58	MG	1A	3209	1/1	0.96	0.17	24,24,24,24	0
58	MG	2A	3023	1/1	0.96	0.13	57,57,57,57	0
58	MG	1A	3284	1/1	0.96	0.18	21,21,21,21	0
58	MG	1a	1683	1/1	0.96	0.09	59,59,59,59	0
58	MG	1A	3726	1/1	0.96	0.26	40,40,40,40	0
58	MG	2A	3241	1/1	0.96	0.20	40,40,40,40	0
58	MG	2A	3029	1/1	0.96	0.47	54,54,54,54	0
58	MG	2A	3243	1/1	0.96	0.27	39,39,39,39	0
58	MG	2A	3461	1/1	0.96	0.10	52,52,52,52	0
58	MG	1A	3392	1/1	0.96	0.17	17,17,17,17	0
58	MG	2A	3735	1/1	0.96	0.20	40,40,40,40	0
58	MG	2A	3737	1/1	0.96	0.09	54,54,54,54	0
58	MG	1A	3728	1/1	0.96	0.22	29,29,29,29	0
58	MG	2A	3739	1/1	0.96	0.13	49,49,49,49	0
58	MG	1A	3037	1/1	0.96	0.21	16,16,16,16	0
58	MG	1O	202	1/1	0.96	0.34	49,49,49,49	0
58	MG	1A	3731	1/1	0.96	0.25	41,41,41,41	0
58	MG	1A	3021	1/1	0.96	0.14	12,12,12,12	0
58	MG	2A	3038	1/1	0.96	0.22	35,35,35,35	0
58	MG	2A	3746	1/1	0.96	0.22	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3043	1/1	0.96	0.20	24,24,24,24	0
58	MG	2A	3476	1/1	0.96	0.41	60,60,60,60	0
58	MG	2A	3749	1/1	0.96	0.24	46,46,46,46	0
58	MG	1A	4020	1/1	0.96	0.16	37,37,37,37	0
58	MG	1A	3336	1/1	0.96	0.26	41,41,41,41	0
58	MG	2A	3753	1/1	0.96	0.13	37,37,37,37	0
58	MG	1a	1694	1/1	0.96	0.12	47,47,47,47	0
58	MG	2A	3755	1/1	0.96	0.18	41,41,41,41	0
58	MG	1A	3879	1/1	0.96	0.09	32,32,32,32	0
58	MG	1A	4023	1/1	0.96	0.12	34,34,34,34	0
58	MG	1A	3293	1/1	0.96	0.30	26,26,26,26	0
58	MG	2A	3048	1/1	0.96	0.29	49,49,49,49	0
58	MG	1A	3737	1/1	0.96	0.13	35,35,35,35	0
58	MG	1A	3535	1/1	0.96	0.13	26,26,26,26	0
58	MG	1A	3620	1/1	0.96	0.17	24,24,24,24	0
58	MG	1A	3399	1/1	0.96	0.08	61,61,61,61	0
58	MG	1A	3622	1/1	0.96	0.21	17,17,17,17	0
58	MG	2A	3765	1/1	0.96	0.15	40,40,40,40	0
58	MG	2a	1699	1/1	0.96	0.13	47,47,47,47	0
58	MG	2A	3766	1/1	0.96	0.18	35,35,35,35	0
58	MG	2A	3267	1/1	0.96	0.26	49,49,49,49	0
58	MG	2A	3491	1/1	0.96	0.10	54,54,54,54	0
58	MG	1A	3623	1/1	0.96	0.18	19,19,19,19	0
58	MG	1A	3624	1/1	0.96	0.16	9,9,9,9	0
58	MG	1T	201	1/1	0.96	0.18	54,54,54,54	0
58	MG	1A	3625	1/1	0.96	0.18	27,27,27,27	0
58	MG	1a	1707	1/1	0.96	0.25	32,32,32,32	0
58	MG	2A	3062	1/1	0.96	0.22	35,35,35,35	0
58	MG	2a	1710	1/1	0.96	0.17	56,56,56,56	0
58	MG	2A	3775	1/1	0.96	0.17	40,40,40,40	0
58	MG	2A	3776	1/1	0.96	0.06	65,65,65,65	0
58	MG	1A	3626	1/1	0.96	0.19	23,23,23,23	0
58	MG	1A	3400	1/1	0.96	0.18	22,22,22,22	0
58	MG	1A	3628	1/1	0.96	0.25	20,20,20,20	0
58	MG	1A	3401	1/1	0.96	0.11	19,19,19,19	0
58	MG	2A	3502	1/1	0.96	0.13	46,46,46,46	0
58	MG	2a	1718	1/1	0.96	0.10	51,51,51,51	0
58	MG	1A	3631	1/1	0.96	0.14	31,31,31,31	0
58	MG	1A	3539	1/1	0.96	0.28	37,37,37,37	0
58	MG	1A	3044	1/1	0.96	0.13	33,33,33,33	0
58	MG	1A	3065	1/1	0.96	0.23	30,30,30,30	0
58	MG	2A	3284	1/1	0.96	0.15	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3031	1/1	0.96	0.21	21,21,21,21	0
58	MG	1a	1718	1/1	0.96	0.16	28,28,28,28	0
58	MG	1A	3758	1/1	0.96	0.12	44,44,44,44	0
58	MG	1A	3253	1/1	0.96	0.20	25,25,25,25	0
58	MG	2A	3076	1/1	0.96	0.20	29,29,29,29	0
58	MG	1a	1721	1/1	0.96	0.28	48,48,48,48	0
58	MG	1A	3068	1/1	0.96	0.17	22,22,22,22	0
58	MG	2A	3521	1/1	0.96	0.09	34,34,34,34	0
58	MG	1W	203	1/1	0.96	0.20	45,45,45,45	0
58	MG	2a	1734	1/1	0.96	0.13	61,61,61,61	0
58	MG	1A	3764	1/1	0.96	0.24	44,44,44,44	0
58	MG	1A	3300	1/1	0.96	0.29	40,40,40,40	0
58	MG	1A	3346	1/1	0.96	0.25	49,49,49,49	0
58	MG	1A	3547	1/1	0.96	0.16	35,35,35,35	0
58	MG	2A	3297	1/1	0.96	0.26	48,48,48,48	0
58	MG	2a	1740	1/1	0.96	0.39	29,29,29,29	0
58	MG	1A	3255	1/1	0.96	0.25	39,39,39,39	0
58	MG	1A	3770	1/1	0.96	0.23	34,34,34,34	0
58	MG	2a	1744	1/1	0.96	0.18	48,48,48,48	0
58	MG	1A	4053	1/1	0.96	0.20	25,25,25,25	0
58	MG	1A	3549	1/1	0.96	0.14	50,50,50,50	0
58	MG	2A	3535	1/1	0.96	0.11	41,41,41,41	0
58	MG	2A	3092	1/1	0.96	0.18	27,27,27,27	0
58	MG	2A	3303	1/1	0.96	0.30	34,34,34,34	0
58	MG	1A	3480	1/1	0.96	0.16	33,33,33,33	0
58	MG	2a	1754	1/1	0.96	0.10	53,53,53,53	0
58	MG	2A	3094	1/1	0.96	0.15	33,33,33,33	0
58	MG	1A	3145	1/1	0.96	0.23	9,9,9,9	0
58	MG	1A	3046	1/1	0.96	0.23	23,23,23,23	0
58	MG	1A	3147	1/1	0.96	0.10	29,29,29,29	0
58	MG	2A	3099	1/1	0.96	0.10	37,37,37,37	0
58	MG	1A	3923	1/1	0.96	0.13	25,25,25,25	0
58	MG	1A	3653	1/1	0.96	0.13	25,25,25,25	0
58	MG	1A	4063	1/1	0.96	0.15	14,14,14,14	0
58	MG	10	109	1/1	0.96	0.12	31,31,31,31	0
58	MG	1a	1742	1/1	0.96	0.11	38,38,38,38	0
58	MG	1A	3925	1/1	0.96	0.18	40,40,40,40	0
58	MG	1A	3654	1/1	0.96	0.12	21,21,21,21	0
58	MG	2A	3318	1/1	0.96	0.12	44,44,44,44	0
58	MG	2a	1769	1/1	0.96	0.15	56,56,56,56	0
58	MG	1A	3070	1/1	0.96	0.29	18,18,18,18	0
58	MG	2a	1771	1/1	0.96	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
58	MG	1A	4069	1/1	0.96	0.09	36,36,36,36	0
58	MG	1A	3072	1/1	0.96	0.30	27,27,27,27	0
58	MG	1A	3309	1/1	0.96	0.22	42,42,42,42	0
58	MG	2A	3324	1/1	0.96	0.15	33,33,33,33	0
58	MG	1A	3658	1/1	0.96	0.18	44,44,44,44	0
58	MG	2A	3326	1/1	0.96	0.23	49,49,49,49	0
58	MG	1A	3261	1/1	0.96	0.11	17,17,17,17	0
58	MG	2a	1782	1/1	0.96	0.19	53,53,53,53	0
58	MG	2A	3567	1/1	0.96	0.23	36,36,36,36	0
58	MG	1A	4077	1/1	0.96	0.14	51,51,51,51	0
58	MG	2A	3569	1/1	0.96	0.17	51,51,51,51	0
58	MG	1A	3933	1/1	0.96	0.08	39,39,39,39	0
58	MG	1A	3785	1/1	0.96	0.18	26,26,26,26	0
58	MG	1a	1756	1/1	0.96	0.09	45,45,45,45	0
58	MG	2A	3332	1/1	0.96	0.15	34,34,34,34	0
58	MG	15	102	1/1	0.96	0.24	31,31,31,31	0
58	MG	2A	3578	1/1	0.96	0.15	62,62,62,62	0
58	MG	2A	3120	1/1	0.96	0.23	38,38,38,38	0
58	MG	2A	3121	1/1	0.96	0.11	66,66,66,66	0
58	MG	2A	3581	1/1	0.96	0.13	40,40,40,40	0
58	MG	2A	3582	1/1	0.96	0.18	23,23,23,23	0
58	MG	1A	3421	1/1	0.96	0.25	39,39,39,39	0
58	MG	1A	3073	1/1	0.96	0.18	15,15,15,15	0
58	MG	2a	1801	1/1	0.96	0.12	57,57,57,57	0
58	MG	2A	3585	1/1	0.96	0.30	64,64,64,64	0
58	MG	1A	3788	1/1	0.96	0.14	33,33,33,33	0
58	MG	16	101	1/1	0.96	0.25	46,46,46,46	0
58	MG	2A	3864	1/1	0.96	0.16	45,45,45,45	0
58	MG	17	103	1/1	0.96	0.21	25,25,25,25	0
58	MG	2A	3590	1/1	0.96	0.24	52,52,52,52	0
58	MG	1A	4085	1/1	0.96	0.28	48,48,48,48	0
58	MG	1A	3425	1/1	0.96	0.26	41,41,41,41	0
58	MG	1A	3790	1/1	0.96	0.18	18,18,18,18	0
58	MG	1A	3664	1/1	0.96	0.16	32,32,32,32	0
58	MG	1A	3564	1/1	0.96	0.26	29,29,29,29	0
58	MG	1A	3361	1/1	0.96	0.15	41,41,41,41	0
58	MG	1a	1771	1/1	0.96	0.14	51,51,51,51	0
58	MG	2A	3598	1/1	0.96	0.21	32,32,32,32	0
58	MG	1A	3429	1/1	0.96	0.18	22,22,22,22	0
58	MG	1A	3227	1/1	0.96	0.24	30,30,30,30	0
58	MG	2A	3601	1/1	0.96	0.20	33,33,33,33	0
58	MG	1A	3228	1/1	0.96	0.21	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3799	1/1	0.96	0.23	41,41,41,41	0
58	MG	1A	3364	1/1	0.96	0.18	34,34,34,34	0
58	MG	1A	3571	1/1	0.96	0.15	19,19,19,19	0
58	MG	1A	3572	1/1	0.96	0.17	11,11,11,11	0
58	MG	1a	1780	1/1	0.96	0.23	63,63,63,63	0
58	MG	1A	3015	1/1	0.96	0.22	26,26,26,26	0
58	MG	2a	1831	1/1	0.96	0.24	57,57,57,57	0
58	MG	1a	1608	1/1	0.96	0.20	48,48,48,48	0
58	MG	2A	3359	1/1	0.96	0.20	44,44,44,44	0
58	MG	2B	219	1/1	0.96	0.16	52,52,52,52	0
58	MG	2a	1835	1/1	0.96	0.30	51,51,51,51	0
58	MG	1A	3191	1/1	0.96	0.16	38,38,38,38	0
58	MG	2D	301	1/1	0.96	0.21	39,39,39,39	0
58	MG	1B	202	1/1	0.96	0.24	36,36,36,36	0
58	MG	2f	201	1/1	0.96	0.27	39,39,39,39	0
58	MG	1A	3368	1/1	0.96	0.23	46,46,46,46	0
58	MG	2A	3147	1/1	0.96	0.31	36,36,36,36	0
58	MG	2A	3616	1/1	0.96	0.25	43,43,43,43	0
58	MG	2j	201	1/1	0.96	0.07	57,57,57,57	0
58	MG	1A	3682	1/1	0.96	0.18	17,17,17,17	0
58	MG	1a	1787	1/1	0.96	0.13	61,61,61,61	0
58	MG	1A	3808	1/1	0.96	0.15	53,53,53,53	0
58	MG	1A	3076	1/1	0.96	0.22	15,15,15,15	0
58	MG	1A	3269	1/1	0.96	0.15	24,24,24,24	0
58	MG	1B	209	1/1	0.96	0.20	31,31,31,31	0
58	MG	1A	3685	1/1	0.96	0.18	22,22,22,22	0
58	MG	1a	1620	1/1	0.96	0.10	46,46,46,46	0
58	MG	1A	3194	1/1	0.96	0.21	37,37,37,37	0
58	MG	1A	3963	1/1	0.96	0.15	36,36,36,36	0
58	MG	1a	1623	1/1	0.96	0.12	49,49,49,49	0
58	MG	1A	3819	1/1	0.96	0.13	28,28,28,28	0
58	MG	1A	3820	1/1	0.96	0.13	48,48,48,48	0
58	MG	1a	1803	1/1	0.96	0.09	52,52,52,52	0
58	MG	1A	3099	1/1	0.96	0.13	16,16,16,16	0
58	MG	2F	306	1/1	0.96	0.19	40,40,40,40	0
58	MG	1A	3580	1/1	0.96	0.10	30,30,30,30	0
58	MG	1A	3058	1/1	0.96	0.26	16,16,16,16	0
58	MG	2A	3171	1/1	0.96	0.08	62,62,62,62	0
58	MG	1a	1630	1/1	0.96	0.21	59,59,59,59	0
58	MG	2A	3639	1/1	0.96	0.23	38,38,38,38	0
58	MG	2A	3384	1/1	0.96	0.28	66,66,66,66	0
58	MG	1A	3236	1/1	0.96	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3643	1/1	0.96	0.08	34,34,34,34	0
58	MG	1a	1810	1/1	0.96	0.30	45,45,45,45	0
58	MG	1A	3826	1/1	0.96	0.11	34,34,34,34	0
58	MG	1A	3827	1/1	0.96	0.09	25,25,25,25	0
58	MG	1A	3583	1/1	0.96	0.38	32,32,32,32	0
58	MG	1A	3831	1/1	0.96	0.14	17,17,17,17	0
58	MG	1A	3445	1/1	0.96	0.23	23,23,23,23	0
58	MG	1A	3693	1/1	0.96	0.33	50,50,50,50	0
58	MG	2X	103	1/1	0.96	0.17	40,40,40,40	0
58	MG	1e	201	1/1	0.96	0.17	59,59,59,59	0
58	MG	1B	221	1/1	0.97	0.22	45,45,45,45	0
58	MG	1A	3168	1/1	0.97	0.22	47,47,47,47	0
58	MG	15	101	1/1	0.97	0.20	15,15,15,15	0
58	MG	1A	3665	1/1	0.97	0.18	24,24,24,24	0
58	MG	1A	3444	1/1	0.97	0.15	30,30,30,30	0
58	MG	15	104	1/1	0.97	0.17	24,24,24,24	0
58	MG	15	105	1/1	0.97	0.22	21,21,21,21	0
58	MG	1A	3200	1/1	0.97	0.12	20,20,20,20	0
58	MG	1A	3170	1/1	0.97	0.16	26,26,26,26	0
58	MG	2A	3039	1/1	0.97	0.23	16,16,16,16	0
58	MG	1A	3350	1/1	0.97	0.20	31,31,31,31	0
58	MG	2A	3777	1/1	0.97	0.23	38,38,38,38	0
58	MG	1A	3351	1/1	0.97	0.16	34,34,34,34	0
58	MG	2A	3779	1/1	0.97	0.12	38,38,38,38	0
58	MG	1a	1733	1/1	0.97	0.19	25,25,25,25	0
58	MG	1A	3202	1/1	0.97	0.20	21,21,21,21	0
58	MG	2A	3376	1/1	0.97	0.22	29,29,29,29	0
58	MG	2A	3211	1/1	0.97	0.20	51,51,51,51	0
58	MG	1A	3830	1/1	0.97	0.14	21,21,21,21	0
58	MG	2A	3574	1/1	0.97	0.21	30,30,30,30	0
58	MG	2A	3575	1/1	0.97	0.11	52,52,52,52	0
58	MG	1A	3018	1/1	0.97	0.22	20,20,20,20	0
58	MG	1B	232	1/1	0.97	0.13	33,33,33,33	0
58	MG	1A	3675	1/1	0.97	0.13	15,15,15,15	0
58	MG	1A	3748	1/1	0.97	0.11	41,41,41,41	0
58	MG	2A	3050	1/1	0.97	0.21	21,21,21,21	0
58	MG	1A	3087	1/1	0.97	0.17	20,20,20,20	0
58	MG	1A	3039	1/1	0.97	0.28	24,24,24,24	0
58	MG	1A	3931	1/1	0.97	0.11	48,48,48,48	0
58	MG	2a	1669	1/1	0.97	0.17	59,59,59,59	0
58	MG	2a	1670	1/1	0.97	0.25	32,32,32,32	0
58	MG	1A	4029	1/1	0.97	0.13	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1672	1/1	0.97	0.10	49,49,49,49	0
58	MG	1A	3075	1/1	0.97	0.15	27,27,27,27	0
58	MG	1D	305	1/1	0.97	0.23	25,25,25,25	0
58	MG	1D	306	1/1	0.97	0.21	24,24,24,24	0
58	MG	1A	3679	1/1	0.97	0.17	13,13,13,13	0
58	MG	1A	3314	1/1	0.97	0.32	50,50,50,50	0
58	MG	1D	309	1/1	0.97	0.24	31,31,31,31	0
58	MG	1A	3756	1/1	0.97	0.10	30,30,30,30	0
58	MG	1a	1611	1/1	0.97	0.22	16,16,16,16	0
58	MG	1A	3240	1/1	0.97	0.24	20,20,20,20	0
58	MG	2A	3231	1/1	0.97	0.20	47,47,47,47	0
58	MG	1A	3937	1/1	0.97	0.15	10,10,10,10	0
58	MG	1A	3064	1/1	0.97	0.29	34,34,34,34	0
58	MG	1E	303	1/1	0.97	0.12	21,21,21,21	0
58	MG	1A	3759	1/1	0.97	0.11	31,31,31,31	0
58	MG	1A	3407	1/1	0.97	0.12	34,34,34,34	0
58	MG	1E	307	1/1	0.97	0.14	25,25,25,25	0
58	MG	1A	3242	1/1	0.97	0.16	16,16,16,16	0
58	MG	1a	1762	1/1	0.97	0.13	34,34,34,34	0
58	MG	1A	3763	1/1	0.97	0.28	50,50,50,50	0
58	MG	1A	3848	1/1	0.97	0.09	27,27,27,27	0
58	MG	2a	1696	1/1	0.97	0.17	40,40,40,40	0
58	MG	2a	1697	1/1	0.97	0.25	49,49,49,49	0
58	MG	2a	1698	1/1	0.97	0.33	61,61,61,61	0
58	MG	1A	3182	1/1	0.97	0.16	21,21,21,21	0
58	MG	1F	303	1/1	0.97	0.20	20,20,20,20	0
58	MG	1F	304	1/1	0.97	0.12	22,22,22,22	0
58	MG	2A	3245	1/1	0.97	0.12	58,58,58,58	0
58	MG	1a	1768	1/1	0.97	0.18	40,40,40,40	0
58	MG	1A	3619	1/1	0.97	0.09	35,35,35,35	0
58	MG	1A	3508	1/1	0.97	0.18	41,41,41,41	0
58	MG	2A	3416	1/1	0.97	0.24	48,48,48,48	0
58	MG	1A	3562	1/1	0.97	0.16	19,19,19,19	0
58	MG	2A	3418	1/1	0.97	0.13	43,43,43,43	0
58	MG	1F	308	1/1	0.97	0.17	20,20,20,20	0
58	MG	2A	3086	1/1	0.97	0.19	34,34,34,34	0
58	MG	2A	3620	1/1	0.97	0.15	39,39,39,39	0
58	MG	2A	3087	1/1	0.97	0.15	33,33,33,33	0
58	MG	1a	1631	1/1	0.97	0.23	38,38,38,38	0
58	MG	2A	3089	1/1	0.97	0.14	41,41,41,41	0
58	MG	2A	3424	1/1	0.97	0.18	51,51,51,51	0
58	MG	1F	309	1/1	0.97	0.11	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3842	1/1	0.97	0.13	39,39,39,39	0
58	MG	1A	3768	1/1	0.97	0.15	29,29,29,29	0
58	MG	2A	3257	1/1	0.97	0.16	40,40,40,40	0
58	MG	2A	3628	1/1	0.97	0.18	30,30,30,30	0
58	MG	1A	3056	1/1	0.97	0.22	23,23,23,23	0
58	MG	1A	3245	1/1	0.97	0.29	34,34,34,34	0
58	MG	2A	3849	1/1	0.97	0.17	42,42,42,42	0
58	MG	1a	1778	1/1	0.97	0.13	39,39,39,39	0
58	MG	1A	3856	1/1	0.97	0.14	44,44,44,44	0
58	MG	1A	3213	1/1	0.97	0.14	33,33,33,33	0
58	MG	1G	201	1/1	0.97	0.10	38,38,38,38	0
58	MG	1A	3953	1/1	0.97	0.13	42,42,42,42	0
58	MG	1A	3028	1/1	0.97	0.19	26,26,26,26	0
58	MG	1G	204	1/1	0.97	0.14	48,48,48,48	0
58	MG	1G	205	1/1	0.97	0.17	41,41,41,41	0
58	MG	2A	3859	1/1	0.97	0.18	36,36,36,36	0
58	MG	2A	3103	1/1	0.97	0.16	23,23,23,23	0
58	MG	1A	3513	1/1	0.97	0.24	40,40,40,40	0
58	MG	2A	3862	1/1	0.97	0.21	37,37,37,37	0
58	MG	1A	3109	1/1	0.97	0.14	28,28,28,28	0
58	MG	2A	3644	1/1	0.97	0.13	28,28,28,28	0
58	MG	2A	3272	1/1	0.97	0.10	62,62,62,62	0
58	MG	1A	4056	1/1	0.97	0.16	12,12,12,12	0
58	MG	2a	1742	1/1	0.97	0.18	47,47,47,47	0
58	MG	1N	203	1/1	0.97	0.24	33,33,33,33	0
58	MG	2A	3444	1/1	0.97	0.23	37,37,37,37	0
58	MG	2a	1745	1/1	0.97	0.17	55,55,55,55	0
58	MG	2a	1746	1/1	0.97	0.34	51,51,51,51	0
58	MG	1A	3282	1/1	0.97	0.14	22,22,22,22	0
58	MG	2A	3109	1/1	0.97	0.15	60,60,60,60	0
58	MG	1a	1792	1/1	0.97	0.15	42,42,42,42	0
58	MG	2A	3652	1/1	0.97	0.11	38,38,38,38	0
58	MG	1A	3776	1/1	0.97	0.15	22,22,22,22	0
58	MG	2B	204	1/1	0.97	0.18	55,55,55,55	0
58	MG	2A	3654	1/1	0.97	0.28	35,35,35,35	0
58	MG	1a	1649	1/1	0.97	0.16	55,55,55,55	0
58	MG	1A	3041	1/1	0.97	0.17	25,25,25,25	0
58	MG	2A	3281	1/1	0.97	0.09	54,54,54,54	0
58	MG	1A	3867	1/1	0.97	0.28	37,37,37,37	0
58	MG	2A	3453	1/1	0.97	0.27	60,60,60,60	0
58	MG	1A	3630	1/1	0.97	0.18	20,20,20,20	0
58	MG	2a	1761	1/1	0.97	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1O	204	1/1	0.97	0.13	49,49,49,49	0
58	MG	1A	4062	1/1	0.97	0.10	28,28,28,28	0
58	MG	1P	201	1/1	0.97	0.21	19,19,19,19	0
58	MG	1A	3964	1/1	0.97	0.09	38,38,38,38	0
58	MG	2A	3665	1/1	0.97	0.12	41,41,41,41	0
58	MG	2B	217	1/1	0.97	0.17	43,43,43,43	0
58	MG	2A	3459	1/1	0.97	0.19	28,28,28,28	0
58	MG	1A	3111	1/1	0.97	0.22	21,21,21,21	0
58	MG	1A	3519	1/1	0.97	0.18	21,21,21,21	0
58	MG	1A	3286	1/1	0.97	0.17	26,26,26,26	0
58	MG	1A	4068	1/1	0.97	0.24	10,10,10,10	0
58	MG	1A	3374	1/1	0.97	0.29	41,41,41,41	0
58	MG	1A	3289	1/1	0.97	0.13	31,31,31,31	0
58	MG	2a	1776	1/1	0.97	0.11	39,39,39,39	0
58	MG	1A	3874	1/1	0.97	0.19	20,20,20,20	0
58	MG	2A	3674	1/1	0.97	0.15	36,36,36,36	0
58	MG	1A	3424	1/1	0.97	0.15	44,44,44,44	0
58	MG	2A	3471	1/1	0.97	0.14	30,30,30,30	0
58	MG	1A	4074	1/1	0.97	0.15	42,42,42,42	0
58	MG	1a	1667	1/1	0.97	0.07	52,52,52,52	0
58	MG	2A	3475	1/1	0.97	0.15	37,37,37,37	0
58	MG	1R	203	1/1	0.97	0.12	34,34,34,34	0
58	MG	1A	3973	1/1	0.97	0.15	35,35,35,35	0
58	MG	2a	1787	1/1	0.97	0.11	57,57,57,57	0
58	MG	1A	4076	1/1	0.97	0.13	25,25,25,25	0
58	MG	1A	3707	1/1	0.97	0.24	35,35,35,35	0
58	MG	1A	3975	1/1	0.97	0.13	36,36,36,36	0
58	MG	1A	3976	1/1	0.97	0.21	47,47,47,47	0
58	MG	2A	3304	1/1	0.97	0.11	44,44,44,44	0
58	MG	1k	201	1/1	0.97	0.20	38,38,38,38	0
58	MG	1A	3022	1/1	0.97	0.12	31,31,31,31	0
58	MG	1A	3114	1/1	0.97	0.22	20,20,20,20	0
58	MG	1A	3010	1/1	0.97	0.18	25,25,25,25	0
58	MG	2G	201	1/1	0.97	0.21	51,51,51,51	0
58	MG	1A	4083	1/1	0.97	0.19	33,33,33,33	0
58	MG	1A	3192	1/1	0.97	0.18	30,30,30,30	0
58	MG	1U	204	1/1	0.97	0.28	42,42,42,42	0
58	MG	2Q	201	1/1	0.97	0.09	45,45,45,45	0
58	MG	1U	206	1/1	0.97	0.19	30,30,30,30	0
58	MG	1A	3881	1/1	0.97	0.20	31,31,31,31	0
58	MG	1A	3882	1/1	0.97	0.12	23,23,23,23	0
58	MG	2a	1809	1/1	0.97	0.23	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3883	1/1	0.97	0.19	26,26,26,26	0
58	MG	1A	3642	1/1	0.97	0.14	22,22,22,22	0
58	MG	1w	105	1/1	0.97	0.17	52,52,52,52	0
58	MG	1V	205	1/1	0.97	0.13	34,34,34,34	0
58	MG	1A	3792	1/1	0.97	0.21	29,29,29,29	0
58	MG	2A	3706	1/1	0.97	0.27	51,51,51,51	0
58	MG	1V	207	1/1	0.97	0.12	48,48,48,48	0
58	MG	2A	3154	1/1	0.97	0.27	44,44,44,44	0
58	MG	1A	3478	1/1	0.97	0.22	42,42,42,42	0
58	MG	2A	3323	1/1	0.97	0.18	53,53,53,53	0
58	MG	2A	3504	1/1	0.97	0.11	31,31,31,31	0
58	MG	1A	3224	1/1	0.97	0.15	31,31,31,31	0
58	MG	2a	1822	1/1	0.97	0.19	48,48,48,48	0
58	MG	2A	3157	1/1	0.97	0.18	46,46,46,46	0
58	MG	2a	1824	1/1	0.97	0.14	49,49,49,49	0
58	MG	1A	3584	1/1	0.97	0.08	36,36,36,36	0
58	MG	1W	204	1/1	0.97	0.16	22,22,22,22	0
58	MG	1A	3432	1/1	0.97	0.18	35,35,35,35	0
58	MG	2A	3510	1/1	0.97	0.17	36,36,36,36	0
58	MG	1A	3588	1/1	0.97	0.23	21,21,21,21	0
58	MG	1X	101	1/1	0.97	0.12	28,28,28,28	0
58	MG	1A	3650	1/1	0.97	0.20	34,34,34,34	0
58	MG	1X	103	1/1	0.97	0.20	39,39,39,39	0
58	MG	2A	3515	1/1	0.97	0.28	40,40,40,40	0
58	MG	2A	3516	1/1	0.97	0.22	24,24,24,24	0
58	MG	1A	3894	1/1	0.97	0.17	17,17,17,17	0
58	MG	2A	3727	1/1	0.97	0.17	23,23,23,23	0
58	MG	1A	3895	1/1	0.97	0.16	19,19,19,19	0
58	MG	2A	3729	1/1	0.97	0.12	47,47,47,47	0
58	MG	1A	3071	1/1	0.97	0.20	9,9,9,9	0
58	MG	1A	3652	1/1	0.97	0.17	17,17,17,17	0
58	MG	1A	3160	1/1	0.97	0.18	25,25,25,25	0
58	MG	2A	3523	1/1	0.97	0.11	49,49,49,49	0
58	MG	1A	3534	1/1	0.97	0.25	23,23,23,23	0
58	MG	1B	205	1/1	0.97	0.15	38,38,38,38	0
58	MG	2A	3736	1/1	0.97	0.17	47,47,47,47	0
58	MG	1A	3900	1/1	0.97	0.14	19,19,19,19	0
58	MG	1A	3804	1/1	0.97	0.17	21,21,21,21	0
58	MG	2A	3529	1/1	0.97	0.12	50,50,50,50	0
58	MG	1A	3098	1/1	0.97	0.18	27,27,27,27	0
58	MG	1A	3007	1/1	0.97	0.15	30,30,30,30	0
58	MG	1A	3299	1/1	0.97	0.16	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3596	1/1	0.97	0.18	32,32,32,32	0
58	MG	2A	3744	1/1	0.97	0.24	23,23,23,23	0
58	MG	1A	3809	1/1	0.97	0.05	40,40,40,40	0
58	MG	1A	3659	1/1	0.97	0.16	25,25,25,25	0
58	MG	1A	3811	1/1	0.97	0.12	14,14,14,14	0
58	MG	1A	3085	1/1	0.97	0.22	25,25,25,25	0
58	MG	2A	3184	1/1	0.97	0.13	31,31,31,31	0
58	MG	1A	3198	1/1	0.97	0.42	41,41,41,41	0
58	MG	2A	3541	1/1	0.97	0.21	51,51,51,51	0
58	MG	2A	3752	1/1	0.97	0.22	45,45,45,45	0
58	MG	1A	3815	1/1	0.97	0.16	16,16,16,16	0
58	MG	2a	1624	1/1	0.97	0.15	52,52,52,52	0
58	MG	1A	3231	1/1	0.97	0.12	19,19,19,19	0
58	MG	2A	3354	1/1	0.97	0.15	61,61,61,61	0
58	MG	2A	3545	1/1	0.97	0.25	36,36,36,36	0
58	MG	2A	3189	1/1	0.97	0.11	62,62,62,62	0
58	MG	2A	3022	1/1	0.97	0.24	39,39,39,39	0
58	MG	1A	3914	1/1	0.97	0.13	48,48,48,48	0
58	MG	2a	1631	1/1	0.97	0.15	43,43,43,43	0
58	MG	1A	3263	1/1	0.97	0.18	32,32,32,32	0
59	K	1A	3568	1/1	0.97	0.17	37,37,37,37	0
58	MG	2A	3550	1/1	0.97	0.18	36,36,36,36	0
58	MG	2A	3551	1/1	0.97	0.11	39,39,39,39	0
58	MG	13	101	1/1	0.97	0.20	32,32,32,32	0
58	MG	2A	3194	1/1	0.97	0.21	49,49,49,49	0
60	ZN	29	102	1/1	0.97	0.08	56,56,56,56	0
58	MG	2A	3026	1/1	0.97	0.17	33,33,33,33	0
58	MG	1A	3174	1/1	0.98	0.28	9,9,9,9	0
58	MG	2A	3028	1/1	0.98	0.13	43,43,43,43	0
58	MG	2A	3160	1/1	0.98	0.21	53,53,53,53	0
58	MG	2A	3161	1/1	0.98	0.21	32,32,32,32	0
58	MG	1A	3079	1/1	0.98	0.19	19,19,19,19	0
58	MG	2A	3576	1/1	0.98	0.25	38,38,38,38	0
58	MG	1U	205	1/1	0.98	0.35	27,27,27,27	0
58	MG	1A	3281	1/1	0.98	0.18	14,14,14,14	0
58	MG	1A	3107	1/1	0.98	0.16	29,29,29,29	0
58	MG	2A	3033	1/1	0.98	0.22	29,29,29,29	0
58	MG	1A	3419	1/1	0.98	0.16	55,55,55,55	0
58	MG	1V	201	1/1	0.98	0.28	25,25,25,25	0
58	MG	1A	3179	1/1	0.98	0.16	17,17,17,17	0
58	MG	1V	203	1/1	0.98	0.14	24,24,24,24	0
58	MG	1A	3593	1/1	0.98	0.17	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3586	1/1	0.98	0.27	21,21,21,21	0
58	MG	1A	3476	1/1	0.98	0.28	43,43,43,43	0
58	MG	1A	3722	1/1	0.98	0.16	10,10,10,10	0
58	MG	2E	304	1/1	0.98	0.18	34,34,34,34	0
58	MG	1A	3723	1/1	0.98	0.16	47,47,47,47	0
58	MG	1A	3957	1/1	0.98	0.19	38,38,38,38	0
58	MG	1a	1651	1/1	0.98	0.16	36,36,36,36	0
58	MG	1A	3958	1/1	0.98	0.11	30,30,30,30	0
58	MG	2E	309	1/1	0.98	0.20	23,23,23,23	0
58	MG	2A	3046	1/1	0.98	0.28	62,62,62,62	0
58	MG	1A	3067	1/1	0.98	0.22	30,30,30,30	0
58	MG	1A	3214	1/1	0.98	0.19	22,22,22,22	0
58	MG	1A	3287	1/1	0.98	0.18	28,28,28,28	0
58	MG	1W	206	1/1	0.98	0.28	20,20,20,20	0
58	MG	1A	3288	1/1	0.98	0.15	25,25,25,25	0
58	MG	1A	3729	1/1	0.98	0.18	15,15,15,15	0
58	MG	2F	307	1/1	0.98	0.14	44,44,44,44	0
58	MG	2A	3053	1/1	0.98	0.16	56,56,56,56	0
58	MG	1A	3426	1/1	0.98	0.08	26,26,26,26	0
58	MG	1A	3181	1/1	0.98	0.27	15,15,15,15	0
58	MG	1X	104	1/1	0.98	0.19	32,32,32,32	0
58	MG	1X	105	1/1	0.98	0.17	35,35,35,35	0
58	MG	1X	106	1/1	0.98	0.21	50,50,50,50	0
58	MG	1A	3732	1/1	0.98	0.13	50,50,50,50	0
58	MG	1D	304	1/1	0.98	0.17	14,14,14,14	0
58	MG	2T	201	1/1	0.98	0.17	52,52,52,52	0
58	MG	1A	3483	1/1	0.98	0.19	32,32,32,32	0
58	MG	1A	3149	1/1	0.98	0.20	20,20,20,20	0
58	MG	1A	3034	1/1	0.98	0.16	21,21,21,21	0
58	MG	1A	3218	1/1	0.98	0.17	28,28,28,28	0
58	MG	2A	3466	1/1	0.98	0.25	15,15,15,15	0
58	MG	2a	1749	1/1	0.98	0.13	65,65,65,65	0
58	MG	1A	3012	1/1	0.98	0.22	21,21,21,21	0
58	MG	1D	310	1/1	0.98	0.20	20,20,20,20	0
58	MG	2A	3615	1/1	0.98	0.19	44,44,44,44	0
58	MG	1a	1788	1/1	0.98	0.05	37,37,37,37	0
58	MG	2A	3470	1/1	0.98	0.17	41,41,41,41	0
58	MG	10	103	1/1	0.98	0.16	38,38,38,38	0
58	MG	10	104	1/1	0.98	0.22	29,29,29,29	0
58	MG	1A	3972	1/1	0.98	0.09	26,26,26,26	0
58	MG	2A	3072	1/1	0.98	0.18	45,45,45,45	0
58	MG	1A	3669	1/1	0.98	0.14	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3130	1/1	0.98	0.21	31,31,31,31	0
58	MG	2A	3478	1/1	0.98	0.15	17,17,17,17	0
58	MG	1A	3892	1/1	0.98	0.15	14,14,14,14	0
58	MG	1A	3893	1/1	0.98	0.23	26,26,26,26	0
58	MG	2A	3209	1/1	0.98	0.19	47,47,47,47	0
58	MG	1A	3036	1/1	0.98	0.23	30,30,30,30	0
58	MG	1E	305	1/1	0.98	0.20	22,22,22,22	0
58	MG	1A	3112	1/1	0.98	0.21	29,29,29,29	0
58	MG	2A	3631	1/1	0.98	0.14	32,32,32,32	0
58	MG	1a	1800	1/1	0.98	0.15	44,44,44,44	0
58	MG	2A	3081	1/1	0.98	0.13	40,40,40,40	0
58	MG	1A	3027	1/1	0.98	0.13	59,59,59,59	0
58	MG	1A	3023	1/1	0.98	0.20	9,9,9,9	0
58	MG	28	103	1/1	0.98	0.14	45,45,45,45	0
58	MG	2a	1774	1/1	0.98	0.07	53,53,53,53	0
58	MG	1E	310	1/1	0.98	0.20	18,18,18,18	0
58	MG	1A	4066	1/1	0.98	0.22	32,32,32,32	0
58	MG	1A	3438	1/1	0.98	0.25	27,27,27,27	0
58	MG	1A	3190	1/1	0.98	0.31	27,27,27,27	0
58	MG	2A	3640	1/1	0.98	0.22	33,33,33,33	0
58	MG	1A	3008	1/1	0.98	0.18	21,21,21,21	0
58	MG	1A	3341	1/1	0.98	0.20	49,49,49,49	0
58	MG	1a	1809	1/1	0.98	0.17	34,34,34,34	0
58	MG	13	103	1/1	0.98	0.13	35,35,35,35	0
58	MG	1A	3342	1/1	0.98	0.14	43,43,43,43	0
58	MG	1A	3680	1/1	0.98	0.20	20,20,20,20	0
58	MG	1A	4073	1/1	0.98	0.14	12,12,12,12	0
58	MG	1A	3750	1/1	0.98	0.20	13,13,13,13	0
58	MG	2a	1789	1/1	0.98	0.12	53,53,53,53	0
58	MG	1A	3389	1/1	0.98	0.33	39,39,39,39	0
58	MG	2A	3097	1/1	0.98	0.15	53,53,53,53	0
58	MG	1A	3390	1/1	0.98	0.23	21,21,21,21	0
58	MG	1A	3829	1/1	0.98	0.13	25,25,25,25	0
58	MG	2a	1794	1/1	0.98	0.12	54,54,54,54	0
58	MG	1A	3030	1/1	0.98	0.16	18,18,18,18	0
58	MG	1A	3558	1/1	0.98	0.14	18,18,18,18	0
58	MG	17	101	1/1	0.98	0.16	22,22,22,22	0
58	MG	1A	3052	1/1	0.98	0.29	19,19,19,19	0
58	MG	17	104	1/1	0.98	0.18	36,36,36,36	0
58	MG	1A	3833	1/1	0.98	0.20	33,33,33,33	0
58	MG	18	102	1/1	0.98	0.26	36,36,36,36	0
58	MG	1A	3834	1/1	0.98	0.14	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	18	104	1/1	0.98	0.31	31,31,31,31	0
58	MG	1A	3913	1/1	0.98	0.14	14,14,14,14	0
58	MG	1A	3393	1/1	0.98	0.05	40,40,40,40	0
58	MG	2a	1806	1/1	0.98	0.26	38,38,38,38	0
58	MG	2a	1807	1/1	0.98	0.24	44,44,44,44	0
58	MG	1A	3138	1/1	0.98	0.10	31,31,31,31	0
58	MG	2A	3518	1/1	0.98	0.15	17,17,17,17	0
58	MG	2A	3818	1/1	0.98	0.18	34,34,34,34	0
58	MG	2A	3819	1/1	0.98	0.25	42,42,42,42	0
58	MG	2A	3820	1/1	0.98	0.10	41,41,41,41	0
58	MG	18	108	1/1	0.98	0.18	33,33,33,33	0
58	MG	1A	3042	1/1	0.98	0.18	21,21,21,21	0
58	MG	2a	1635	1/1	0.98	0.09	52,52,52,52	0
58	MG	1A	3347	1/1	0.98	0.14	33,33,33,33	0
58	MG	1A	3761	1/1	0.98	0.17	14,14,14,14	0
58	MG	1a	1714	1/1	0.98	0.25	28,28,28,28	0
58	MG	2A	3826	1/1	0.98	0.13	54,54,54,54	0
58	MG	1A	3348	1/1	0.98	0.32	26,26,26,26	0
58	MG	2A	3828	1/1	0.98	0.17	50,50,50,50	0
58	MG	1A	3920	1/1	0.98	0.18	18,18,18,18	0
58	MG	1A	3140	1/1	0.98	0.18	21,21,21,21	0
58	MG	1N	206	1/1	0.98	0.24	32,32,32,32	0
58	MG	2A	3528	1/1	0.98	0.17	39,39,39,39	0
58	MG	1A	4093	1/1	0.98	0.10	46,46,46,46	0
58	MG	1A	3163	1/1	0.98	0.19	25,25,25,25	0
58	MG	1A	3308	1/1	0.98	0.20	18,18,18,18	0
58	MG	1A	3164	1/1	0.98	0.16	17,17,17,17	0
58	MG	2A	3837	1/1	0.98	0.17	41,41,41,41	0
58	MG	2A	3838	1/1	0.98	0.18	53,53,53,53	0
58	MG	1A	3695	1/1	0.98	0.11	23,23,23,23	0
58	MG	2A	3840	1/1	0.98	0.23	21,21,21,21	0
58	MG	1A	3402	1/1	0.98	0.23	25,25,25,25	0
58	MG	1A	3166	1/1	0.98	0.21	23,23,23,23	0
58	MG	1A	3141	1/1	0.98	0.19	20,20,20,20	0
58	MG	1Q	201	1/1	0.98	0.26	33,33,33,33	0
58	MG	1A	3119	1/1	0.98	0.16	22,22,22,22	0
58	MG	2A	3846	1/1	0.98	0.17	28,28,28,28	0
58	MG	2A	3264	1/1	0.98	0.21	45,45,45,45	0
58	MG	1Q	203	1/1	0.98	0.21	24,24,24,24	0
58	MG	1A	3169	1/1	0.98	0.16	32,32,32,32	0
58	MG	2A	3850	1/1	0.98	0.18	37,37,37,37	0
58	MG	1a	1618	1/1	0.98	0.16	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3357	1/1	0.98	0.16	40,40,40,40	0
58	MG	2A	3692	1/1	0.98	0.25	49,49,49,49	0
58	MG	1A	3120	1/1	0.98	0.27	28,28,28,28	0
58	MG	1A	3463	1/1	0.98	0.18	51,51,51,51	0
58	MG	1A	3204	1/1	0.98	0.19	20,20,20,20	0
58	MG	2A	3696	1/1	0.98	0.25	22,22,22,22	0
58	MG	1A	3640	1/1	0.98	0.14	14,14,14,14	0
58	MG	1A	3706	1/1	0.98	0.18	17,17,17,17	0
58	MG	2A	3699	1/1	0.98	0.30	43,43,43,43	0
58	MG	1A	3004	1/1	0.98	0.16	14,14,14,14	0
58	MG	1A	3858	1/1	0.98	0.10	25,25,25,25	0
58	MG	2A	3012	1/1	0.98	0.17	36,36,36,36	0
58	MG	2A	3410	1/1	0.98	0.30	31,31,31,31	0
58	MG	2a	1679	1/1	0.98	0.12	38,38,38,38	0
58	MG	2A	3013	1/1	0.98	0.12	35,35,35,35	0
58	MG	1S	201	1/1	0.98	0.21	33,33,33,33	0
58	MG	1a	1628	1/1	0.98	0.27	39,39,39,39	0
58	MG	2a	1683	1/1	0.98	0.16	43,43,43,43	0
58	MG	2A	3868	1/1	0.98	0.15	40,40,40,40	0
58	MG	2A	3707	1/1	0.98	0.11	57,57,57,57	0
58	MG	2A	3557	1/1	0.98	0.26	29,29,29,29	0
58	MG	2A	3016	1/1	0.98	0.16	53,53,53,53	0
58	MG	1A	3411	1/1	0.98	0.07	34,34,34,34	0
58	MG	1A	3781	1/1	0.98	0.12	20,20,20,20	0
58	MG	2A	3561	1/1	0.98	0.22	27,27,27,27	0
58	MG	1A	3206	1/1	0.98	0.27	12,12,12,12	0
58	MG	1A	3207	1/1	0.98	0.18	24,24,24,24	0
58	MG	2A	3151	1/1	0.98	0.11	46,46,46,46	0
58	MG	1A	3863	1/1	0.98	0.14	12,12,12,12	0
60	ZN	1Y	206	1/1	0.98	0.12	52,52,52,52	0
60	ZN	14	102	1/1	0.98	0.06	81,81,81,81	0
58	MG	2A	3153	1/1	0.98	0.22	37,37,37,37	0
60	ZN	1n	103	1/1	0.98	0.10	51,51,51,51	0
58	MG	1A	3864	1/1	0.98	0.18	16,16,16,16	0
58	MG	1A	3032	1/1	0.98	0.14	17,17,17,17	0
60	ZN	25	106	1/1	0.98	0.11	73,73,73,73	0
58	MG	1A	3585	1/1	0.98	0.14	21,21,21,21	0
58	MG	1a	1751	1/1	0.98	0.20	34,34,34,34	0
58	MG	2A	3503	1/1	0.99	0.28	42,42,42,42	0
58	MG	1A	3825	1/1	0.99	0.14	24,24,24,24	0
58	MG	2a	1700	1/1	0.99	0.23	26,26,26,26	0
58	MG	17	102	1/1	0.99	0.17	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3178	1/1	0.99	0.21	18,18,18,18	0
58	MG	1A	3090	1/1	0.99	0.30	34,34,34,34	0
58	MG	2A	3057	1/1	0.99	0.09	45,45,45,45	0
58	MG	1F	301	1/1	0.99	0.16	25,25,25,25	0
58	MG	1F	302	1/1	0.99	0.17	20,20,20,20	0
58	MG	1A	3369	1/1	0.99	0.27	28,28,28,28	0
58	MG	2a	1648	1/1	0.99	0.14	50,50,50,50	0
58	MG	2A	3725	1/1	0.99	0.21	36,36,36,36	0
58	MG	1A	3797	1/1	0.99	0.11	14,14,14,14	0
58	MG	1A	3666	1/1	0.99	0.26	24,24,24,24	0
58	MG	1Y	204	1/1	0.99	0.31	38,38,38,38	0
58	MG	1A	3717	1/1	0.99	0.13	28,28,28,28	0
58	MG	1A	3598	1/1	0.99	0.14	17,17,17,17	0
58	MG	2D	305	1/1	0.99	0.20	21,21,21,21	0
58	MG	1a	1728	1/1	0.99	0.20	51,51,51,51	0
58	MG	1A	3643	1/1	0.99	0.16	17,17,17,17	0
58	MG	2a	1779	1/1	0.99	0.13	44,44,44,44	0
58	MG	2A	3678	1/1	0.99	0.17	37,37,37,37	0
58	MG	1A	3303	1/1	0.99	0.28	18,18,18,18	0
58	MG	1A	3126	1/1	0.99	0.16	20,20,20,20	0
58	MG	2A	3021	1/1	0.99	0.19	16,16,16,16	0
58	MG	1A	3127	1/1	0.99	0.14	19,19,19,19	0
58	MG	1A	3171	1/1	0.99	0.23	22,22,22,22	0
58	MG	1A	3038	1/1	0.99	0.11	16,16,16,16	0
58	MG	1A	3752	1/1	0.99	0.16	13,13,13,13	0
58	MG	2A	3474	1/1	0.99	0.14	44,44,44,44	0
58	MG	1D	301	1/1	0.99	0.16	20,20,20,20	0
58	MG	1A	3649	1/1	0.99	0.18	10,10,10,10	0
58	MG	1A	3561	1/1	0.99	0.19	25,25,25,25	0
58	MG	1A	3003	1/1	0.99	0.25	19,19,19,19	0
58	MG	2a	1731	1/1	0.99	0.15	52,52,52,52	0
58	MG	1A	3165	1/1	0.99	0.19	14,14,14,14	0
58	MG	1A	3812	1/1	0.99	0.18	14,14,14,14	0
58	MG	1A	3422	1/1	0.99	0.25	34,34,34,34	0
58	MG	1U	208	1/1	0.99	0.28	28,28,28,28	0
58	MG	1A	4006	1/1	0.99	0.08	25,25,25,25	0
58	MG	2A	3035	1/1	0.99	0.21	36,36,36,36	0
58	MG	2A	3537	1/1	0.99	0.20	24,24,24,24	0
58	MG	1A	3586	1/1	0.99	0.27	26,26,26,26	0
58	MG	1A	3285	1/1	0.99	0.18	23,23,23,23	0
58	MG	1A	3033	1/1	0.99	0.21	25,25,25,25	0
58	MG	1A	3817	1/1	0.99	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3818	1/1	0.99	0.12	23,23,23,23	0
58	MG	2A	3188	1/1	0.99	0.15	32,32,32,32	0
58	MG	1a	1795	1/1	0.99	0.07	38,38,38,38	0
58	MG	1A	3017	1/1	0.99	0.11	39,39,39,39	0
58	MG	1A	4046	1/1	0.99	0.20	27,27,27,27	0
58	MG	2V	201	1/1	0.99	0.27	42,42,42,42	0
58	MG	1a	1752	1/1	0.99	0.12	41,41,41,41	0
58	MG	1A	3177	1/1	0.99	0.13	24,24,24,24	0
58	MG	1A	3366	1/1	0.99	0.20	24,24,24,24	0
58	MG	1A	3428	1/1	0.99	0.16	21,21,21,21	0
60	ZN	16	102	1/1	0.99	0.15	37,37,37,37	0
60	ZN	19	102	1/1	0.99	0.16	36,36,36,36	0
58	MG	1A	4084	1/1	0.99	0.11	38,38,38,38	0
58	MG	2a	1693	1/1	0.99	0.15	44,44,44,44	0
58	MG	1P	203	1/1	0.99	0.29	24,24,24,24	0
58	MG	1E	308	1/1	0.99	0.15	35,35,35,35	0
60	ZN	26	102	1/1	0.99	0.14	52,52,52,52	0
58	MG	1A	3514	1/1	0.99	0.10	17,17,17,17	0
58	MG	1A	3533	1/1	0.99	0.20	29,29,29,29	0
61	SF4	1d	302	8/8	0.99	0.10	51,52,59,61	0
61	SF4	2d	303	8/8	0.99	0.09	52,61,73,73	0
58	MG	1A	3724	1/1	1.00	0.14	18,18,18,18	0

6.5 Other polymers

There are no such residues in this entry.